Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(4-methylphenyl)pyridine-2,6-dicarboxamide

Jian Ying Qi,[a,b]* Qi Yun Yang,[a] Kim Hung Lam,[b] Zhong Yuan Zhou[b] and Albert S. C. Chan[b]†

[a]Department of Chemistry, Changsha University of Electric Power, Changsha, Hunan, People's Republic of China, and [b]Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, People's Republic of China

† Additional correspondence author, e-mail: bcachan@polyu.edu.hk.

Correspondence e-mail: bcqijy@polyu.edu.hk

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.089
wR factor = 0.181
Data-to-parameter ratio = 17.4

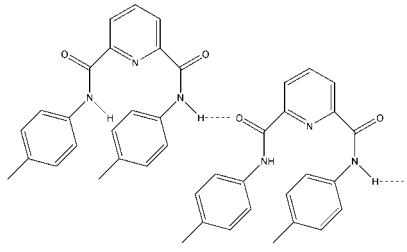
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 28 January 2003
Accepted 27 February 2003
Online 7 March 2003

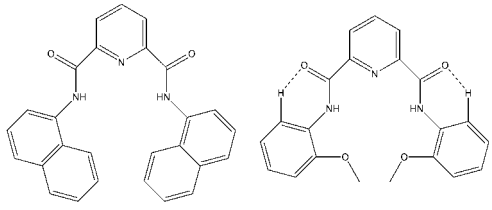
The title molecule, $C_{21}H_{19}N_3O_2$, lies on a crystallographic twofold axis which runs through the central C and N atoms of the pyridine ring. The aryl rings are slightly twisted out of the pyridine-ring plane by an angle of 15.7 (14)°. Molecules are linked by N—H···O intermolecular hydrogen bonds to form chains in the *c* direction.

Comment

Our research has shown that the previously reported ligands (II) and (III) (Qi *et al.*, 2001; Yang *et al.*, 2001) easily form Co^{III} complexes *via* the coordination of the pyridine N and the amide N atoms. However, these Co^{III} complexes are difficult to crystallize and this may be due to the steric effect of the bulky naphthyl ring of ligand (II) or the 2-methoxy group on the phenyl ring of ligand (III). Therefore, ligand (I), with less steric hindrance of the coordinated amide N atom, was prepared. We expect that it will be easier to form metal complexes of this ligand and grow single crystals for X-ray analysis.



(I)



(II) (III)

Compound (I) has a roughly planar structure, similar to those in (II) and (III). The molecule lies on a crystallographic twofold axis which runs through C11 and N2. The two substituted phenyl rings are twisted from coplanarity with the pyridine-ring plane and form dihedral angles of 15.7 (14)°. The dihedral angle between the two phenyl rings is 25.0 (15)°. Intermolecular N—H···O hydrogen bonds, formed *via* the carbonyl O and amide H atoms, link molecules into chains in the *c* direction (see Table 1).

Experimental

The title compound was synthesized from 2,6-pyridinedicarboxylic acid and 4-toluidine by a published procedure (Ray *et al.*, 1997). The

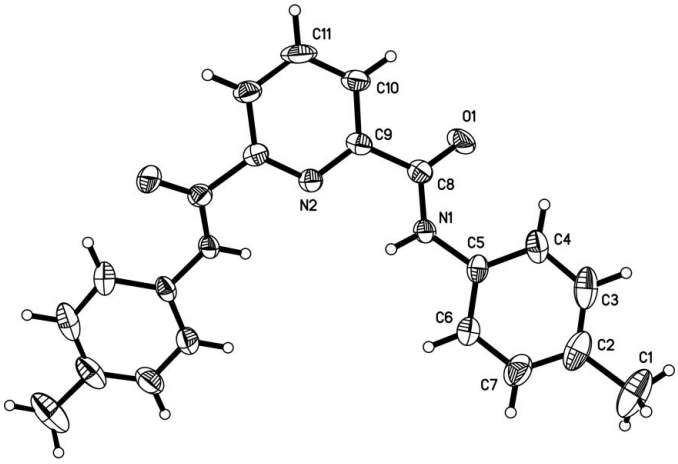


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level (Siemens, 1995). The unlabelled part of the molecule is related to the labelled part by the symmetry operation ($-x$, y, $-z+\frac{1}{2}$).

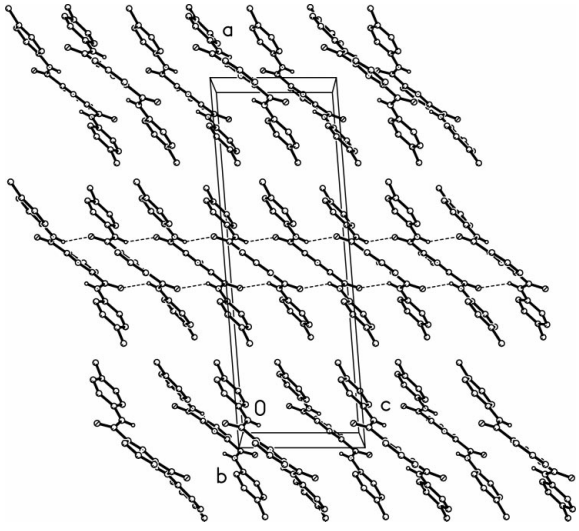


Figure 2
The molecular packing, showing the hydrogen bonding (dashed lines) in the *c* direction.

crystal used for the data collection was obtained by slow evaporation from a saturated solution in dimethylformamide and water at room temperature.

Crystal data

$C_{21}H_{19}N_3O_2$
$M_r = 345.39$
Monoclinic, $C2/c$
$a = 25.140\ (5)$ Å
$b = 8.5779\ (17)$ Å
$c = 8.5295\ (17)$ Å
$\beta = 94.46\ (3)^\circ$
$V = 1833.8\ (6)$ Å^3
$Z = 4$
$D_x = 1.251$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2125 reflections
$\theta = 1$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 294\ (2)$ K
Prism, yellow
$0.22 \times 0.20 \times 0.10$ mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.992$
5712 measured reflections
2084 independent reflections
734 reflections with $I > 2\sigma(I)$
$R_{int} = 0.137$
$\theta_{max} = 27.6^\circ$
$h = -32 \rightarrow 25$
$k = -10 \rightarrow 11$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.089$
$wR(F^2) = 0.181$
$S = 1.02$
2084 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.31	3.068 (4)	147

Symmetry code: (i) $x, -y, \frac{1}{2}+z$.

The H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation. The percentage of observed data was only 35% of the unique data available to a θ_{max} of 27.5°. Inclusion of such a high percentage of essentially unobserved data into the structure refinement restricts the precision of the results. The weak data also lead to a high value of R_{int} of 0.137.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995) and *SHELXTL-NT* (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-NT*; software used to prepare material for publication: *SHELXTL-NT*.

The Hong Kong Polytechnic University ASD fund and the National Natural Science Foundation of China (No. D20063002), as well as the Natural Science Foundation of Hunan Province (No. 02 JJy2015), are thanked for their financial support of this study.

References

Qi, J. Y., Zhou, Z. Y. & Chan, A. S. C. (2001). *Acta Cryst.* E**57**, o749–o750.
Ray, M., Ghosh, D., Shirin, Z. & Mukheerjee, R. (1997). *Inorg. Chem.* **36**, 3568–3572.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1995). *SMART* (Version 5.0), *SAINT* (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**, o1161–o1162.