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N-Phenylcyclohexanecarboxamide

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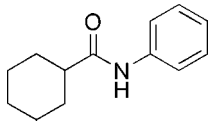
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.080; data-to-parameter ratio = 10.1.

In the title compound, $C_{13}H_{17}NO$, the cyclohexane ring adopts a chair conformation and the amide C(=O)—N moiety is almost coplanar with the phenyl ring [C—N—C—O = 4.1 (2)°]. In the crystal, molecules are linked to form a $C(4)$ infinite [001] chain *via* N—H···O hydrogen bonds, unlike the cyclic motif seen in related structures.

Related literature

For hydrogen-bonding motifs in amides, see: Taylor *et al.* (1984); Leiserowitz & Schmidt (1969). For related structures, see: Lemmerer & Michael (2008).



Experimental

Crystal data

$C_{13}H_{17}NO$
M_r = 203.28
Orthorhombic, $Pca2_1$
a = 9.943 (2) Å
b = 11.839 (2) Å
c = 9.6514 (19) Å
V = 1136.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 K
0.24 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.982, T_{max} = 0.993
8926 measured reflections
1431 independent reflections
1308 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
S = 1.09
1431 reflections
141 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.85 (3)	1.98 (3)	2.8145 (19)	171.7 (18)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5665).

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Taylor, R., Kennard, O. & Versichel, W. (1984). *Acta Cryst.* B**40**, 280–288.

supporting information

Acta Cryst. (2010). E**66**, o2763 [https://doi.org/10.1107/S1600536810039267]

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S1. Comment

The amides are an important H-bonding supramolecular synthon (Taylor *et al.*, 1984; Leiserowitz & Schmidt, 1969), and we herein report the crystal structure of the title compound (I).

In the crystal structure of the title compound, Fig. 1, the cyclohexane group adopts a chair conformation [torsion angles: C1/C2/C3/C4 54.67 (19)°, C2/C3/C4/C5 - 55.3 (2)°]. The amide C(=O)—N moiety is almost coplanar with the phenyl ring [torsion angles: C8/N1/C7/O1 4.1 (2)°, C8/N1/C7/C6 - 175.38 (13)°]. Molecules are linked to form an infinite chain down the *c* axis *via* N—H···O hydrogen bonds (Fig. 2 and Table 1), being different from the reported secondary graph set $R_6^4(16)$ in 1-phenylcylcopentane- carboxamide and 1-(2-bromphenyl)cyclopentanecarboxamide (Lemmerer & Michael, 2008).

S2. Experimental

The title compound was prepared from cyclohexoyl chloride and aniline. Colourless blocks of (I) were grown out *via* recrystallization from ethanol.

S3. Refinement

Anomalous dispersion was negligible and Friedel pairs were merged before refinement. The amide H atom was located in a difference Fourier map and refined freely. The other H atoms were positioned geometrically and allowed to ride on their parent atoms [C—H = 1.00 (aliphic CH), 0.95(aromatic CH) or 0.99Å (CH_2), and U_{iso}(H) = 1.2 U_{eq}(C)]

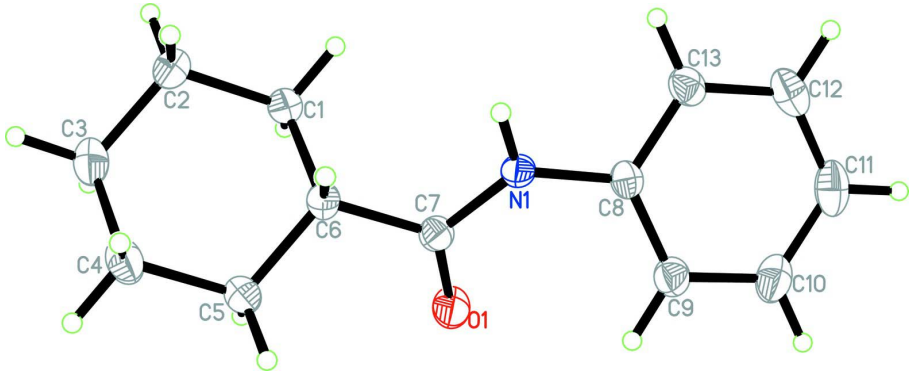

Figure 1

The molecule of (I) showing displacement ellipsoids drawn at the 50% probability level.

