Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-[(2,3,5,6-Tetrafluoro-1,4-phenylene)-dimethylene]bis(pyridine-2-carboxamide)

Sheng-Chun Chen,[a] Fang-Hua Yin,[a] Ming-Yang He,[a] Kang Yan[b] and Qun Chen[a]*

[a]Key Laboratory of Fine Petro-Chemical Technology, Jiangsu Polytechnic University, Changzhou 213164, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Nanjing University of Technology, Nanjing 210009, People's Republic of China

Correspondence e-mail: chenqunjpu@yahoo.com

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.067
wR factor = 0.138
Data-to-parameter ratio = 14.0

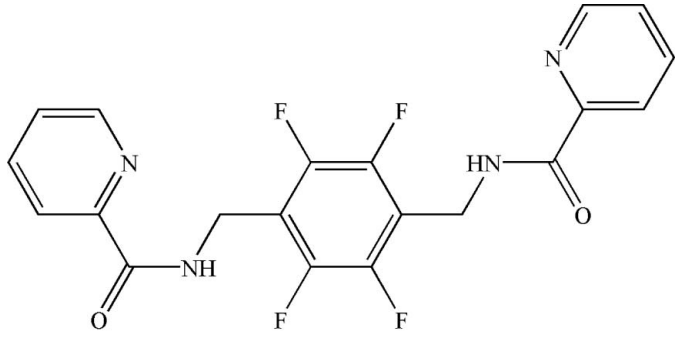
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 March 2007
Accepted 7 April 2007

The title compound, $C_{20}H_{14}F_4N_4O_2$, is centrosymmetric. The dihedral angle between the pyridine and benzene ring is 64.8 (4)°. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonding.

Comment

Pyridinecarboxamide derivatives have attracted much attention because of their biological activity, for example, anticancer (Liu *et al.*, 1996) and anti-allergic activities (Tsuzurahara *et al.*, 1987). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule of (I) is centrosymmetric, with the centroid of the benzene ring located on an inversion center. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyridine ring is twisted with respect to the benzene ring, the dihedral angle being 64.8 (4)°. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds (Table 1).

Experimental

Compound (I) was prepared according to He *et al.* (2006). Single crystals were obtained by slow evaporation of a methanol solution.

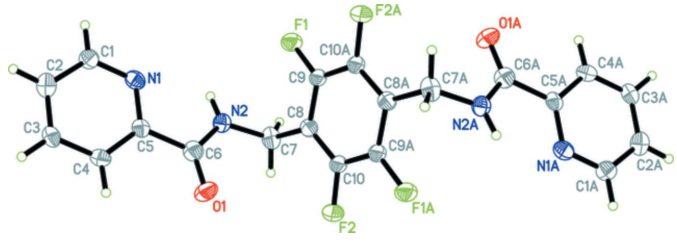


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids [symmetry code: (A) 1 − *x*, 2 − *y*, 1 − *z*].

Crystal data

$C_{20}H_{14}F_4N_4O_2$
M_r = 418.35
Triclinic, $P\overline{1}$
a = 5.4300 (11) Å
b = 7.0430 (14) Å
c = 11.216 (2) Å
α = 86.88 (3)°
β = 86.30 (3)°
γ = 78.08 (3)°
V = 418.44 (14) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 291 (2) K
0.30 × 0.24 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: none
3539 measured reflections
1822 independent reflections
1477 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.138
S = 1.02
1822 reflections
130 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 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
N2—H2B···O1^{i}	0.86	2.49	3.203 (3)	141
N2—H2B···N1	0.86	2.29	2.666 (3)	107

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

H atoms were placed in calculated positions and refined in riding mode, with N—H = 0.86 Å, C—H = 0.97 (methylene) or 0.93 Å (aromatic) and U_{iso}(H) = 1.2U_{eq}(N,C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Center for Testing and Analysis of Nanjing University for support.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2000). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
He, M.-Y., Chen, S.-C. & Chen, Q. (2006). *Acta Cryst.* E**62**, o3716–o3717.
Liu, Q., Zhang, S.-W., Wei, Y. G. & Shao, M.-C. (1996). *Acta Cryst.* C**52**, 2260–2261.
Tsuzurahara, K., Ishikawa, S., Ono, Y., Murata, T., Kikuchi, M. & Takeyama, S. (1987). *Jpn J. Pharmacol.* **45**, 55–62.