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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.041
wR factor = 0.104
Data-to-parameter ratio = 10.2

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

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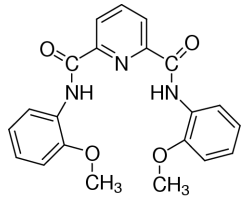
In the title tridentate ligand, $C_{21}H_{19}N_3O_4$, the phenyl rings are slightly twisted out of the pyridine-ring plane. C—H···O intramolecular and intermolecular hydrogen bonds are observed in the structure.

Comment

In our recent research, the *N*,*N*′-di-2-naphthylpyridine-2,6-dicarboxamide (Qi *et al.*, 2001) ligand easily formed a cobalt(III) complex in basic media *via* the coordination of pyridine nitrogen and deprotonated amide nitrogen. However, it is difficult to crystallize this complex, which may be due to the steric effect of the bulky naphthyl group in the ligand. Therefore, the title ligand, (I), with less steric hindrance, 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)

In (I), the two phenyl rings are twisted from coplanarity with the pyridine-ring plane and form dihedral angles of 9.0 (2) and 23.4 (2)° with this plane. The dihedral angle between the two phenyl rings is 31.1 (2)°. One of the methoxy groups is coplanar with the attached phenyl ring [C1—O2—C2—C3 −1.3 (5)°], whereas, the other is slightly twisted from the phenyl ring [C21—O4—C20—C19 8.4 (5)°]. Two intramolecular C—H···O hydrogen bonds are observed in the structure (Table 1).

Experimental

The title compound was synthesized following a published procedure (Ray *et al.*, 1997). Single crystals were obtained by slow evaporation from a DMF–water (8:1) saturated solution of the compound at room temperature.

Crystal data

$C_{21}H_{19}N_3O_4$
M_r = 377.39
Orthorhombic, $P2_12_12_1$
a = 4.7919 (9) Å
b = 15.775 (3) Å
c = 25.228 (5) Å
V = 1907.1 (6) Å^3
Z = 4
D_x = 1.314 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 4522 reflections
θ = 1–27.5°
μ = 0.09 mm^{-1}
T = 294 (2) K
Plate, colourless
0.24 × 0.20 × 0.18 mm

Data collection

Siemens CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.984
12 538 measured reflections
2571 independent reflections
1007 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 27.5°
$h = -6 \rightarrow 5$
$k = -20 \rightarrow 19$
$l = -29 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.104
S = 0.85
2571 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2	0.86	2.19	2.602 (4)	110
N2—H2A···N1	0.86	2.26	2.700 (4)	112
N3—H3A···O4	0.86	2.22	2.580 (4)	105
N3—H3A···N1	0.86	2.25	2.678 (4)	111
C6—H6A···O1	0.93	2.28	2.891 (5)	123
C11—H11A···O3^{i}	0.93	2.57	3.260 (4)	132
C16—H16A···O3	0.93	2.37	2.917 (4)	118
C21—H21B···O1^{ii}	0.96	2.49	3.124 (5)	124

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$; (ii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

The Friedel data were merged during the final stages of the refinement. All the H atoms were positioned geometrically and were allowed to ride on their respective parent atoms with *SHELXL*97 (Sheldrick, 1997) defaults for bond lengths and displacement parameters.

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

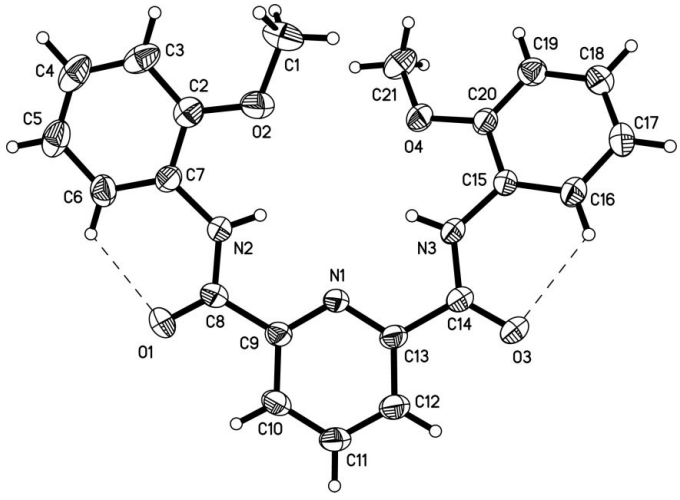


Figure 1
The molecular structure of (I). Displacement ellipsoids are shown at the 30% probability level (Siemens, 1995).

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