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N,*N*′-Di-2-pyridylbenzene-1,3-dicarboxamide dimethyl sulfoxide solvate

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Key indicators

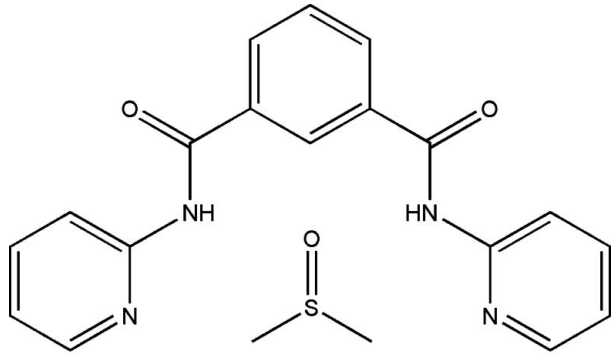
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.113
Data-to-parameter ratio = 15.9

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

In the crystal structure of the title compound, $C_{18}H_{14}N_4O_2\cdot C_2H_6OS$, the *N*,*N*′-di-2-pyridylbenzene-1,3-dicarboxamide molecule is non-planar, the two pyridine rings being twisted with respect to the benzene ring by 30.0 (2) and 27.5 (1)°. The two imino groups are hydrogen bonded with the dimethyl sulfoxide solvent molecule.

Comment

N,*N*′-Di-2-pyridylbenzene-1,3-dicarboxamide has improved actions on insulin biosynthesis and hypoglycemic activity (Nagai *et al.*, 1982). Recently, we obtained single crystals of *N*,*N*′-di-2-pyridylbenzene-1,3-dicarboxamide dimethylsulfoxide solvate, (I), and determined its structure by X-ray diffraction.



(I)

The asymmetric unit of (I) is shown in Fig. 1. In the molecule of *N*,*N*′-di-2-pyridylbenzene-1,3-dicarboxamide, the two pyridine rings (N2/C8–C12 and N4/C14–C18) adopt a *syn* configuration with respect to the benzene ring, with dihedral angles of 30.0 (2) and 27.5 (1)°, respectively. The two imino groups are hydrogen bonded with the dimethyl sulfoxide solvent molecule (Table 1).

Experimental

The title compound was prepared according to the procedure reported by Singha *et al.* (1997). Recrystallization from a dimethyl sulfoxide solution gave single crystals of (I).

Crystal data

$C_{18}H_{14}N_4O_2\cdot C_2H_6OS$
M_r = 396.46
Monoclinic, $P2_1/n$
a = 10.4852 (17) Å
b = 16.274 (3) Å
c = 12.101 (2) Å
β = 104.921 (3)°
V = 1995.3 (6) Å^3
Z = 4
D_x = 1.320 Mg m^{-3}
Mo *Kα* radiation
μ = 0.19 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
11180 measured reflections
4059 independent reflections
2168 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.113$
$S = 0.98$
4059 reflections
255 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.1524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.86	2.26	3.106 (3)	168
N3—H3···O3	0.86	2.19	2.994 (3)	156

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

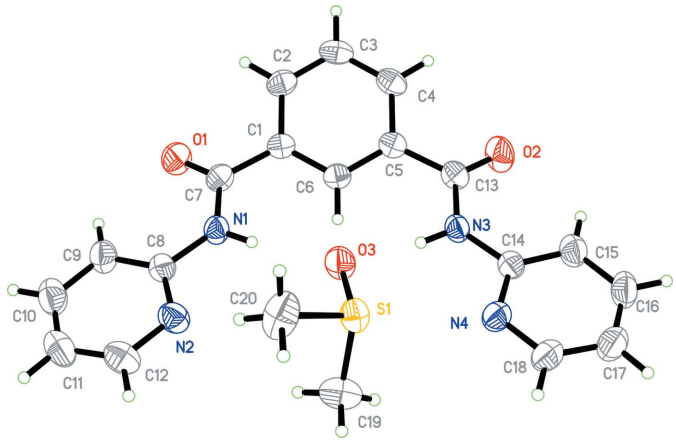


Figure 1
The asymmetric unit of (I), shown with 40% probability displacement ellipsoids (arbitrary spheres for H atoms).

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