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N,N'-Bis(4-pyridylformyl)piperazine

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: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.117
Data-to-parameter ratio = 10.7

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

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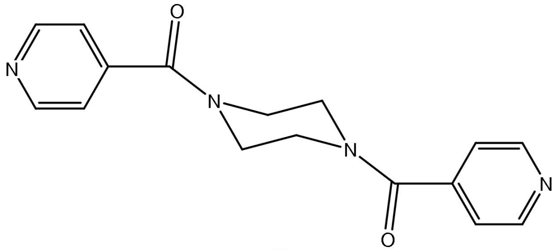
In the title compound, $C_{16}H_{16}N_4O_2$, the piperazine ring adopts a chair conformation. The title molecule has a crystallographically imposed centre of symmetry with half the molecule constituting the asymmetric unit. Molecules of (I) are linked into a three-dimensional framework by weak C—H···O and C—H···N interactions. The packing is further stabilized by C—H···π and π–π interactions.

Comment

Self-assembly of coordination polymers from the basic building blocks is of considerable interest due to the intriguing diverse architectures and potential applications of these polymers in catalysis and advanced materials, such as magnetic, optical and electronic materials (Yaghi *et al.*, 1995; Chui *et al.*, 1999). The simple ligands pyrazine and 4,4-bipyridine are good candidates for designs using rod-like spacers, which afford a wide variety of structural types with transition metals (Sunahara *et al.*, 2004). For this reason, and as a continuation of our search for new pyridyl-donor ligands, we report here the crystal structure of N,N'-bis(4-pyridylformyl)piperazine, (I).



(I)

The title molecule has a crystallographically imposed centre of symmetry. All bond lengths and angles have normal values (Allen *et al.*, 1987). In contrast to the planar conformation of piperazinedione (Wen *et al.*, 2004), the piperazine ring in (I) adopts a chair conformation (Fig. 1). The sum of the bond angles around atom N2 (359.26°) indicates a planar configuration. The two aromatic rings are parallel to one another. In the crystal structure, the molecues are linked into a three-dimensional framework by weak C2—H2···O1 and C7—H7*A*···N1 intermolecular interactions. The packing is further stabilized by C—H···π (Table 2) and π–π interactions involving the pyridine rings: *Cg*1 is the centroid of the pyridine ring; $Cg1(x, y, z)\cdots Cg1(-x, -1-y, -1-z) = 3.941$ Å.

Experimental

To a solution of 4-pyridinecarboxylic acid (1.23 g, 10 mmol) in pyridine (20 ml) was added piperazine (0.431 g, 50 mmol) in pyridine

(20 ml). After the addition of triphenyl phosphite (3.1 g, 10 mmol), the mixture was heated on a steam bath for 8 h and the solution was then reduced to 10 ml by vacuum evaporation. A yellow precipitate was obtained from the solution after allowing it to stand overnight at room temperature. 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

$C_{16}H_{16}N_4O_2$
$M_r = 296.32$
Monoclinic, $P2_1/c$
$a = 9.206$ (3) Å
$b = 8.282$ (3) Å
$c = 11.347$ (3) Å
$\beta = 123.255$ (17)°
$V = 723.5$ (4) Å^3
$Z = 2$
$D_x = 1.360$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1942 reflections
$\theta = 3.3$–26.0°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Column, yellow
0.30 × 0.28 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.973$, $T_{\max} = 0.988$
3862 measured reflections
1410 independent reflections
1270 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.1°$
$h = -11 \rightarrow 9$
$k = -7 \rightarrow 10$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.117$
$S = 1.09$
1410 reflections
132 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.1396P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.2255 (17)	N2—C8	1.4660 (17)
N2—C6	1.3490 (17)	C5—C6	1.5028 (18)
N2—C7	1.4636 (16)		
C6—N2—C7	125.84 (11)	C7—N2—C8	112.80 (10)
C6—N2—C8	120.62 (11)	N2—C6—C5	118.23 (11)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$O1$^{\rm i}$	0.97 (2)	2.54 (2)	3.435 (3)	154 (1)
C7—H7$A\cdots$N1$^{\rm ii}$	0.97 (2)	2.50 (2)	3.327 (2)	142 (1)
C8—H8$B\cdots$O1	0.96 (2)	2.36 (2)	2.777 (2)	105 (1)

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

All H atoms were located in difference Fourier maps and refined isotropically. The C—H distances lie in the range 0.96 (2)–1.034 (17) Å.

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).

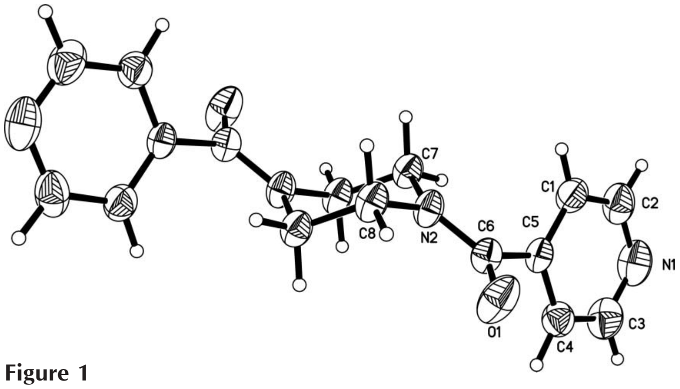


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $-x-1, -y-1, -z-2$.

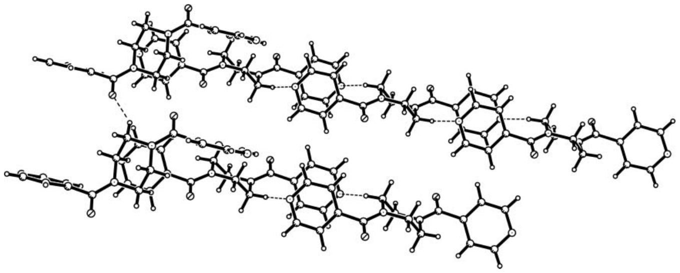


Figure 2
Packing diagram of (I), showing the π–π interactions and hydrogen bonds (dashed lines).

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