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N-Propylurea: the missing link

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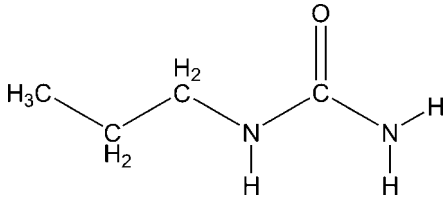
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.172; data-to-parameter ratio = 9.8.

The title molecule, $C_4H_{10}N_2O$, is planar and its alkyl chain displays an all-*trans* configuration, which is typical for *n*-alkylurea structures. Pairs of molecules are hydrogen bonded across crystallographic inversion centres [N···O = 2.962 (4) Å], with each O atom involved in two additional hydrogen bonds, linking adjacent urea molecules into chains along *c* [N···O = 2.924 (3) and 3.042 (3) Å]. Each chain is propagated by a *c*-glide operation and planes containing adjacent urea molecules intercept at an angle of 50.14 (9)°.

Related literature

The title compound is the third member (n = 3) of the straight-chain alkylurea series, $H_2NCONHC_nH_{2n+1}$. Crystal structures for the analogous compounds with n = 1 (Huiszoon & Tiemessen, 1976) and n = 2, 4–14 (Hashimoto *et al.*, 2005) have been published previously.



Experimental

Crystal data

$C_4H_{10}N_2O$
M_r = 102.14
Monoclinic, $P2_1/c$
a = 7.8473 (10) Å
b = 7.7271 (10) Å
c = 9.2429 (14) Å
β = 95.777 (6)°
V = 557.61 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 150 (2) K
0.3 × 0.25 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)
T_{min} = 0.925, T_{max} = 1.000
(expected range = 0.923–0.998)
3437 measured reflections
1017 independent reflections
710 reflections with $I > 2\sigma(I)$
R_{int} = 0.167

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.172
S = 1.10
1017 reflections
104 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.19 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—H1A···O1^{i}	0.96 (4)	2.00 (4)	2.962 (4)	175 (3)
N1—H1B···O1^{ii}	0.96 (3)	2.02 (3)	2.924 (3)	156 (3)
N2—H2A···O1^{ii}	0.92 (3)	2.24 (3)	3.042 (3)	145 (2)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the use of the EPSRC's Chemical Database Service at Daresbury (Allen, 2002; Fletcher *et al.*, 1996) and EPSRC support for the purchase of equipment.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2331).

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supplementary materials

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N-Propylurea: the missing link

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Comment

For the purpose of this paper, n-propylurea will be referred to as C_3—U in compliance with the system used by Hashimoto *et al.*. (2005) and is derived from the number of carbon atoms in the alkyl group, $H_2NCONHC_nH_{2n+1}$.

In common with all the members of the $C_{4–14}$—U series, C_3—U is planar and its alkyl chain displays an all-*trans* configuration (Fig. 1). This contrasts with non-planar C_2—U, in which the terminal methyl group is in a skew position with respect to the N—C bond.

The H-bonding network in the title compound (Fig. 2) is typical for the longer chain n-alkylurea crystal structures and consists of pairs of molecules linked across crystallographic inversion centres (N···O 2.962 (4) Å). Furthermore, each oxygen is involved in two additional H-bonds, which link adjacent urea moieties into chains along *c* (N···O 2.924 (3), 3.042 (3) Å). All three N···O values agree well with those in the $C_{5–14}$—U series, for which the corresponding distances fall in the ranges 2.95 (1), 3.06 (2) and 2.93 (2) Å.

Each chain is propogated by a c-glide operation and planes containing adjacent urea moieties intercept at an angle of 50.14 (9)°. This value is slightly more acute than in the analogous $C_{5–14}$—U structures (54.0–55.4°, except for C_5—U, 57.5°). Interestingly, although the crystal packing in C_4—U is somewhat different to the remainder of the series, the structure has retained the above H-bonded chains, albeit with coplanar urea moieties.

Experimental

The n-propylurea (C_3—U) crystals were grown by evaporation, using 30% weight % H_2O_2 as the solvent. This was a failed attempt at preparing an n-propylurea H_2O_2 adduct.

