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N-Cyclohexyl-2-oxo-2-phenylacetamide

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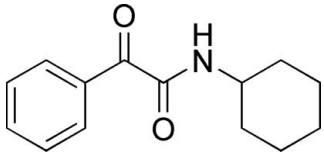
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.082; data-to-parameter ratio = 11.3.

In the title compound, $C_{14}H_{17}NO_2$, the two carbonyl groups are oriented with respect to each other with a torsion angle of −129.9 (3)°. The cyclohexane ring adopts a chair conformation. In the crystal, molecules are linked by N—H···O hydrogen bonds into a chain running along the *a* axis.

Related literature

For related *N*-substituted 2-oxo-2-phenylacetamides, see: Boryczka *et al.* (1998); Dai & Wu (2011).



Experimental

Crystal data

$C_{14}H_{17}NO_2$
M_r = 231.29
Orthorhombic, $P2_12_12_1$
a = 9.6942 (4) Å
b = 10.4394 (6) Å
c = 13.2100 (8) Å
V = 1336.87 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 153 K
0.25 × 0.16 × 0.12 mm

Data collection

Bruker SMART 1000 CCD diffractometer
5120 measured reflections
1737 independent reflections
845 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.082
S = 1.00
1737 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.08 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 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}	0.88	2.02	2.863 (2)	159

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* ; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank Mr J. Gu for valuable suggestions and Mr J. Liu for assistance with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5541).

References

Boryczka, S., Suwinska, K., Le Guillanton, G., Do, Q. T. & Elothmani, D. (1998). *J. Chem. Crystallogr.* **28**, 555–560.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2012). E**68**, o1948 [doi:10.1107/S1600536812023549]

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Comment

Several crystals of N-substituted phenylglyoxamide have been reported, and their great differences of the cystal form due to the N—H···O hydrogen bond linking form have been observed (Boryczka *et al.*, 1998; Dai & Wu, 2011). In our research for exploring the effect rule of the N-substituted group of phenylglyoxamide to the crystal form, we have synthesized the title compound by condensation of phenylglyoxic acid with cyclohexylamine. The structure of the title compound has been characterized by spectroscopic methods and further confirmation by X-ray analysis. We report here its crystal structure. The two carbonyl groups of the molecule are oriented to each other with a torsion angle of -129.9 (3)°. Molecules are linked by intermolecular hydrogen bonds N—H···O into a one-dimensional chain (Fig. 2).

Experimental

Into a suspension of phenylglyoxylic acid (400 mg, 2.67 mmol) and cyclohexylamine (0.272 ml, 2.38 mmol) in methylene chloride (10 ml), *N*,*N*′-dicyclohexylcarbodiimide (DCC) (540 mg, 2.62 mmol) and 4-(dimethylamino)pyridine (DMAP) (66 mg, 0.54 mmol) was added respectively at room temperature and continuted stirring for 10 h. The reaction mixture was filtered and the filtrate was concentrated under reduced pressure, the residue was purified by colum chromatography (silica gel, 30% of ethyl acetate in hexane) to afford the title compound in 69% yield (379 mg) as a white solid, m.p. 384–385 K. Single crystals suitable for X-ray diffraction of the title compound were grown in a mixture of ethyl acetate and hexane.

Refinement

The H atoms were placed in calculated positions with C—H = 0.93–0.98 Å, N—H = 0.88 Å and included in the refinement as riding their carrier atoms with U_{iso}(H) = 1.2U_{eq}(C,N).

