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N,*N*′-Di-2-naphthylpyridine-2,6-dicarboxamide

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Key indicators

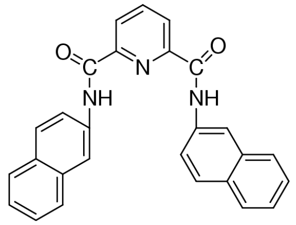
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.105
Data-to-parameter ratio = 16.2

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

The title tridentate ligand, $C_{27}H_{19}N_3O_2$, is essentially planar.

Comment

A series of Cu^{II}, Fe^{III}, Co^{III} and Ni^{II} complexes of ligands containing pyridine-2,6-dicarboxamide moieties have been synthesized in recent years (Chavez *et al.*, 1996, 1998; Marlin *et al.*, 1999; Hiratani & Taguchi, 1990). It has been well documented that amidate ligands have the ability to stabilize high formal oxidation states of metal ions due to the good σ-donor properties of the deprotonated N atom (Patra & Mukherjee, 1999).



(I)

In order to develop further the coordination chemistry of pyridine–amide ligands toward metal ions, we synthesized the title ligand, (I), with a naphthyl instead of a phenyl group connected to the amide N atom. It is estimated that the conjugation effect of the naphthyl ring is in favor of the coordination of the deprotonated nitrogen but the steric effect of the bulk aromatic ring will hinder the coordination. In the process of forming a complex, the naphthyl ring will probably rotate to another position where it is far away from the inside of the molecule, so that the amide N atom can easily coordinate with a metal ion.

Experimental

The title compound was synthesized according to the procedure of Ray *et al.* (1997). The crystal used for data collection was obtained by slow evaporation from a saturated DMF–water (10:1) solution at room temperature.

Crystal data

$C_{27}H_{19}N_3O_2$
M_r = 417.45
Monoclinic, $P2_1/c$
a = 8.816 (3) Å
b = 14.965 (4) Å
c = 15.936 (5) Å
β = 104.122 (6)°
V = 2039.0 (10) Å^3
Z = 4

D_x = 1.360 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8732 reflections
θ = 1–27.5°
μ = 0.09 mm^{-1}
T = 294 (2) K
Prism, colorless
0.28 × 0.10 × 0.06 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.976$, $T_{\max} = 0.995$
13 601 measured reflections
4710 independent reflections
1538 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.090$
$\theta_{\max} = 27.6^\circ$
$h = -11 \rightarrow 10$
$k = -16 \rightarrow 19$
$l = -17 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.105$
$S = 0.75$
4710 reflections
290 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0050 (4)

The C-bound 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-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

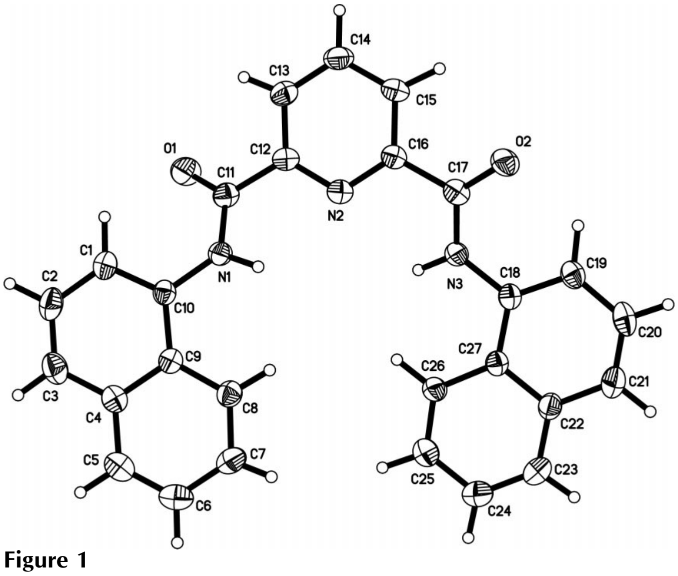


Figure 1
The molecular structure of (I) showing 30% probability displacement ellipsoids (Siemens, 1995).

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