Refinement

The extremely thin, easily-distorted n-propylurea crystals produced a streaked diffraction pattern, which resulted in an elevated R_{int}. H atoms were refined isotropically.

Figures

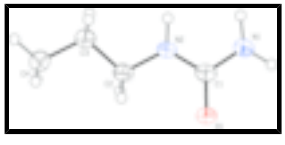

Fig. 1. The molecular structure of C_3—U, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

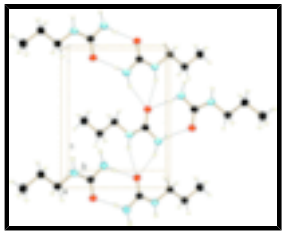

Fig. 2. The packing of C_3—U, viewed perpendicular to the *c* axis, showing the H-bonding scheme (dashed lines).

N-Propylurea

Crystal data

$C_4H_{10}N_2O_1$	F_{000} = 224
M_r = 102.14	D_x = 1.217 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3437 reflections
a = 7.8473 (10) Å	θ = 2–26º
b = 7.7271 (10) Å	μ = 0.09 mm^{-1}
c = 9.2429 (14) Å	*T* = 150 (2) K
β = 95.777 (6)º	Plate, colourless
V = 557.61 (13) Å^3	0.3 × 0.25 × 0.02 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.167
CCD rotation images, thick slices scans	θ_{max} = 25.5º
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)	θ_{min} = 3.4º
T_{min} = 0.925, T_{max} = 1.000	*h* = −9→9
3437 measured reflections	*k* = −9→9
1017 independent reflections	*l* = −9→11
710 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	All H-atom parameters refined
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.3434P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.064	$(\Delta/\sigma)_{max}$ = 0.015
$wR(F^2)$ = 0.172	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 1.10	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
1017 reflections	Extinction correction: none
104 parameters	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1361 (4)	0.2221 (4)	0.5775 (3)	0.0316 (7)
C2	0.2539 (4)	0.5134 (4)	0.5468 (3)	0.0334 (7)
C3	0.3388 (5)	0.6552 (4)	0.6406 (3)	0.0383 (8)
C4	0.3912 (5)	0.8063 (5)	0.5506 (4)	0.0428 (9)
N1	0.0878 (4)	0.1021 (3)	0.6715 (3)	0.0390 (7)
N2	0.2076 (3)	0.3678 (3)	0.6358 (3)	0.0355 (7)
O1	0.1154 (3)	0.2001 (3)	0.44264 (19)	0.0365 (6)
H1A	0.025 (5)	0.005 (5)	0.629 (4)	0.055 (10)*
H1B	0.092 (4)	0.135 (4)	0.772 (4)	0.043 (9)*
H2A	0.221 (4)	0.378 (4)	0.736 (3)	0.029 (7)*
H2B	0.328 (4)	0.469 (4)	0.467 (3)	0.037 (8)*
H2C	0.149 (4)	0.564 (4)	0.486 (3)	0.037 (8)*
H3A	0.437 (4)	0.608 (4)	0.702 (4)	0.047 (9)*
H3B	0.262 (5)	0.691 (5)	0.720 (4)	0.060 (11)*
H4A	0.286 (5)	0.857 (5)	0.492 (4)	0.059 (11)*
H4B	0.474 (5)	0.771 (5)	0.486 (4)	0.061 (11)*
H4C	0.443 (5)	0.903 (6)	0.610 (4)	0.069 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0314 (16)	0.0381 (17)	0.0255 (15)	0.0049 (13)	0.0038 (12)	0.0001 (12)
C2	0.0356 (16)	0.0382 (17)	0.0258 (14)	−0.0018 (14)	0.0008 (12)	0.0017 (12)
C3	0.0464 (19)	0.0381 (17)	0.0293 (15)	−0.0034 (15)	−0.0018 (14)	0.0018 (13)
C4	0.047 (2)	0.0408 (19)	0.0391 (19)	−0.0076 (17)	−0.0011 (16)	−0.0006 (15)
N1	0.0540 (18)	0.0368 (14)	0.0266 (14)	−0.0058 (13)	0.0066 (12)	−0.0001 (11)
N2	0.0480 (16)	0.0379 (14)	0.0205 (13)	−0.0068 (12)	0.0020 (10)	0.0005 (11)
O1	0.0484 (14)	0.0372 (12)	0.0233 (11)	−0.0038 (10)	0.0005 (9)	−0.0012 (8)

