Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dicyclohexyl(hydroxy)acetonitrile

Richard Betz and Peter Klüfers*

Ludwig-Maximilians Universität, Department Chemie und Biochemie, Butenandtstrasse 5–13 (Haus D), 81377 München, Germany
Correspondence e-mail: kluef@cup.uni-muenchen.de

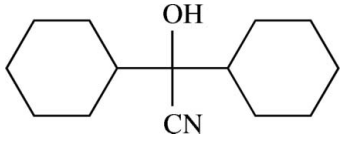
Received 20 July 2007; accepted 21 August 2007

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.100; data-to-parameter ratio = 21.2.

The title compound, $C_{14}H_{23}NO$, the cyanohydrin of dicyclohexyl ketone, was prepared as an intermediate in the synthesis of dicyclohexyl(hydroxy)acetic acid. The cyclohexyl rings adopt chair conformations. The central C atom is in a slightly distorted tetrahedral environment of three C atoms and one O atom. Intermolecular hydrogen bonds are present in the crystal structure, forming dimers.

Related literature

The title compound was prepared according to standard procedures (Becker *et al.*, 2001).



Experimental

Crystal data

$C_{14}H_{23}NO$
M_r = 221.34
Monoclinic, $P2_1/c$
a = 10.1300 (11) Å
b = 10.8140 (8) Å
c = 12.5540 (13) Å
β = 108.548 (12)°
V = 1303.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 200 (2) K
0.43 × 0.32 × 0.26 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997)
T_{min} = 0.979, T_{max} = 0.985
10944 measured reflections
3117 independent reflections
2073 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
S = 0.92
3117 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.84	2.07	2.8982 (14)	167

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

Data collection: *IPDS Software* (Stoe & Cie, 1996); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

The authors thank Sandra Albrecht and Dr Peter Mayer for professional support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2449).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Becker, H. G. O., Beckert, R., Domschke, G., Fanghänel, E., Habicher, W. D., Metz, P., Pavel, D. & Schwetlick, K. (2001). *Organikum – Organisch-chemisches Grundpraktikum*. Weinheim, Germany: Wiley-VCH.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA. Windows version (L. J. Farrugia, University of Glasgow, Scotland) used.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (1996). *IPDS Software*. Stoe Publication 4801-007. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (1997). *X-RED*. Version 1.09. Stoe & Cie GmbH, Darmstadt, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, o3893 [**doi:10.1107/S160053680704127X**]

Dicyclohexyl(hydroxy)acetonitrile

R. Betz and P. Klüfers

Comment

The title compound, $C_{14}H_{23}NO$, the cyanohydrin of dicyclohexyl ketone, was prepared as intermediate in the synthesis of α-hydroxy-dicyclohexyl- acetic acid. It was obtained as the product of the acid catalyzed addition of potassium cyanide to dicyclohexylketone.

The cyclohexyl rings adopt chair conformations. The central C atom is in a slightly distorted tetrahedral environment of three C atoms and one O atom. Intramolecular hydrogen bonds are present in the crystal structure.

The molecular structure (Fig. 1) shows two cyclohexane rings, a cyano- and a hydroxy-group attached to one central C atom. The central C atom connects to both rings as equatorial substituent. It is in a slightly distorted tetrahedral environment comprised of C11, C21, C2 and O1.

The molecular packing (Fig. 2) shows intermolecular hydrogen bonds between the O bonded H atom and the N atom of the next molecule.

Experimental

The title compound was prepared according to standard procedures (Becker *et al.*, 2001) by reaction of dicyclohexylketone and potassium cyanide in acidified water. Recrystallization of the product was performed from chloroform at room temperature upon free evaporation of the solvent.

Refinement

All H atoms were located in a difference map and refined as riding on their parent atoms. One common isotropic displacement parameter for all H atoms was refined to U_{iso}(H) = 0.0420 (17).

Figures

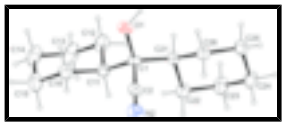


Fig. 1. The molecular structure of (I), with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

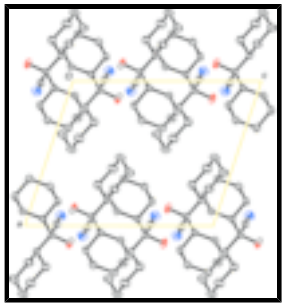


Fig. 2. The packing of (I), viewed along [0 1 0]. H atoms omitted for clarity except the O bonded H atom.

