Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Acetyl-1,3-dicyclohexylurea

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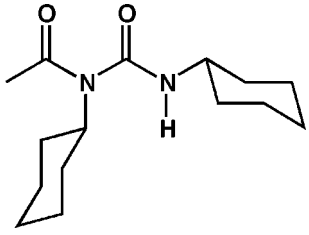
Received 4 September 2007; accepted 5 September 2007

Key indicators: single-crystal X-ray study; T = 183 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.108; data-to-parameter ratio = 20.2.

The title compound, $C_{15}H_{26}N_2O_2$, was prepared from dicyclohexylcarbodiimide and acetic acid. The crystal structure is established by strong N—H···O interactions between the amide H atom and the acetyl O atom, producing dimeric units which are connected into infinite chains by additional C—H···O hydrogen bonds.

Related literature

For related literature, see: Ball *et al.* (1990); Banerjee *et al.* (2000); Bechtel *et al.* (1979); Behrens & Rehder (2006); Chérioux *et al.* (2002); Orea Flores *et al.* (2006); Gallagher *et al.* (1999); Goel *et al.* (2003); Ishida *et al.* (1983); Mazumdar *et al.* (2003); Perollier *et al.* (1999); Salas-Coronado *et al.* (2001); Toniolo *et al.* (1990); Detar & Silverstein (1966*a*,*b*); Khorana (1953); Ogawa *et al.* (1990); Ramsden & Rose (1997); Smart *et al.* (1960); Smith *et al.* (1958); Wei *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{26}N_2O_2$
M_r = 266.38
Monoclinic, $P2_1/n$
a = 10.6174 (4) Å
b = 14.2451 (9) Å
c = 10.8862 (6) Å
β = 111.795 (3)°
V = 1528.80 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 183 (2) K
0.3 × 0.2 × 0.2 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
5982 measured reflections
3494 independent reflections
2103 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 0.95
3494 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^{i}	0.88	2.04	2.907 (3)	171
C12—H12B···O1^{ii}	0.99	2.57	3.469 (3)	151

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1990); software used to prepare material for publication: *SHELXL97* and *XP*.

The author thanks the Deutsche Forschungsgemeinschaft for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2203).

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supplementary materials

Acta Cryst. (2007). E**63**, o4036-o4037 [**doi:10.1107/S1600536807043656**]

1-Acetyl-1,3-dicyclohexylurea

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Comment

Acylated *N*-aryl- and *N*-alkylurea derivatives have been investigated, *e.g.* as intermediates in the synthesis of amidines and heterocyclic compounds derived therefrom, as well as precursors for poly(amide-imide)s (Wei *et al.* 2006, Ramsden & Rose 1997, Khorana 1953, Smith *et al.* 1958, Detar & Silverstein 1966*a*,b, Ogawa *et al.* 1990, Smart *et al.* 1960). Although quite a number of acylated dicyclohexylurea derivatives have been structurally characterized (Ball *et al.* 1990, Banerjee *et al.* 2000, Bechtel *et al.* 1979, Behrens & Rehder 2006, Chérioux *et al.* 2002, Orea Flores *et al.* 2006, Gallagher *et al.* 1999, Goel *et al.* 2003, Ishida *et al.* 1983, Mazumdar *et al.* 2003, Perollier *et al.* 1999, Salas-Coronado *et al.* 2001, Toniolo *et al.* 1990), the structure of the most simple derivative, with an acetyl group, has not yet been reported.

The molecular structure of the title compound (Fig. 1) shows the two urea nitrogen atoms N1 and N2 having a planar geometry, with an angle of 69.00 (6)° between [C6, N1, H1N, C7] and [C7, N2, C8, C14]. The bond lengths and angles have expected values. The crystal structure is determined by hydrogen bonds. The strongest interactions are observed between the amide N1—H1N group and the acetyl oxygen atom (H···O 2.035 Å). Two of these hydrogen bonds link two molecules, forming a dimeric cyclic unit. These dimers are linked to produce infinite chains by additional C—H···O bonds from one of the cyclohexyl substituents to the carbonyl oxygen atom of the urea unit (Fig. 2, Table 1).

