S1—C21	1.758 (4)	N2—C9	1.474 (5)
S2—O4	1.433 (3)	O5—C13	1.193 (6)
S2—O3	1.432 (3)	O6—C13	1.346 (6)
S2—N2	1.634 (4)	O6—C14	1.444 (6)
S2—C15	1.761 (4)		
C11—N1—C1	107.9 (3)	C2—C1—N1	129.6 (4)
C11—N1—S1	125.2 (3)	N2—C9—C8	113.8 (3)
C1—N1—S1	126.2 (3)	N2—C10—C11	108.5 (3)
C10—N2—C9	113.7 (3)	C7—C11—N1	109.5 (3)
C10—N2—S2	119.5 (3)	N1—C11—C10	126.3 (3)
C9—N2—S2	117.4 (3)	O5—C13—O6	123.3 (4)
C13—O6—C14	116.0 (4)	O5—C13—C12	128.0 (4)
C6—C1—N1	107.7 (4)	O6—C13—C12	108.7 (4)
S1—N1—C1—C2	−6.1 (7)	S2—N2—C9—C8	−90.3 (4)

The H atoms of C14 were fixed by a riding model. All the other H atoms were refined isotropically.

Data collection: Rigaku *AFC-7R* diffractometer. Cell refinement: *MSC/AFC Diffraction Control Software* (Molecular Structure Corporation, 1988). Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1993). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*92 (Vickovic, 1994). Software used to prepare material for publication: *PARST* (Nardelli, 1983, 1995).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1278). Services for accessing these data are described at the back of the journal.

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N,N'-Dicyclohexylurea†

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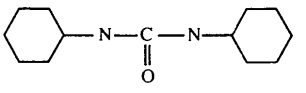
Abstract

The title molecule, $C_{13}H_{24}N_2O$, possesses twofold symmetry, with the C=O group lying on a crystallographic twofold axis in the unit cell. The cyclohexane rings adopt a chair conformation. Successive molecules along the twofold axis are related by the short *b* translation and interact through two identical diad-related N—H···O hydrogen bonds [2.962 (5) Å] in which the O atom lying on the twofold axis acts as a common acceptor for the diad-related amino protons.

Comment

An interesting aspect of the title structure, (I), is that the asymmetric unit consists of mainly the *N*-cyclohexyl group and half of the C=O moiety. The C=O group lies on a crystallographic twofold axis and thus the title molecule possesses a twofold symmetry relating the *N*-cyclohexyl groups. The bond lengths and angles observed in the cyclohexane ring, as well as their variations around the ring, are found to be within the observed range of values reported for related structures, such as *N,N'*-dicyclohexyl-*N*-4-phenylbutyrylurea (Ball, Brown & Bennet, 1990) and 3-cyclohexyl-1-[2-(1*H*-indol-3-yl)ethyl]urea (Ishida, Yamashita, Takai & Inoue, 1983).



(I)

An *ORTEP* diagram (Johnson, 1965; Vickovic, 1994) of the title molecule is shown in Fig. 1. For the cyclohexane ring, the average value of the bond angle, 112.8°, and that of the absolute torsion angle, 50.7°, as well as the distribution of the torsion angles around the ring, agree closely with the theoretically predicted values of 111.5 and 54.7° for chair conformations (Bixon & Lifson, 1967). As stated in the abstract, the molecules interact through two identical intermolecular N—H···O hydrogen bonds. This interaction gives rise to an infinite sheet-like structure, similar to the parallel

† DCB contribution No. 878.

β sheet structure observed in peptides. Crystal packing involves stacking of these sheets in which the hydrophobic cyclohexyl groups are clustered together in a pseudo-hexagonal packing arrangement (Fig. 2).