Dicyclohexyl(hydroxy)acetonitrile

Crystal data

$C_{14}H_{23}NO$	F_{000} = 488
M_r = 221.34	D_x = 1.128 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5000 reflections
a = 10.1300 (11) Å	θ = 2.2–27.9º
b = 10.8140 (8) Å	μ = 0.07 mm^{-1}
c = 12.5540 (13) Å	T = 200 (2) K
β = 108.548 (12)º	Block, colourless
V = 1303.8 (2) Å^3	0.43 × 0.32 × 0.26 mm
Z = 4	

Data collection

Stoe IPDS diffractometer	3117 independent reflections
Radiation source: fine-focus sealed tube	2073 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048
T = 200(2) K	θ_{max} = 28.0º
area detection scans	θ_{min} = 2.5º
Absorption correction: numerical (XRED; Stoe & Cie, 1997)	h = −13→13
T_{min} = 0.979, T_{max} = 0.985	k = −13→14
10944 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H-atom parameters constrained
$wR(F^2)$ = 0.100	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.92	$(\Delta/\sigma)_{max} < 0.001$

3117 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
147 parameters	$\Delta\rho_{min} = -0.16$ 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}
O1	0.12139 (9)	0.76034 (8)	0.27055 (6)	0.0276 (2)
H1	0.1015	0.6855	0.2747	0.0367 (8)*
N2	−0.06931 (12)	1.00845 (10)	0.17481 (10)	0.0342 (3)
C1	0.06155 (12)	0.80206 (10)	0.15801 (9)	0.0192 (2)
C2	−0.01281 (13)	0.91914 (11)	0.16750 (10)	0.0228 (3)
C11	0.17886 (12)	0.83620 (11)	0.10885 (9)	0.0220 (3)
H11	0.1347	0.8776	0.0348	0.0367 (8)*
C12	0.25527 (13)	0.72163 (13)	0.08798 (11)	0.0311 (3)
H121	0.2969	0.6770	0.1597	0.0367 (8)*
H122	0.1881	0.6655	0.0355	0.0367 (8)*
C13	0.36959 (14)	0.75672 (16)	0.03856 (12)	0.0405 (4)
H131	0.4206	0.6813	0.0300	0.0367 (8)*
H132	0.3267	0.7931	−0.0370	0.0367 (8)*
C14	0.47133 (14)	0.84872 (16)	0.11226 (13)	0.0423 (4)
H141	0.5226	0.8091	0.1847	0.0367 (8)*
H142	0.5399	0.8736	0.0750	0.0367 (8)*
C15	0.39607 (14)	0.96243 (15)	0.13399 (13)	0.0390 (3)
H151	0.3539	1.0074	0.0625	0.0367 (8)*
H152	0.4638	1.0183	0.1863	0.0367 (8)*
C16	0.28235 (13)	0.92723 (13)	0.18439 (11)	0.0288 (3)
H161	0.3256	0.8894	0.2592	0.0367 (8)*
H162	0.2323	1.0027	0.1945	0.0367 (8)*
C21	−0.04689 (11)	0.70938 (11)	0.08676 (9)	0.0188 (2)
H21	0.0009	0.6275	0.0927	0.0367 (8)*
C22	−0.10254 (12)	0.74228 (12)	−0.03845 (9)	0.0255 (3)
H221	−0.1505	0.8233	−0.0478	0.0367 (8)*
H222	−0.0238	0.7495	−0.0687	0.0367 (8)*
C23	−0.20376 (13)	0.64389 (14)	−0.10405 (10)	0.0317 (3)