Experimental

1.96 g Dicyclohexylcarbodiimide (9.51 mmol) were stirred at room temperature for 5 h together with 5 ml glacial acetic acid and 1 mol% (110 mg) [$Pd(PPh_3)_4$] in 10 ml THF. On standing at −20° for three days, colorless crystals of the title compound were produced; these were identified by their melting point and ^{1}H NMR spectrum (Ogawa *et al.* 1990, Smart *et al.* 1960). ^{13}C NMR ($CDCl_3$, 293 K) [p.p.m.]: 23.9 (CH_3), 24.6 (CH_2), 25.2 (CH_2), 25.4 (CH_2), 26.2 (CH_2), 30.7 (CH_2), 32.6 (CH_2), 55.6 (CH), 56,4 (CH), 153.9 (C=O), 170.9 (C=O).

Refinement

Hydrogen atoms were placed in idealized positions and refined using a riding model, with distances of N—H = 0.88 Å and C—H = 0.98–1.00 Å; U_{iso}(H) = 1.5U_{eq}(C,*N*).

Figures

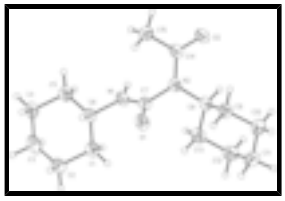

Fig. 1. The molecular structure of the title compound, showing the labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

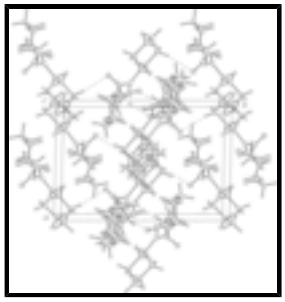

Fig. 2. Crystal structure of the title compound. Dashed lines indicate hydrogen bonds.

1-Acetyl-1,3-dicyclohexyurea

Crystal data

$C_{15}H_{26}N_2O_2$	F_{000} = 584
M_r = 266.38	D_x = 1.157 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2yn	Cell parameters from 5982 reflections
a = 10.6174 (4) Å	θ = 2.5–27.5º
b = 14.2451 (9) Å	μ = 0.08 mm^{-1}
c = 10.8862 (6) Å	T = 183 (2) K
β = 111.795 (3)º	Cuboid, colourless
V = 1528.80 (14) Å^3	0.3 × 0.2 × 0.2 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	2103 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.030
Monochromator: graphite	θ_{max} = 27.5º
T = 183(2) K	θ_{min} = 2.5º
phi–scan, ω–scan	h = −13→13
Absorption correction: none	k = −16→18
5982 measured reflections	l = −14→14
3494 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H-atom parameters constrained
$wR(F^2)$ = 0.108	$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max} < 0.001$
3494 reflections	$\Delta\rho_{max}$ = 0.17 e Å^{-3}

173 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.06204 (15)	0.63488 (12)	0.96118 (14)	0.0552 (4)
H1A	0.1613	0.6441	0.9905	0.083*
H1B	0.0443	0.5666	0.9597	0.083*
C2	0.01037 (16)	0.68244 (14)	1.05960 (14)	0.0639 (5)
H2A	0.0525	0.6522	1.1473	0.096*
H2B	0.0376	0.7493	1.0690	0.096*
C3	−0.14216 (16)	0.67575 (12)	1.01465 (16)	0.0576 (4)
H3A	−0.1688	0.6092	1.0153	0.086*
H3B	−0.1730	0.7108	1.0769	0.086*
C4	−0.20999 (14)	0.71539 (13)	0.87715 (14)	0.0584 (4)
H4A	−0.1919	0.7837	0.8789	0.088*
H4B	−0.3093	0.7064	0.8478	0.088*
C5	−0.15866 (13)	0.66796 (12)	0.77887 (14)	0.0571 (4)
H5A	−0.1864	0.6012	0.7692	0.086*
H5B	−0.2006	0.6984	0.6913	0.086*
C6	−0.00597 (12)	0.67416 (9)	0.82379 (12)	0.0348 (3)
H6	0.0198	0.7418	0.8251	0.052*
N1	0.03787 (10)	0.62479 (8)	0.72894 (10)	0.0384 (3)
H1N	−0.0132	0.5789	0.6825	0.058*
C7	0.15079 (12)	0.64555 (9)	0.70914 (12)	0.0350 (3)
O1	0.23242 (9)	0.70596 (7)	0.76652 (9)	0.0460 (3)
N2	0.17255 (10)	0.58545 (7)	0.61161 (10)	0.0348 (3)
C8	0.28978 (12)	0.52058 (9)	0.65772 (12)	0.0345 (3)
H8	0.2645	0.4638	0.5997	0.052*
C9	0.41480 (12)	0.56302 (10)	0.64319 (14)	0.0420 (3)
H9A	0.4454	0.6183	0.7020	0.063*
H9B	0.3927	0.5840	0.5508	0.063*
C10	0.52742 (14)	0.48970 (11)	0.67961 (15)	0.0526 (4)
H10A	0.4983	0.4363	0.6173	0.079*
H10B	0.6095	0.5176	0.6717	0.079*