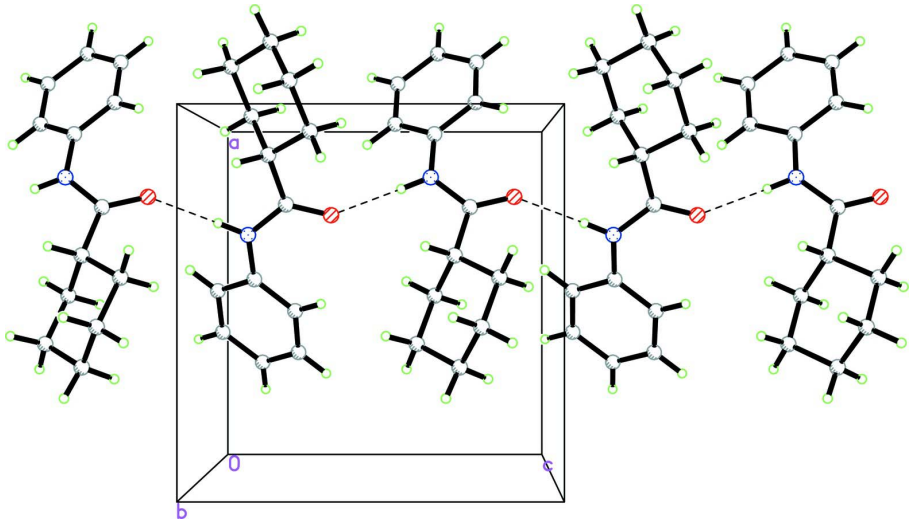

Figure 2

The infinite chain formed *via* N—H···O down the *c* axis.

N-Phenylcyclohexanecarboxamide

Crystal data

$C_{13}H_{17}NO$
$M_r = 203.28$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 9.943$ (2) Å
$b = 11.839$ (2) Å
$c = 9.6514$ (19) Å
$V = 1136.1$ (4) Å^3
$Z = 4$
$F(000) = 440$
$D_x = 1.188$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3664 reflections
$\theta = 2.9$–$27.8°$
$\mu = 0.08$ mm^{-1}
$T = 113$ K
Block, colorless
0.24 × 0.18 × 0.10 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.982$, $T_{max} = 0.993$
8926 measured reflections
1431 independent reflections
1308 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.4°$
$h = -13 \rightarrow 11$
$k = -15 \rightarrow 13$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.080$
$S = 1.09$
1431 reflections
141 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 0.0154P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}

$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^{2}\lambda^{3}$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.174 (16)