Computing details

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

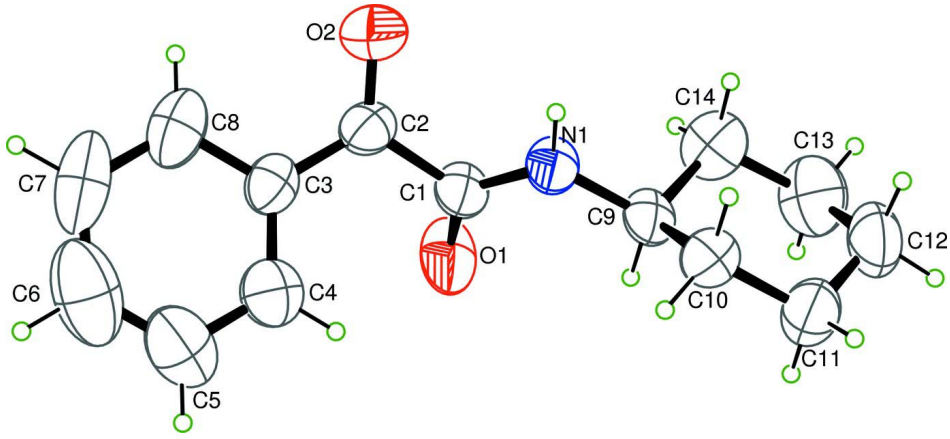

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 40% probability level. H atoms are presented as small spheres of arbitrary radius.

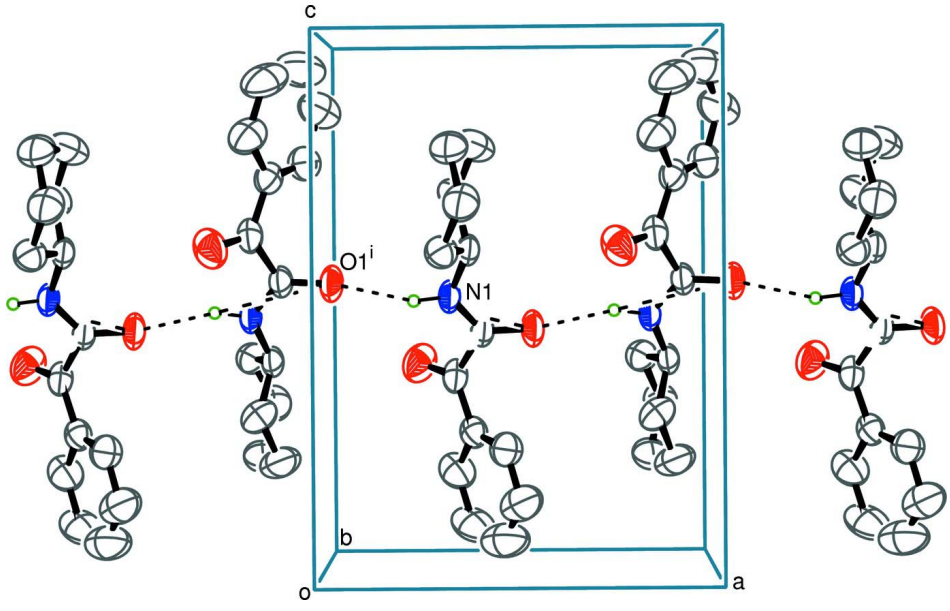

Figure 2

One-dimensional chain molecules of the title compound linked by two adjacent moleculars N—H···O hydrogen bonds (dotted lines). Symmetry code: (i) -0.5 + *x*, 0.5 - *y*, 1 - *z*.

N-Cyclohexyl-2-oxo-2-phenylacetamide

Crystal data

$C_{14}H_{17}NO_2$
$M_r = 231.29$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 9.6942\ (4)$ Å
$b = 10.4394\ (6)$ Å
$c = 13.2100\ (8)$ Å
$V = 1336.87\ (12)$ Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.149$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6354 reflections
$\theta = 3.2–27.5°$
$\mu = 0.08$ mm^{-1}
$T = 153$ K
Block, colourless
0.25 × 0.16 × 0.12 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
5120 measured reflections
1737 independent reflections
845 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -10 \rightarrow 12$
$k = -9 \rightarrow 13$
$l = -10 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.082$
$S = 1.00$
1737 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.08$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4098 (2)	0.2794 (2)	0.45295 (19)	0.0663 (6)
C2	0.3397 (2)	0.3534 (2)	0.3683 (2)	0.0684 (7)
C3	0.3856 (2)	0.3354 (2)	0.2645 (2)	0.0667 (6)
C4	0.4675 (3)	0.2327 (3)	0.2370 (3)	0.0863 (7)
H4	0.4986	0.1749	0.2876	0.104*
C5	0.5046 (4)	0.2127 (4)	0.1389 (4)	0.1220 (11)
H5	0.5598	0.1408	0.1216	0.146*
C6	0.4629 (6)	0.2948 (6)	0.0663 (3)	0.1472 (17)
H6	0.4902	0.2810	−0.0019	0.177*
C7	0.3812 (4)	0.3986 (5)	0.0898 (4)	0.1328 (15)
H7	0.3525	0.4561	0.0382	0.159*
C8	0.3411 (3)	0.4187 (3)	0.1896 (3)	0.0992 (9)
H8	0.2834	0.4891	0.2064	0.119*
C9	0.37782 (19)	0.1451 (2)	0.60266 (19)	0.0663 (6)
H9	0.4801	0.1356	0.5966	0.080*
C10	0.3146 (2)	0.0142 (2)	0.6000 (2)	0.0774 (7)
H10A	0.3387	−0.0284	0.5355	0.093*
H10B	0.2130	0.0217	0.6035	0.093*

