Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(pyridin-4-ylmethyl)succinamide–terephthalic acid (1/1)

Clive L. Oliver,* Gareth O. Lloyd and Elise J.C. de Vries

Department of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland 7602, South Africa

Correspondence e-mail: oli@sun.ac.za

Received 21 June 2005
Accepted 4 July 2005
Online 16 July 2005

Key indicators

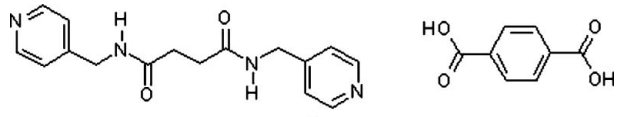
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.146
Data-to-parameter ratio = 15.0

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

Alternate molecules of *N*,*N*′-bis(pyridin-4-ylmethyl)-succinamide and terephthalic acid, each of which is located about a centre of inversion, are linked by strong O—H···N hydrogen bonds to form strands in the title compound, $C_{16}H_{18}N_4O_2\cdot C_8H_6O_4$. In addition, strong N—H···O hydrogen bonds between the *N*,*N*′-bis(pyridin-4-ylmethyl)succinamide molecules of adjacent strands link the latter to form sheets.

Comment

N,*N*′-Bis-pyridin-4-ylmethyl-succinamide, (1), forms part of a series of compounds under investigation by us that possess biologically relevant functional groups, such as aromatic rings and amide groups (Atwood *et al.*, 1998; Barbour *et al.*, 2000). It has recently been used in the assembly of harmonic single and triple helices in a polymeric coordination complex (Lloyd *et al.*, 2005). Co-crystallization of terephthalic acid, (2), with (1) forms part of a structural study in which various acids were co-crystallized with the latter. The structure of (1) co-crystallized with (2) is described here.



(I)

Compounds (1) and (2) crystallize in a 1:1 ratio, (I), with each molecule located about a centre of inversion (Fig. 1). Hydrogen bonding plays an important role in the crystal

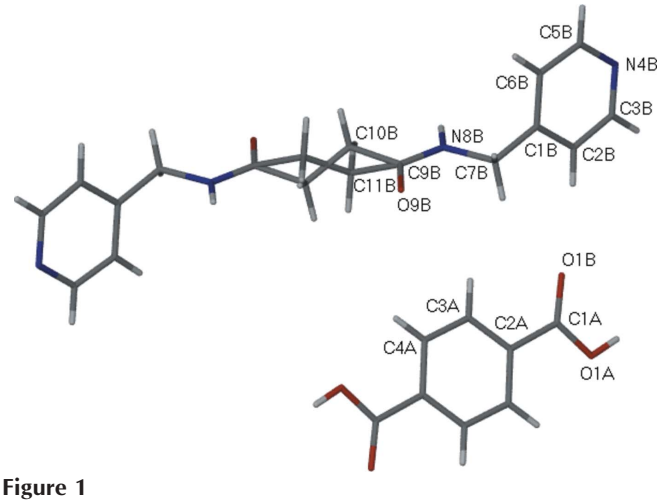


Figure 1
The molecular structures of (1) and (2). Only the atoms of the asymmetric unit are numbered. Unlabelled atoms are related to labelled atoms by $(-x, -y+1, -z+1)$ in (1) and $(-x+1, -y+1, -z)$ in (2).

assembly (Fig. 2). The termini of (1) and (2) are linked to each other *via* O—H···N^{ii} hydrogen bonds [symmetry code: (ii) $-x-1$, $-y+2$, $-z$], forming infinite one-dimensional strands; see Table 1 for parameters describing the hydrogen-bonding scheme. Neigbouring strands are in turn linked by two centrosymmetrically related N—H···O^{i} hydrogen bonds [symmetry code: (i) $x-1$, y, z] which involve molecule (1). These hydrogen bonds link the strands to form infinite two-dimensional sheets. The sheets stack along the diagonal of the *bc* plane and the amide hydrogen-bonding pattern displayed is similar to that observed in β-sheets of protein molecules (Sasaki & Lieberman, 1996). Hydrogen-bonding patterns of this type have recently been used in the rational design of coordination polymers (Sarkar & Biradha, 2005).

The absence of significant π–π interactions [centroid···centroid distances are ∼4.8 Å] is ascribed to the more favourable amide hydrogen bonding, which prevents close approach of aromatic rings in the structure.