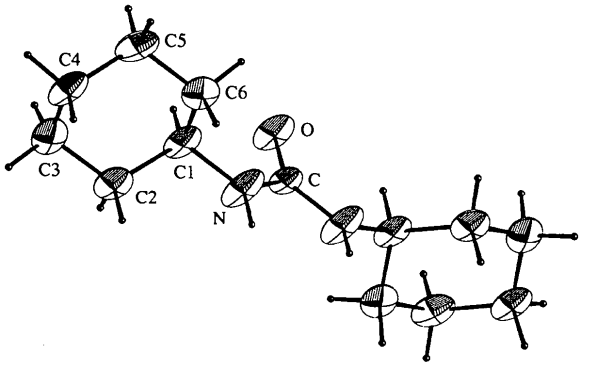


Fig. 1. *ORTEP*92 (Johnson, 1965; Vickovic, 1994) plot of the molecule with numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

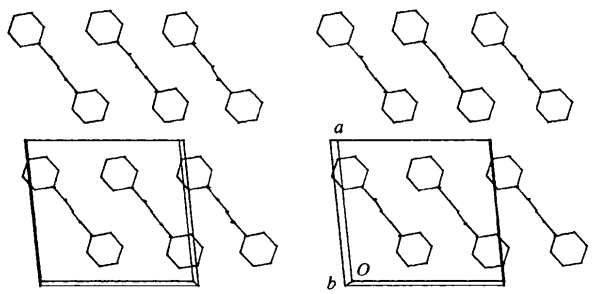


Fig. 2. Stereoview of the crystal packing arrangement down the *b* axis.

Experimental

The title compound was obtained from the Sigma Chemical Company.

Crystal data

$C_{13}H_{24}N_2O$
M_r = 224.34
Monoclinic
$P2/c$
a = 11.520 (1) Å
b = 4.700 (1) Å
c = 12.040 (1) Å
β = 95.44 (1)°
V = 649.0 (2) Å^3
Z = 2
D_x = 1.148 Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 15 reflections
θ = 10–15°
μ = 0.565 mm^{-1}
T = 293 (2) K
Plate-like
0.20 × 0.15 × 0.15 mm
Colourless transparent

Data collection

Picker FACS–I four-circle diffractometer
$w/2\theta$ scans
Absorption correction: none
812 measured reflections
812 independent reflections
468 reflections with $I > 2\sigma(I)$
θ_{max} = 55°
$h = -12 \rightarrow 12$
$k = 0 \rightarrow 4$
$l = 0 \rightarrow 12$
3 standard reflections
every 200 reflections
frequency: 120 min
intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0646
$wR(F^2)$ = 0.1807
S = 0.930
812 reflections
74 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.1072P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.598 e Å^{-3}
$\Delta\rho_{min}$ = −0.148 e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\sum_i\sum_j U^{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
O	1/2	0.5834 (8)	1/4	0.0526 (12)
N	0.4192 (3)	0.1663 (7)	0.2957 (3)	0.0612 (12)
C	1/2	0.3145 (12)	1/4	0.0413 (14)
C1	0.3291 (3)	0.2772 (8)	0.3593 (3)	0.0458 (11)
C2	0.2100 (3)	0.1785 (10)	0.3166 (3)	0.0618 (13)
C3	0.1153 (3)	0.2839 (11)	0.3849 (3)	0.0661 (14)
C4	0.1410 (4)	0.2257 (9)	0.5072 (3)	0.0594 (13)
C5	0.2601 (3)	0.3261 (10)	0.5517 (3)	0.0651 (14)
C6	0.3550 (3)	0.2218 (9)	0.4839 (3)	0.0553 (12)

Table 2. *Selected geometric parameters (Å, °)*

O—C	1.264 (6)	N—C1	1.444 (5)
N—C	1.324 (4)		
O—C—N	121.8 (3)	N—C—N^i	116.5 (5)
C1—N—C—O	−6.2 (4)	C—N—C1—C2	127.3 (4)
C1—N—C—N^i	173.8 (4)	C—N—C1—C6	−105.2 (4)

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

Data collection: local program. Cell refinement: local program. Data reduction: local program. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*92 (Johnson, 1965; Vickovic, 1994). Software used to prepare material for publication: *PARST* (Nardelli, 1983, 1995).

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