C11	0.3656 (3)	−0.0661 (3)	0.6877 (2)	0.0963 (9)
H11A	0.3203	−0.1511	0.6857	0.116*
H11B	0.4663	−0.0794	0.6811	0.116*
C12	0.3357 (3)	−0.0036 (3)	0.7859 (2)	0.1077 (10)
H12A	0.3754	−0.0557	0.8413	0.129*
H12B	0.2346	0.0002	0.7960	0.129*
C13	0.3938 (3)	0.1297 (3)	0.7912 (2)	0.1173 (11)
H13A	0.4958	0.1252	0.7919	0.141*
H13B	0.3635	0.1709	0.8549	0.141*
C14	0.3468 (3)	0.2104 (3)	0.7015 (2)	0.0926 (8)
H14A	0.2463	0.2259	0.7067	0.111*
H14B	0.3941	0.2944	0.7035	0.111*
N1	0.32939 (16)	0.22256 (17)	0.51791 (15)	0.0709 (6)
H1	0.2397	0.2315	0.5102	0.085*
O1	0.53605 (14)	0.27896 (19)	0.45723 (13)	0.1065 (7)
O2	0.24786 (18)	0.42743 (18)	0.39078 (16)	0.1070 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0406 (12)	0.0839 (14)	0.0744 (18)	−0.0046 (11)	0.0022 (12)	0.0129 (15)
C2	0.0468 (12)	0.0696 (14)	0.089 (2)	0.0002 (12)	0.0027 (14)	0.0158 (15)
C3	0.0585 (13)	0.0672 (14)	0.074 (2)	−0.0106 (13)	−0.0036 (14)	0.0135 (15)
C4	0.0808 (16)	0.0898 (18)	0.088 (2)	−0.0109 (17)	0.0028 (17)	0.0012 (17)
C5	0.137 (3)	0.125 (3)	0.104 (3)	−0.020 (2)	0.027 (3)	−0.016 (3)
C6	0.188 (4)	0.167 (4)	0.087 (3)	−0.077 (4)	0.014 (3)	−0.015 (3)
C7	0.158 (3)	0.148 (3)	0.093 (3)	−0.044 (3)	−0.029 (3)	0.054 (3)
C8	0.107 (2)	0.0941 (18)	0.097 (3)	−0.0214 (17)	−0.015 (2)	0.030 (2)
C9	0.0369 (10)	0.0915 (15)	0.0706 (18)	−0.0062 (11)	0.0024 (12)	0.0167 (16)
C10	0.0801 (15)	0.0763 (16)	0.0757 (19)	0.0060 (14)	−0.0005 (16)	0.0040 (15)
C11	0.0945 (19)	0.0939 (17)	0.101 (3)	0.0056 (16)	0.0059 (19)	0.0259 (19)
C12	0.102 (2)	0.144 (3)	0.077 (3)	0.005 (2)	0.005 (2)	0.037 (2)
C13	0.131 (2)	0.145 (3)	0.076 (2)	−0.012 (2)	−0.026 (2)	−0.007 (2)
C14	0.0999 (19)	0.0907 (17)	0.087 (2)	−0.0083 (17)	−0.0252 (18)	−0.0073 (18)
N1	0.0344 (8)	0.0975 (13)	0.0809 (15)	−0.0005 (9)	0.0012 (9)	0.0273 (12)
O1	0.0367 (8)	0.1821 (17)	0.1007 (15)	−0.0129 (10)	−0.0007 (9)	0.0534 (14)
O2	0.0890 (12)	0.1142 (14)	0.1178 (17)	0.0351 (12)	0.0181 (13)	0.0217 (14)