Geometric parameters (Å, °)

C1—O1	1.252 (3)	C3—H3A	0.98 (3)
C1—N2	1.346 (4)	C3—H3B	1.03 (4)
C1—N1	1.351 (4)	C4—H4A	1.02 (4)
C2—N2	1.461 (4)	C4—H4B	0.96 (4)
C2—C3	1.510 (4)	C4—H4C	0.99 (4)
C2—H2B	1.05 (3)	N1—H1A	0.96 (4)

C2—H2C	1.03 (3)	N1—H1B	0.96 (3)
C3—C4	1.515 (4)	N2—H2A	0.92 (3)
O1—C1—N2	121.3 (3)	H3A—C3—H3B	100 (3)
O1—C1—N1	122.0 (3)	C3—C4—H4A	110 (2)
N2—C1—N1	116.7 (2)	C3—C4—H4B	111 (2)
N2—C2—C3	110.8 (2)	H4A—C4—H4B	110 (3)
N2—C2—H2B	109.5 (17)	C3—C4—H4C	113 (2)
C3—C2—H2B	113.6 (17)	H4A—C4—H4C	106 (3)
N2—C2—H2C	112.0 (17)	H4B—C4—H4C	107 (3)
C3—C2—H2C	108.6 (18)	C1—N1—H1A	116 (2)
H2B—C2—H2C	102 (2)	C1—N1—H1B	117 (2)
C2—C3—C4	111.9 (3)	H1A—N1—H1B	125 (3)
C2—C3—H3A	109.7 (19)	C1—N2—C2	122.4 (2)
C4—C3—H3A	111 (2)	C1—N2—H2A	118.4 (18)
C2—C3—H3B	110 (2)	C2—N2—H2A	119.1 (18)
C4—C3—H3B	113 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{i}	0.96 (4)	2.00 (4)	2.962 (4)	175 (3)
N1—H1B···O1^{ii}	0.96 (3)	2.02 (3)	2.924 (3)	156 (3)
N2—H2A···O1^{ii}	0.92 (3)	2.24 (3)	3.042 (3)	145 (2)

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

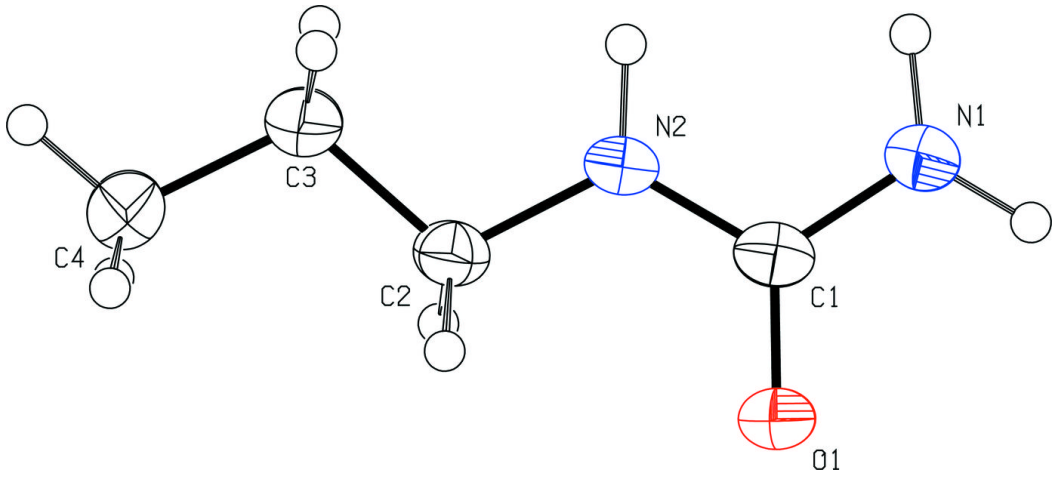

Fig. 2