Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,6-Bis(pyridine-4-carboxamido)hexane

Cai-Feng Ding,[a] Mei Zhu,[a] Xue-Mei Li,[a] Shu-Sheng Zhang,[a]* Hong Xu[b] and Ping-Kai Ouyang[b]

[a]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China, and [b]College of Life Science and Pharmaceutical Engineering, Nanjing University of Technology, 210093 Nanjing, Jiangsu, People's Republic of China

Correspondence e-mail: zhangshush@public.qd.sd.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.113
Data-to-parameter ratio = 14.8

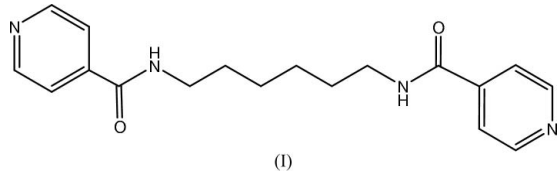
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 March 2005
Accepted 17 March 2005
Online 25 March 2005

In the title compound, $C_{18}H_{22}N_4O_2$, the molecule has a crystallographically imposed centre of symmetry. Intermolecular N—H···O hydrogen bonds link the molecules into ribbons along the *a* axis. The crystal packing is further stabilized by weak C—H···N interactions.

Comment

In recent years, the synthesis and characterization of coordination polymers have attracted increased interest, owing to their fascinating structural diversity and potential applications as functional materials (Tang & Guloy, 1999; Debajyoti *et al.*, 2004). As a good candidate for rigid rodlike spacers in the construction of metal-organic polymers, 4,4′-bipyridine has been relatively well known and has shown hundreds of interesting supramolecular architectures (Chen *et al.*, 2001). For this reason, and as a continuation of our search for new pyridyl-donor ligands, we have synthesized the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles (Table 1) in (I) show normal values (Allen *et al.*, 1987). The molecule has a crystallographic inversion centre. Intermolecular N—H···O hydrogen bonds (Table 2) link the molecules into ribbons along the *a* axis. The packing is further stabilized into a three-dimensional framework by weak intermolecular C—H···N hydrogen bonds (Table 2).

Experimental

Hexane-1,6-diamine (1 g, 17 mmol) was added slowly to a pyridine solution (50 ml) of pyridine-4-carboxylic acid (4.23 g, 34 mmol). The

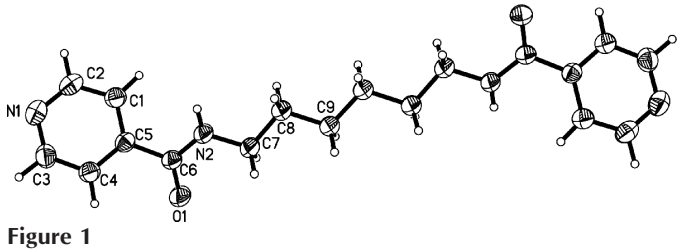


Figure 1
View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by (−1 − *x*, −*y*, −*z*).

mixture was stirred for 15 min and triphenyl phosphite (9 ml, 34 mmol) was added slowly through a dropping funnel over a period of 15 min. The mixture was refluxed for 6 h and the volume was then reduced to 10 ml by vacuum evaporation. A white precipitate was obtained from the solution after allowing it to stand at room temperature for 24 h. The solid was filtered off and washed with cold water. Yellow crystals were obtained by slow evaporation of an ethanol solution of the compound.

Crystal data

$C_{18}H_{22}N_4O_2$	D_x = 1.308 Mg m^{-3}
M_r = 326.40	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1592 reflections
a = 5.0940 (9) Å	θ = 2.6–25.9°
b = 5.2911 (10) Å	μ = 0.09 mm^{-1}
c = 30.759 (6) Å	T = 293 (2) K
β = 91.067 (3)°	Plate, yellow
V = 828.9 (3) Å^3	0.41 × 0.22 × 0.06 mm
Z = 2	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	1616 independent reflections
	1363 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.016
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.0°
	$h = -6 \rightarrow 5$
T_{min} = 0.965, T_{max} = 0.995	$k = -6 \rightarrow 6$
4366 measured reflections	$l = -37 \rightarrow 31$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.1501P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.041	
$wR(F^2)$ = 0.113	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
1616 reflections	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
109 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.2315 (16)	N2—C6	1.3325 (18)
N1—C2	1.330 (2)	N2—C7	1.4584 (18)
N1—C3	1.334 (2)		
C6—N2—C7	120.91 (11)	O1—C6—C5	120.73 (13)
O1—C6—N2	122.12 (13)	N2—C6—C5	117.14 (12)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.85	2.16	2.985 (1)	162
C2—H2B···N1^{ii}	0.93	2.60	3.466 (2)	156

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

All H atoms were located in difference Fourier maps and refined isotropically. All H atoms were placed at idealized positions and allowed to ride on their parent C atom, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 and 1.5U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

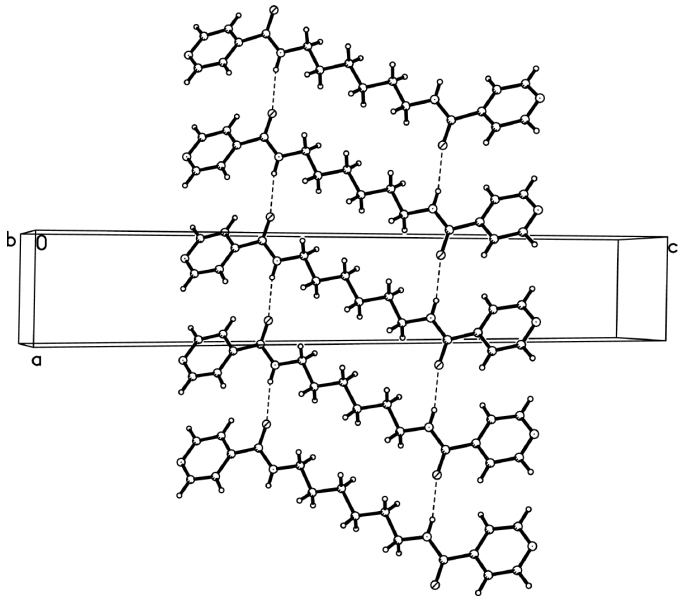


Figure 2
Packing diagram of (I), showing the hydrogen-bonded (dashed lines) ribbons.

This project was supported by the National Natural Science Foundation of China (Nos. 20275020 and 20475030) and the Outstanding Adult–Young Scientific Research Encouraging Foundation of Shandong Province (No. 03BS081).

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.
Chen, B., Eddaoudi, M., Hyde, S. T. & O'Keeffe, M. (2001). *Science*, **291**, 1021–1023.
Debajyoti, G., Tapas Dumor, M. & Golam, M. (2004). *Dalton Trans.* pp.1687–1695.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL.* Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tang, Z. & Guloy, A. M. (1999). *J. Am. Chem. Soc.* **121**, 452–453.