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4-(1*H*-Indol-3-yl)-2,6-bis(4-methoxyphenyl)-pyridine

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.003 Å
R factor = 0.074
wR factor = 0.145
Data-to-parameter ratio = 16.5

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

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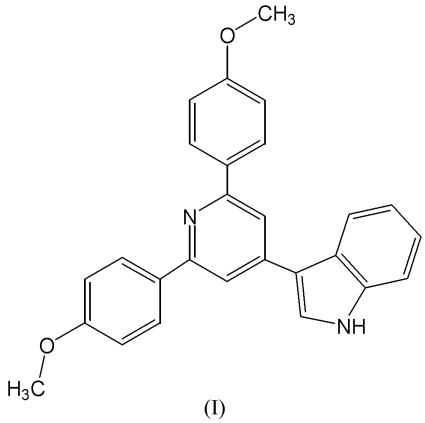
The title compound, $C_{27}H_{22}N_2O_2$, was synthesized by the reaction of indole-3-carbaldehyde with 4-methoxyacetophenone and ammonium acetate in glycol under microwave irradiation. X-ray analysis reveals that N—H···N hydrogen bonds link the molecules into zigzag chains along [01$\bar{1}$].

Comment

2,4,6-Trisubstituted pyridines are important because of their biological activity (Shirai *et al.*, 1993) and optical (fluorescence and scintillation) properties (Knyazhanskii *et al.*, 1996; Kurfurst *et al.*, 1989) and their quaternary salts have synthetic applications (Katritzky, 1980; Katritzky & Marson, 1984). We report here the crystal structure of the title compound, (I).



(I)

The asymmetric unit contains two molecules (Fig. 1). The corresponding bond distances and angles agree with each other. In one molecule, the two methoxyphenyl rings form dihedral angles of 43.81 (5) and 42.22 (8)° with the pyridine ring [40.54 (5) and 43.78 (7)° in the other molecule] and the dihedral angle between the indole and pyridine rings is

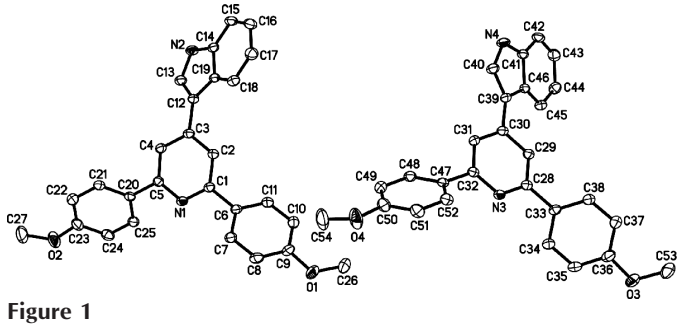


Figure 1
The asymmetric unit of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.

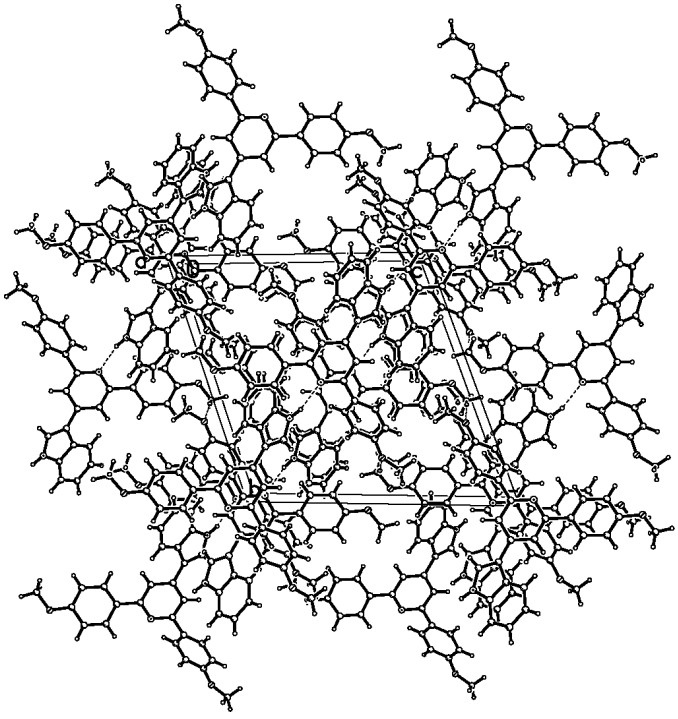


Figure 2
Molecular packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

33.58 (7)° [34.30 (6)° in the other molecule]. In the crystal structure, intermolecular N—H···N hydrogen bonds (Table 2) link the molecules into chains along [01$\bar{1}$] (Fig. 2).