C11	0.56119 (15)	0.45453 (11)	0.82013 (16)	0.0591 (4)
H11A	0.6302	0.4043	0.8395	0.089*
H11B	0.6001	0.5066	0.8831	0.089*
C12	0.43630 (15)	0.41690 (10)	0.83923 (15)	0.0526 (4)
H12A	0.4601	0.4000	0.9334	0.079*
H12B	0.4056	0.3591	0.7859	0.079*
C13	0.32072 (14)	0.48780 (10)	0.79900 (13)	0.0434 (3)
H13A	0.3463	0.5423	0.8597	0.065*
H13B	0.2388	0.4586	0.8056	0.065*
C14	0.09682 (12)	0.59270 (9)	0.47971 (13)	0.0363 (3)
O2	0.11724 (8)	0.53978 (7)	0.39946 (9)	0.0435 (3)
C15	−0.00869 (13)	0.66818 (10)	0.43522 (13)	0.0449 (4)
H15A	−0.0302	0.6815	0.3413	0.067*
H15B	0.0259	0.7252	0.4871	0.067*
H15C	−0.0908	0.6472	0.4481	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0564 (9)	0.0703 (11)	0.0422 (8)	0.0220 (8)	0.0222 (7)	0.0044 (8)
C2	0.0658 (10)	0.0937 (14)	0.0366 (8)	0.0233 (9)	0.0240 (7)	0.0030 (9)
C3	0.0711 (10)	0.0585 (10)	0.0630 (10)	−0.0031 (8)	0.0478 (8)	−0.0074 (8)
C4	0.0411 (8)	0.0827 (12)	0.0558 (10)	0.0064 (8)	0.0230 (7)	−0.0156 (9)
C5	0.0386 (8)	0.0856 (12)	0.0474 (9)	0.0047 (8)	0.0163 (6)	−0.0181 (9)
C6	0.0381 (7)	0.0349 (7)	0.0358 (7)	−0.0018 (5)	0.0188 (5)	−0.0058 (6)
N1	0.0375 (6)	0.0437 (7)	0.0386 (6)	−0.0075 (5)	0.0193 (5)	−0.0128 (5)
C7	0.0366 (7)	0.0369 (7)	0.0336 (7)	0.0010 (6)	0.0154 (6)	−0.0016 (6)
O1	0.0426 (5)	0.0449 (6)	0.0549 (6)	−0.0092 (5)	0.0233 (4)	−0.0152 (5)
N2	0.0355 (6)	0.0400 (6)	0.0324 (6)	0.0020 (5)	0.0167 (5)	−0.0031 (5)
C8	0.0382 (7)	0.0341 (7)	0.0349 (7)	−0.0003 (6)	0.0176 (5)	−0.0028 (6)
C9	0.0392 (7)	0.0458 (8)	0.0449 (8)	−0.0011 (6)	0.0204 (6)	0.0014 (7)
C10	0.0389 (7)	0.0638 (10)	0.0564 (10)	0.0041 (7)	0.0193 (6)	−0.0021 (8)
C11	0.0510 (9)	0.0614 (10)	0.0542 (10)	0.0149 (8)	0.0072 (7)	−0.0017 (8)
C12	0.0707 (10)	0.0418 (8)	0.0416 (8)	0.0095 (7)	0.0165 (7)	0.0044 (7)
C13	0.0547 (8)	0.0403 (8)	0.0404 (8)	0.0008 (7)	0.0236 (6)	0.0038 (7)
C14	0.0356 (7)	0.0400 (8)	0.0365 (7)	−0.0093 (6)	0.0170 (6)	−0.0052 (6)
O2	0.0484 (6)	0.0479 (6)	0.0368 (5)	−0.0063 (4)	0.0188 (4)	−0.0102 (4)
C15	0.0392 (7)	0.0521 (9)	0.0402 (8)	0.0009 (6)	0.0111 (6)	−0.0006 (7)