H231	−0.2413	0.6693	−0.1838	0.0367 (8)*
H232	−0.1531	0.5650	−0.1009	0.0367 (8)*
C24	−0.32405 (13)	0.62365 (14)	−0.05789 (10)	0.0318 (3)
H241	−0.3834	0.5552	−0.0992	0.0367 (8)*
H242	−0.3818	0.6994	−0.0693	0.0367 (8)*
C25	−0.26967 (13)	0.59256 (13)	0.06700 (10)	0.0269 (3)
H251	−0.3489	0.5856	0.0967	0.0367 (8)*
H252	−0.2213	0.5118	0.0775	0.0367 (8)*
C26	−0.16947 (12)	0.69184 (11)	0.13214 (9)	0.0221 (3)
H261	−0.1335	0.6682	0.2124	0.0367 (8)*
H262	−0.2201	0.7711	0.1267	0.0367 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0398 (5)	0.0232 (5)	0.0157 (4)	−0.0047 (4)	0.0030 (3)	0.0033 (3)
N2	0.0388 (6)	0.0244 (6)	0.0417 (7)	0.0030 (5)	0.0158 (5)	−0.0062 (5)
C1	0.0251 (6)	0.0181 (6)	0.0146 (5)	0.0030 (5)	0.0066 (4)	0.0012 (4)
C2	0.0277 (6)	0.0222 (7)	0.0213 (6)	−0.0028 (5)	0.0114 (5)	−0.0019 (5)
C11	0.0218 (6)	0.0257 (6)	0.0188 (5)	0.0016 (5)	0.0070 (4)	0.0008 (5)
C12	0.0247 (6)	0.0341 (8)	0.0355 (7)	0.0033 (6)	0.0111 (5)	−0.0092 (6)
C13	0.0247 (6)	0.0595 (10)	0.0403 (8)	0.0043 (7)	0.0144 (6)	−0.0111 (7)
C14	0.0224 (7)	0.0643 (11)	0.0411 (8)	−0.0023 (7)	0.0115 (6)	−0.0025 (7)
C15	0.0310 (7)	0.0469 (9)	0.0408 (8)	−0.0108 (7)	0.0137 (6)	−0.0018 (7)
C16	0.0297 (6)	0.0296 (7)	0.0277 (6)	−0.0042 (5)	0.0100 (5)	−0.0024 (5)
C21	0.0218 (5)	0.0189 (6)	0.0169 (5)	0.0025 (5)	0.0080 (4)	−0.0005 (4)
C22	0.0257 (6)	0.0352 (7)	0.0171 (5)	−0.0005 (6)	0.0088 (5)	0.0017 (5)
C23	0.0306 (7)	0.0466 (9)	0.0179 (6)	−0.0052 (6)	0.0078 (5)	−0.0041 (6)
C24	0.0266 (6)	0.0439 (8)	0.0237 (6)	−0.0067 (6)	0.0064 (5)	−0.0020 (6)
C25	0.0260 (6)	0.0317 (7)	0.0246 (6)	−0.0030 (5)	0.0103 (5)	−0.0003 (5)
C26	0.0258 (6)	0.0244 (6)	0.0184 (5)	0.0026 (5)	0.0104 (5)	0.0011 (5)

Geometric parameters (Å, °)

O1—C1	1.4220 (13)	C15—H152	0.9900
O1—H1	0.8400	C16—H161	0.9900
N2—C2	1.1412 (16)	C16—H162	0.9900
C1—C2	1.4972 (16)	C21—C22	1.5335 (15)
C1—C21	1.5447 (16)	C21—C26	1.5338 (15)
C1—C11	1.5479 (16)	C21—H21	1.0000
C11—C12	1.5271 (17)	C22—C23	1.5245 (18)
C11—C16	1.5281 (17)	C22—H221	0.9900
C11—H11	1.0000	C22—H222	0.9900
C12—C13	1.5255 (18)	C23—C24	1.5223 (17)
C12—H121	0.9900	C23—H231	0.9900
C12—H122	0.9900	C23—H232	0.9900
C13—C14	1.517 (2)	C24—C25	1.5249 (17)
C13—H131	0.9900	C24—H241	0.9900
C13—H132	0.9900	C24—H242	0.9900