Experimental

Compound (I) was prepared by the reaction of indole-3-carbaldehyde (2 mmol) with 4-methoxyacetophenone (4 mmol) and ammonium acetate (2 mmol) in glycol (2 ml) under microwave irradiation (yield 73%; m.p. 505–506 K). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{27}H_{22}N_2O_2$
M_r = 406.47
Triclinic, $P\bar{1}$
a = 8.7438 (13) Å
b = 16.341 (2) Å
c = 16.460 (2) Å
α = 68.442 (11)°
β = 76.059 (12)°
γ = 75.827 (12)°
V = 2090.7 (5) Å^3
Z = 4
D_x = 1.291 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7351 reflections
θ = 3.1–27.5°
μ = 0.08 mm^{-1}
T = 193 (2) K
Block, orange
0.51 × 0.42 × 0.20 mm

Data collection

Rigaku Mercury diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.959, T_{max} = 0.984
23621 measured reflections
9420 independent reflections
7619 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.5°
$h = -11 \rightarrow 11$
$k = -21 \rightarrow 21$
$l = -20 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.145
S = 1.16
9420 reflections
571 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0393P)^2 + 1.3567P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.350 (3)	C4—C5	1.391 (3)
N1—C5	1.352 (3)	C5—C20	1.484 (3)
N3—C28	1.349 (3)	C28—C29	1.390 (3)
N3—C32	1.353 (3)	C28—C33	1.488 (3)
C1—C2	1.391 (3)	C29—C30	1.395 (3)
C1—C6	1.486 (3)	C30—C31	1.393 (3)
C2—C3	1.390 (3)	C30—C39	1.466 (3)
C3—C4	1.396 (3)	C31—C32	1.389 (3)
C3—C12	1.464 (3)	C32—C47	1.481 (3)
C1—N1—C5	117.33 (17)	N1—C5—C4	122.70 (19)
C28—N3—C32	117.43 (17)	N3—C28—C29	122.48 (19)
N1—C1—C2	122.44 (18)	C28—C29—C30	120.55 (19)
C3—C2—C1	120.75 (19)	C31—C30—C29	116.47 (18)
C2—C3—C4	116.44 (18)	C32—C31—C30	120.43 (19)
C5—C4—C3	120.31 (19)	N3—C32—C31	122.60 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H28···N1^{i}	0.91 (3)	2.12 (3)	3.001 (3)	163 (2)
N2—H1···N3^{ii}	0.94 (3)	2.10 (3)	3.018 (2)	165 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y, 1+z$.

Amine H atoms were located in a difference Fourier map and were refined isotropically [N—H = 0.91 (3) and 0.94 (3) Å]. All other H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.95–0.98 Å, and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2000–2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Jacobson, R. (1998). Private communication to the Rigaku Corporation.
Katritzky, A. R. (1980). *Tetrahedron*, **36**, 679–699.
Katritzky, A. R. & Marson, C. M. (1984). *Angew. Chem. Int. Ed. Engl.* **23**, 420–429.
Knyazhanskii, M. I., Makarova, N. I., Olekhnovich, E. P., Pichko, V. A. & Kharlanov, V. A. (1996). *Zh. Org. Khim.* **32**, 1097–1103.

Kurfurst, A., Lhotak, P., Petru, M. & Kuthan, J. (1989). *Collect. Czech. Chem. Commun.* **54**, 462–472.
Rigaku (1999). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2000–2003). *CrystalStructure*. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Shirai, H., Hanabusa, K., Takahashi, Y., Mizobe, F. & Hanada, K. (1993). Japan Patent 93126541.