Geometric parameters (Å, °)

C1—C6	1.5065 (19)	N2—C8	1.4802 (15)
C1—C2	1.5311 (19)	C8—C9	1.5194 (17)
C1—H1A	0.9900	C8—C13	1.5219 (18)
C1—H1B	0.9900	C8—H8	1.0000
C2—C3	1.511 (2)	C9—C10	1.5250 (19)
C2—H2A	0.9900	C9—H9A	0.9900
C2—H2B	0.9900	C9—H9B	0.9900
C3—C4	1.509 (2)	C10—C11	1.521 (2)

C3—H3A	0.9900	C10—H10A	0.9900
C3—H3B	0.9900	C10—H10B	0.9900
C4—C5	1.5268 (19)	C11—C12	1.514 (2)
C4—H4A	0.9900	C11—H11A	0.9900
C4—H4B	0.9900	C11—H11B	0.9900
C5—C6	1.5121 (17)	C12—C13	1.5227 (18)
C5—H5A	0.9900	C12—H12A	0.9900
C5—H5B	0.9900	C12—H12B	0.9900
C6—N1	1.4608 (15)	C13—H13A	0.9900
C6—H6	1.0000	C13—H13B	0.9900
N1—C7	1.3278 (15)	C14—O2	1.2325 (15)
N1—H1N	0.8800	C14—C15	1.4977 (18)
C7—O1	1.2165 (15)	C15—H15A	0.9800
C7—N2	1.4477 (15)	C15—H15B	0.9800
N2—C14	1.3645 (16)	C15—H15C	0.9800
C6—C1—C2	111.49 (12)	N2—C8—C9	111.93 (10)
C6—C1—H1A	109.3	N2—C8—C13	111.91 (10)
C2—C1—H1A	109.3	C9—C8—C13	110.99 (11)
C6—C1—H1B	109.3	N2—C8—H8	107.2
C2—C1—H1B	109.3	C9—C8—H8	107.2
H1A—C1—H1B	108.0	C13—C8—H8	107.2
C3—C2—C1	111.40 (13)	C8—C9—C10	109.35 (12)
C3—C2—H2A	109.3	C8—C9—H9A	109.8
C1—C2—H2A	109.3	C10—C9—H9A	109.8
C3—C2—H2B	109.3	C8—C9—H9B	109.8
C1—C2—H2B	109.3	C10—C9—H9B	109.8
H2A—C2—H2B	108.0	H9A—C9—H9B	108.3
C4—C3—C2	110.92 (12)	C11—C10—C9	110.88 (12)
C4—C3—H3A	109.5	C11—C10—H10A	109.5
C2—C3—H3A	109.5	C9—C10—H10A	109.5
C4—C3—H3B	109.5	C11—C10—H10B	109.5
C2—C3—H3B	109.5	C9—C10—H10B	109.5
H3A—C3—H3B	108.0	H10A—C10—H10B	108.1
C3—C4—C5	111.49 (13)	C12—C11—C10	111.31 (12)
C3—C4—H4A	109.3	C12—C11—H11A	109.4
C5—C4—H4A	109.3	C10—C11—H11A	109.4
C3—C4—H4B	109.3	C12—C11—H11B	109.4
C5—C4—H4B	109.3	C10—C11—H11B	109.4
H4A—C4—H4B	108.0	H11A—C11—H11B	108.0
C6—C5—C4	111.49 (11)	C11—C12—C13	112.26 (12)
C6—C5—H5A	109.3	C11—C12—H12A	109.2
C4—C5—H5A	109.3	C13—C12—H12A	109.2
C6—C5—H5B	109.3	C11—C12—H12B	109.2
C4—C5—H5B	109.3	C13—C12—H12B	109.2
H5A—C5—H5B	108.0	H12A—C12—H12B	107.9
N1—C6—C1	111.22 (11)	C12—C13—C8	110.05 (11)
N1—C6—C5	109.15 (10)	C12—C13—H13A	109.7
C1—C6—C5	111.13 (11)	C8—C13—H13A	109.7
N1—C6—H6	108.4	C12—C13—H13B	109.7

