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N-(1-Phenylethyl)indole-2-carboxamide dimethylformamide solvate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.109
Data-to-parameter ratio = 18.8

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

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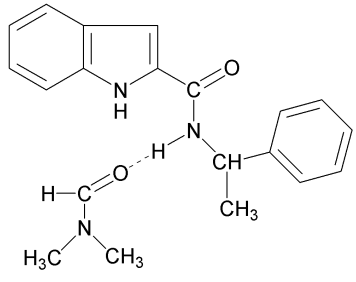
In the title compound, $C_{17}H_{16}N_2O\cdot C_3H_7NO$, containing indolyl and amide groups, the indolyl and phenyl rings are not coplanar, and form a dihedral angle of 88.4 (2)°. There are two intermolecular hydrogen bonds through the indole N and carbonyl O atom of the molecule, as well as through the amide N atom of the molecule and carbonyl O atom of the dimethylformamide solvent molecule.

Comment

We have reported the structure of the bidentate ligand (*R*)-*N*-(1-phenylethyl)quinoline-2-carboxamide (Yang *et al.*, 2001). This ligand was found to be easily coordinated to ruthenium(III) in a basic medium. The resulting Ru complex showed excellent catalytic activity in the epoxidation of cyclic alkenes. In order to further investigate the ligand performance of a new bidentate ligand, (I), containing the indole-2-carboxamide moiety, was synthesized. When the ligand coordinates to a metal ion through the ring N and the amide N atoms, the indolyl ligand, which contains a five-membered ring, will be less sterically hindered than the quinolyl derivative, which contains a six-membered ring. As a result, their catalytic activities should differ.



(I)

The indolyl and phenyl rings in (I) (Fig. 1) are not coplanar, and form a dihedral angle of 88.4 (2)°. The amide group is rotated out of the indole ring plane, forming a dihedral angle of 2.2 (1)°. There are two intermolecular hydrogen bonds; one involves the indole N and carbonyl O atom of the molecule, the other the amide N atom of the molecule and carbonyl O atom of the dimethylformamide (DMF) solvent molecule.

Experimental

The title compound was synthesized from 2-indolecarboxylic acid and methylbenzylamine, according to the general procedure of Johnson *et al.* (1960). The crystal used for the data collection was obtained by slow evaporation from a saturated DMF–water (10:1) solution at room temperature.

Crystal data

$C_{17}H_{16}N_2O\cdot C_3H_7NO$
$M_r = 337.41$
Triclinic, $P\overline{1}$
$a = 7.8166\ (11)$ Å
$b = 11.1683\ (18)$ Å
$c = 11.5769\ (18)$ Å
$\alpha = 73.310\ (3)^\circ$
$\beta = 85.990\ (4)^\circ$
$\gamma = 77.571\ (4)^\circ$
$V = 945.3\ (3)$ Å^3
$Z = 2$
$D_x = 1.185$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3267 reflections
$\theta = 1$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 294\ (2)$ K
Prism, colorless
0.14 × 0.12 × 0.10 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.989$, $T_{max} = 0.992$
6524 measured reflections
4309 independent reflections
1395 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.6^\circ$
$h = -8 \rightarrow 10$
$k = -14 \rightarrow 12$
$l = -12 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.109$
$S = 0.97$
4309 reflections
229 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.86	2.01	2.803 (2)	153
N2—H2A···O2	0.86	2.06	2.863 (3)	155

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

H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

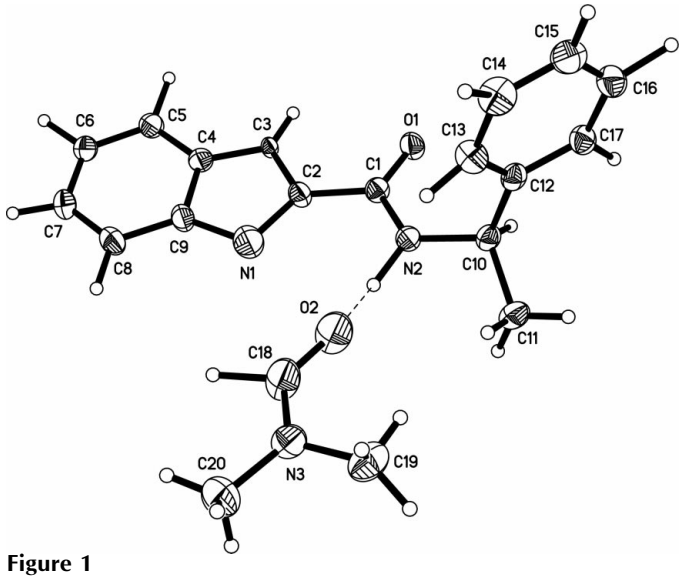


Figure 1
The molecular structure of (I), with ellipsoids at the 30% probability level (Siemens, 1995).

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References

Johnson, A. W., King, T. J. & Turner, J. R. (1960). *J. Chem. Soc.* pp. 1509–1511.
Sheldrick, G. M. (1996). *SADABS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Siemens (1995). *SMART* (Version 5.0) and *SHELXTL*-NT (Version 5.10). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Yang, Q. Y., Zhou, Z. Y. & Qi, J. Y. (2001). *Acta Cryst.* E**57**, o971–o972.