Experimental

Compound (1) was synthesized in an analogous manner to *N*,*N*′-bis-pyridin-4-ylmethylglutarimide (de Vries *et al.*, 2005), except that succinyl dichloride instead of glutaryl dichloride was reacted with 4-aminomethylpyridine. Equimolar amounts of compounds (1) and (2) were dissolved in an excess of dimethylformamide, after which crystallization proceeded by slow evaporation. Colourless plate-like crystals formed after several weeks.

Crystal data

$C_{16}H_{18}N_4O_2\cdot C_8H_6O_4$
M_r = 464.47
Triclinic, $P\overline{1}$
a = 4.8721 (13) Å
b = 9.550 (3) Å
c = 11.547 (3) Å
α = 96.582 (4)°
β = 95.944 (4)°
γ = 94.753 (4)°
V = 528.4 (3) Å^3
Z = 1
D_x = 1.460 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2080 reflections
θ = 2.6–28.3°
μ = 0.11 mm^{-1}
T = 100 (2) K
Plates, colourless
0.30 × 0.30 × 0.10 mm

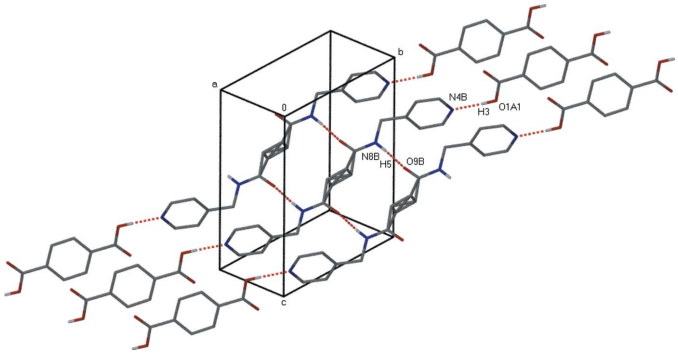


Figure 2
The infinite two-dimensional sheets formed by the N—H···O and O—H···O hydrogen bonding. Dotted red lines indicate the hydrogen-bonding interactions. For clarity, only H atoms involved in the hydrogen bonding are shown.

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.973, T_{max} = 0.989
3480 measured reflections
2330 independent reflections
2156 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.2°
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 11$
$l = -15 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.146
S = 1.07
2330 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2 + 0.3562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N8B—H5···O9B^{i}	0.88	2.01	2.875 (2)	166
O1A—H3···N4B^{ii}	0.84	1.82	2.654 (2)	175

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

All aromatic and methylene H atoms were positioned using the riding-model approximation, with C—H = 0.95 and 0.99 Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(C). The amide H atom was placed in an idealized trigonal–planar position, N—H = 0.88 Å, based on its initial peak position in the difference Fourier map, and U_{iso}(H) = 1.2U_{eq}(N). The hydroxyl H atom was positioned using a hydrogen-bond searching model, with O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(O). Atom C10 of molecule (1) is disordered over two positions, with the major disordered component having a site-occupancy factor of 0.86 (1), as determined from the refinement.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED* (Atwood & Barbour, 2003).

The authors thank the National Research Foundation of South Africa for financial assistance.

References

Atwood, J. L. & Barbour, L. J. (2003). *Cryst. Growth Des.* **3**, 3–8.
Atwood, J. L., Barbour, L. J. & Orr, G. W. (1998). *Nature (London)*, **393**, 671–672.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Barbour, L. J., Orr, G. W. & Atwood, J. L.(2000). *Chem. Commun.* pp. 859–860.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2001). *SMART*. Version 5.625. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *SAINT*. Version 6.36a. Bruker AXS Inc., Madison, Wisconsin, USA.
Lloyd, G. O., Atwood, J. L. & Barbour, L. J. (2005). *Chem. Commun.* pp. 1845–1845.
Sarkar, M. & Biradha, K. (2005). *Chem. Commun.* pp. 2229–2231.
Sasaki, T. & Lieberman, M. (1996). *Comprehensive Supramolecular Chemistry*, edited by J. L. Atwood, J. E. D. Davies, D. D. MacNicol & F. Vögtle, Vol, 4, pp. 193–242. Oxford: Elsevier Science, Oxford.
Sheldrick, G. M. (1997). *SHELXS97*, *SHELXL97* and *SADABS* (Version 2.05). University of Göttingen, Germany.
Vries, E. J. C. de, Oliver, C. L. & Lloyd, G. O. (2005). *Acta Cryst.* E**61**, o1577–o1578.