C1—C6—H6	108.4	C8—C13—H13B	109.7
C5—C6—H6	108.4	H13A—C13—H13B	108.2
C7—N1—C6	123.46 (10)	O2—C14—N2	120.64 (12)
C7—N1—H1N	118.3	O2—C14—C15	121.14 (12)
C6—N1—H1N	118.3	N2—C14—C15	118.19 (11)
O1—C7—N1	126.04 (12)	C14—C15—H15A	109.5
O1—C7—N2	121.17 (11)	C14—C15—H15B	109.5
N1—C7—N2	112.76 (11)	H15A—C15—H15B	109.5
C14—N2—C7	122.34 (11)	C14—C15—H15C	109.5
C14—N2—C8	119.79 (10)	H15A—C15—H15C	109.5
C7—N2—C8	117.62 (9)	H15B—C15—H15C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.88	2.04	2.907 (3)	171
C12—H12B···O1^{ii}	0.99	2.57	3.469 (3)	151

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2.

Fig. 1

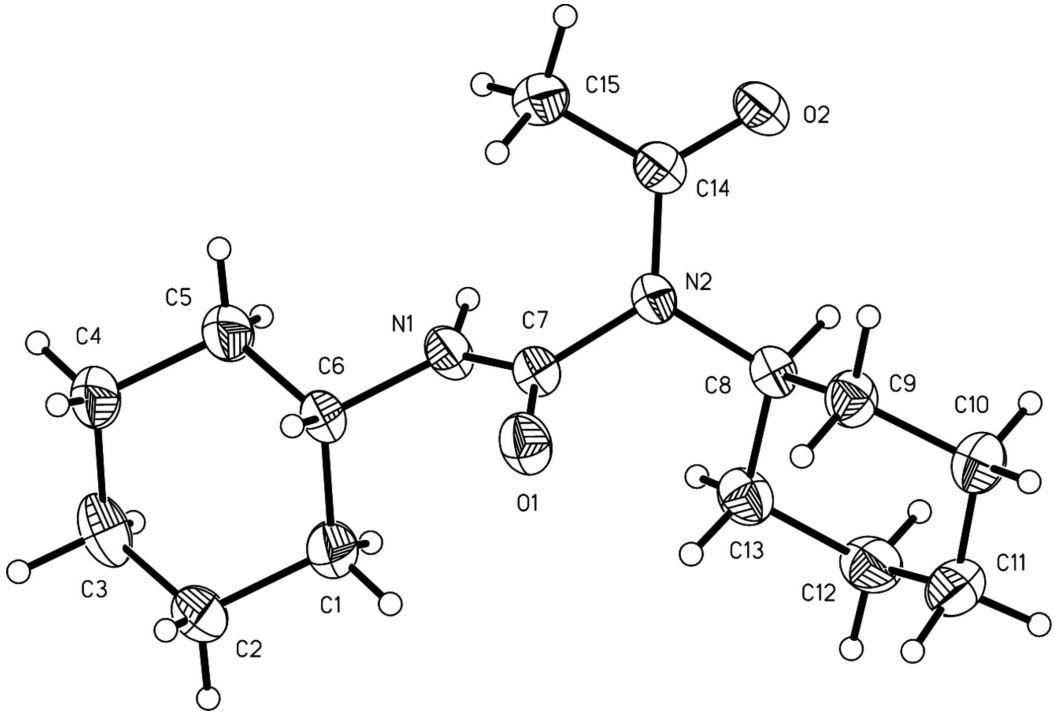

Fig. 2