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 $F^2 > \sigma(F^2)$ 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	0.22562 (12)	0.24856 (10)	0.38081 (13)	0.0311 (3)
N1	0.17317 (13)	0.25866 (10)	0.15287 (15)	0.0201 (3)
C1	0.48835 (17)	0.24779 (12)	0.16381 (19)	0.0254 (4)
H1A	0.4512	0.2918	0.0854	0.031*
H1B	0.5133	0.3014	0.2382	0.031*
C2	0.61342 (18)	0.18387 (14)	0.11590 (18)	0.0282 (4)
H2A	0.5904	0.1367	0.0346	0.034*
H2B	0.6832	0.2387	0.0871	0.034*
C3	0.66924 (17)	0.10871 (15)	0.2307 (2)	0.0344 (4)
H3A	0.7032	0.1566	0.3071	0.041*
H3B	0.7457	0.0642	0.1941	0.041*
C4	0.56207 (18)	0.02845 (14)	0.2867 (2)	0.0334 (4)
H4A	0.5996	−0.0153	0.3651	0.040*
H4B	0.5356	−0.0255	0.2133	0.040*
C5	0.43777 (16)	0.09411 (13)	0.33568 (18)	0.0259 (4)
H5A	0.3681	0.0404	0.3679	0.031*
H5B	0.4625	0.1434	0.4146	0.031*
C6	0.38120 (15)	0.16622 (12)	0.21778 (17)	0.0218 (3)
H6	0.3575	0.1140	0.1401	0.026*
C7	0.25333 (16)	0.22777 (12)	0.25968 (16)	0.0207 (3)
C8	0.05357 (14)	0.32340 (12)	0.16232 (17)	0.0193 (3)
C9	−0.03152 (16)	0.31722 (13)	0.27635 (18)	0.0253 (4)
H9	−0.0110	0.2681	0.3513	0.030*
C10	−0.14675 (18)	0.38349 (15)	0.2797 (2)	0.0325 (4)
H10	−0.2045	0.3798	0.3580	0.039*
C11	−0.17880 (18)	0.45468 (14)	0.1711 (2)	0.0340 (4)
H11	−0.2574	0.5002	0.1750	0.041*
C12	−0.09518 (18)	0.45894 (13)	0.0565 (2)	0.0300 (4)
H12	−0.1174	0.5067	−0.0193	0.036*
C13	0.02102 (16)	0.39388 (13)	0.05141 (18)	0.0240 (3)
H13	0.0782	0.3974	−0.0274	0.029*
H1	0.204 (2)	0.2485 (15)	0.072 (3)	0.035 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0268 (6)	0.0522 (7)	0.0143 (6)	0.0088 (5)	−0.0021 (5)	−0.0028 (5)
N1	0.0190 (7)	0.0273 (6)	0.0138 (6)	0.0021 (5)	0.0007 (5)	−0.0007 (5)
C1	0.0241 (8)	0.0280 (8)	0.0241 (8)	0.0058 (6)	0.0028 (7)	0.0048 (7)
C2	0.0238 (9)	0.0310 (8)	0.0299 (9)	0.0038 (6)	0.0055 (7)	0.0028 (7)
C3	0.0240 (9)	0.0374 (9)	0.0418 (11)	0.0083 (7)	0.0003 (8)	0.0062 (8)
C4	0.0290 (9)	0.0291 (8)	0.0420 (10)	0.0068 (7)	−0.0009 (8)	0.0094 (8)
C5	0.0234 (8)	0.0268 (7)	0.0275 (8)	0.0017 (6)	−0.0010 (7)	0.0065 (7)
C6	0.0189 (7)	0.0242 (7)	0.0222 (7)	0.0028 (6)	−0.0003 (6)	0.0005 (6)
C7	0.0194 (7)	0.0238 (7)	0.0188 (7)	−0.0006 (6)	−0.0015 (6)	−0.0007 (6)
C8	0.0184 (7)	0.0198 (6)	0.0196 (7)	−0.0009 (5)	−0.0043 (6)	−0.0032 (6)
C9	0.0230 (8)	0.0303 (8)	0.0226 (8)	0.0025 (6)	−0.0014 (6)	−0.0008 (7)
C10	0.0226 (8)	0.0405 (9)	0.0345 (9)	0.0044 (7)	0.0008 (7)	−0.0063 (8)
C11	0.0249 (9)	0.0279 (8)	0.0493 (11)	0.0073 (6)	−0.0079 (8)	−0.0078 (8)
C12	0.0317 (10)	0.0219 (8)	0.0366 (9)	−0.0007 (6)	−0.0142 (8)	0.0017 (7)
C13	0.0232 (8)	0.0252 (7)	0.0236 (8)	−0.0040 (6)	−0.0063 (7)	0.0014 (7)

Geometric parameters (Å, º)