C14—C15	1.517 (2)	C25—C26	1.5242 (17)
C14—H141	0.9900	C25—H251	0.9900
C14—H142	0.9900	C25—H252	0.9900
C15—C16	1.5284 (18)	C26—H261	0.9900
C15—H151	0.9900	C26—H262	0.9900
C1—O1—H1	109.5	C15—C16—H161	109.4
O1—C1—C2	104.81 (9)	C11—C16—H162	109.4
O1—C1—C21	111.68 (9)	C15—C16—H162	109.4
C2—C1—C21	108.16 (9)	H161—C16—H162	108.0
O1—C1—C11	109.46 (9)	C22—C21—C26	109.41 (9)
C2—C1—C11	107.43 (9)	C22—C21—C1	113.88 (9)
C21—C1—C11	114.75 (9)	C26—C21—C1	112.07 (9)
N2—C2—C1	179.90 (18)	C22—C21—H21	107.0
C12—C11—C16	110.12 (10)	C26—C21—H21	107.0
C12—C11—C1	111.73 (10)	C1—C21—H21	107.0
C16—C11—C1	111.62 (9)	C23—C22—C21	110.89 (10)
C12—C11—H11	107.7	C23—C22—H221	109.5
C16—C11—H11	107.7	C21—C22—H221	109.5
C1—C11—H11	107.7	C23—C22—H222	109.5
C13—C12—C11	111.09 (12)	C21—C22—H222	109.5
C13—C12—H121	109.4	H221—C22—H222	108.1
C11—C12—H121	109.4	C24—C23—C22	112.15 (10)
C13—C12—H122	109.4	C24—C23—H231	109.2
C11—C12—H122	109.4	C22—C23—H231	109.2
H121—C12—H122	108.0	C24—C23—H232	109.2
C14—C13—C12	111.80 (11)	C22—C23—H232	109.2
C14—C13—H131	109.3	H231—C23—H232	107.9
C12—C13—H131	109.3	C23—C24—C25	110.61 (10)
C14—C13—H132	109.3	C23—C24—H241	109.5
C12—C13—H132	109.3	C25—C24—H241	109.5
H131—C13—H132	107.9	C23—C24—H242	109.5
C15—C14—C13	111.01 (11)	C25—C24—H242	109.5
C15—C14—H141	109.4	H241—C24—H242	108.1
C13—C14—H141	109.4	C26—C25—C24	110.94 (10)
C15—C14—H142	109.4	C26—C25—H251	109.5
C13—C14—H142	109.4	C24—C25—H251	109.5
H141—C14—H142	108.0	C26—C25—H252	109.5
C14—C15—C16	111.15 (12)	C24—C25—H252	109.5
C14—C15—H151	109.4	H251—C25—H252	108.0
C16—C15—H151	109.4	C25—C26—C21	111.56 (9)
C14—C15—H152	109.4	C25—C26—H261	109.3
C16—C15—H152	109.4	C21—C26—H261	109.3
H151—C15—H152	108.0	C25—C26—H262	109.3
C11—C16—C15	111.24 (10)	C21—C26—H262	109.3
C11—C16—H161	109.4	H261—C26—H262	108.0
O1—C1—C11—C12	70.70 (12)	O1—C1—C21—C22	−173.36 (9)
C2—C1—C11—C12	−176.04 (10)	C2—C1—C21—C22	71.82 (12)
C21—C1—C11—C12	−55.75 (13)	C11—C1—C21—C22	−48.06 (13)

O1—C1—C11—C16	−53.09 (13)	O1—C1—C21—C26	61.77 (12)
C2—C1—C11—C16	60.17 (12)	C2—C1—C21—C26	−53.05 (12)
C21—C1—C11—C16	−179.54 (10)	C11—C1—C21—C26	−172.93 (9)
C16—C11—C12—C13	−55.89 (14)	C26—C21—C22—C23	−56.29 (13)
C1—C11—C12—C13	179.48 (10)	C1—C21—C22—C23	177.43 (10)
C11—C12—C13—C14	55.78 (16)	C21—C22—C23—C24	56.30 (14)
C12—C13—C14—C15	−55.19 (17)	C22—C23—C24—C25	−55.17 (16)
C13—C14—C15—C16	55.32 (16)	C23—C24—C25—C26	55.12 (15)
C12—C11—C16—C15	56.47 (14)	C24—C25—C26—C21	−57.23 (13)
C1—C11—C16—C15	−178.83 (11)	C22—C21—C26—C25	57.32 (13)
C14—C15—C16—C11	−56.51 (15)	C1—C21—C26—C25	−175.37 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.84	2.07	2.8982 (14)	167

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

Fig. 1

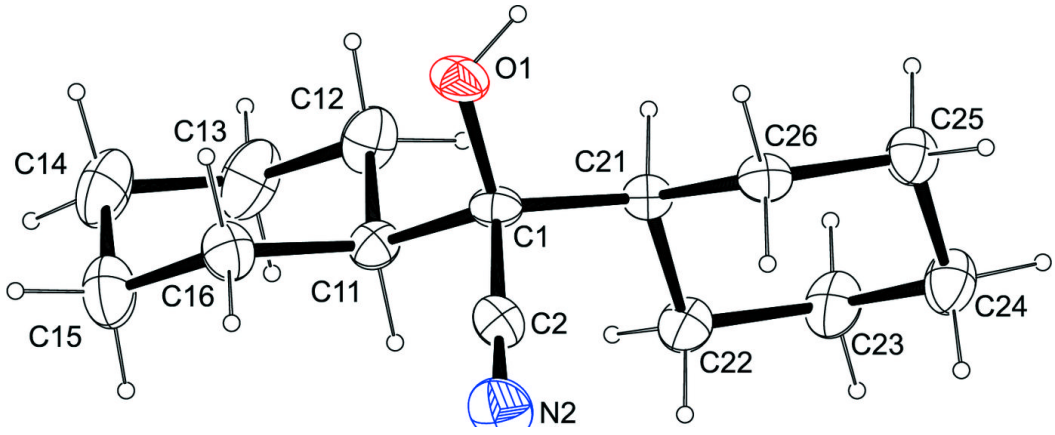


Fig. 2