O1—C7	1.226 (2)	C5—C6	1.530 (2)
N1—C7	1.353 (2)	C5—H5A	0.9900
N1—C8	1.4176 (19)	C5—H5B	0.9900
N1—H1	0.85 (3)	C6—C7	1.520 (2)
C1—C2	1.527 (2)	C6—H6	1.0000
C1—C6	1.529 (2)	C8—C9	1.390 (2)
C1—H1A	0.9900	C8—C13	1.395 (2)
C1—H1B	0.9900	C9—C10	1.389 (2)
C2—C3	1.526 (2)	C9—H9	0.9500
C2—H2A	0.9900	C10—C11	1.383 (3)
C2—H2B	0.9900	C10—H10	0.9500
C3—C4	1.527 (3)	C11—C12	1.385 (3)
C3—H3A	0.9900	C11—H11	0.9500
C3—H3B	0.9900	C12—C13	1.390 (2)
C4—C5	1.535 (2)	C12—H12	0.9500
C4—H4A	0.9900	C13—H13	0.9500
C4—H4B	0.9900		
C7—N1—C8	126.23 (15)	C6—C5—H5B	109.6
C7—N1—H1	116.4 (15)	C4—C5—H5B	109.6
C8—N1—H1	116.4 (14)	H5A—C5—H5B	108.1
C2—C1—C6	110.94 (12)	C7—C6—C1	111.75 (12)
C2—C1—H1A	109.5	C7—C6—C5	112.16 (13)
C6—C1—H1A	109.5	C1—C6—C5	110.46 (13)
C2—C1—H1B	109.5	C7—C6—H6	107.4
C6—C1—H1B	109.5	C1—C6—H6	107.4
H1A—C1—H1B	108.0	C5—C6—H6	107.4

C3—C2—C1	111.43 (14)	O1—C7—N1	122.67 (15)
C3—C2—H2A	109.3	O1—C7—C6	122.53 (14)
C1—C2—H2A	109.3	N1—C7—C6	114.80 (14)
C3—C2—H2B	109.3	C9—C8—C13	119.85 (14)
C1—C2—H2B	109.3	C9—C8—N1	122.21 (14)
H2A—C2—H2B	108.0	C13—C8—N1	117.94 (14)
C2—C3—C4	111.49 (14)	C10—C9—C8	119.40 (15)
C2—C3—H3A	109.3	C10—C9—H9	120.3
C4—C3—H3A	109.3	C8—C9—H9	120.3
C2—C3—H3B	109.3	C11—C10—C9	121.10 (18)
C4—C3—H3B	109.3	C11—C10—H10	119.4
H3A—C3—H3B	108.0	C9—C10—H10	119.4
C3—C4—C5	110.85 (13)	C10—C11—C12	119.33 (16)
C3—C4—H4A	109.5	C10—C11—H11	120.3
C5—C4—H4A	109.5	C12—C11—H11	120.3
C3—C4—H4B	109.5	C11—C12—C13	120.47 (17)
C5—C4—H4B	109.5	C11—C12—H12	119.8
H4A—C4—H4B	108.1	C13—C12—H12	119.8
C6—C5—C4	110.48 (14)	C12—C13—C8	119.83 (16)
C6—C5—H5A	109.6	C12—C13—H13	120.1
C4—C5—H5A	109.6	C8—C13—H13	120.1

C6—C1—C2—C3	−55.5 (2)	C1—C6—C7—N1	78.01 (17)
C1—C2—C3—C4	54.7 (2)	C5—C6—C7—N1	−157.32 (13)
C2—C3—C4—C5	−55.3 (2)	C7—N1—C8—C9	−32.8 (2)
C3—C4—C5—C6	56.9 (2)	C7—N1—C8—C13	148.20 (15)
C2—C1—C6—C7	−177.32 (14)	C13—C8—C9—C10	−1.4 (2)
C2—C1—C6—C5	57.07 (19)	N1—C8—C9—C10	179.54 (15)
C4—C5—C6—C7	176.87 (13)	C8—C9—C10—C11	0.6 (2)
C4—C5—C6—C1	−57.75 (17)	C9—C10—C11—C12	0.7 (3)
C8—N1—C7—O1	4.1 (2)	C10—C11—C12—C13	−1.1 (2)
C8—N1—C7—C6	−175.38 (13)	C11—C12—C13—C8	0.2 (2)
C1—C6—C7—O1	−101.43 (19)	C9—C8—C13—C12	1.0 (2)
C5—C6—C7—O1	23.2 (2)	N1—C8—C13—C12	−179.90 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.85 (3)	1.98 (3)	2.8145 (19)	171.7 (18)

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