Geometric parameters (Å, º)

C1—O1	1.226 (2)	C9—C14	1.504 (3)
C1—N1	1.302 (2)	C9—H9	1.0000
C1—C2	1.519 (3)	C10—C11	1.512 (3)
C2—O2	1.216 (3)	C10—H10A	0.9900
C2—C3	1.454 (3)	C10—H10B	0.9900
C3—C4	1.383 (3)	C11—C12	1.481 (4)
C3—C8	1.386 (3)	C11—H11A	0.9900
C4—C5	1.360 (4)	C11—H11B	0.9900
C4—H4	0.9500	C12—C13	1.502 (4)
C5—C6	1.348 (5)	C12—H12A	0.9900

C5—H5	0.9500	C12—H12B	0.9900
C6—C7	1.378 (5)	C13—C14	1.524 (3)
C6—H6	0.9500	C13—H13A	0.9900
C7—C8	1.390 (5)	C13—H13B	0.9900
C7—H7	0.9500	C14—H14A	0.9900
C8—H8	0.9500	C14—H14B	0.9900
C9—N1	1.459 (3)	N1—H1	0.8800
C9—C10	1.498 (3)		

O1—C1—N1	124.4 (2)	C11—C10—H10A	109.5
O1—C1—C2	118.8 (2)	C9—C10—H10B	109.5
N1—C1—C2	116.70 (18)	C11—C10—H10B	109.5
O2—C2—C3	122.5 (2)	H10A—C10—H10B	108.1
O2—C2—C1	118.1 (3)	C12—C11—C10	111.3 (2)
C3—C2—C1	119.5 (2)	C12—C11—H11A	109.4
C4—C3—C8	118.5 (3)	C10—C11—H11A	109.4
C4—C3—C2	121.6 (2)	C12—C11—H11B	109.4
C8—C3—C2	119.8 (3)	C10—C11—H11B	109.4
C5—C4—C3	121.4 (3)	H11A—C11—H11B	108.0
C5—C4—H4	119.3	C11—C12—C13	112.1 (3)
C3—C4—H4	119.3	C11—C12—H12A	109.2
C6—C5—C4	120.1 (4)	C13—C12—H12A	109.2
C6—C5—H5	120.0	C11—C12—H12B	109.2
C4—C5—H5	120.0	C13—C12—H12B	109.2
C5—C6—C7	120.8 (4)	H12A—C12—H12B	107.9
C5—C6—H6	119.6	C12—C13—C14	111.3 (3)
C7—C6—H6	119.6	C12—C13—H13A	109.4
C6—C7—C8	119.5 (4)	C14—C13—H13A	109.4
C6—C7—H7	120.2	C12—C13—H13B	109.4
C8—C7—H7	120.2	C14—C13—H13B	109.4
C3—C8—C7	119.7 (3)	H13A—C13—H13B	108.0
C3—C8—H8	120.2	C9—C14—C13	111.4 (2)
C7—C8—H8	120.2	C9—C14—H14A	109.4
N1—C9—C10	110.88 (19)	C13—C14—H14A	109.4
N1—C9—C14	110.53 (19)	C9—C14—H14B	109.4
C10—C9—C14	110.6 (2)	C13—C14—H14B	109.4
N1—C9—H9	108.2	H14A—C14—H14B	108.0
C10—C9—H9	108.2	C1—N1—C9	124.46 (16)
C14—C9—H9	108.2	C1—N1—H1	117.8
C9—C10—C11	110.8 (2)	C9—N1—H1	117.8
C9—C10—H10A	109.5		

O1—C1—C2—O2	−129.9 (3)	C2—C3—C8—C7	−177.8 (3)
N1—C1—C2—O2	48.6 (3)	C6—C7—C8—C3	1.1 (5)
O1—C1—C2—C3	49.1 (3)	N1—C9—C10—C11	179.74 (19)
N1—C1—C2—C3	−132.4 (2)	C14—C9—C10—C11	−57.3 (3)
O2—C2—C3—C4	−165.7 (2)	C9—C10—C11—C12	57.3 (3)
C1—C2—C3—C4	15.4 (3)	C10—C11—C12—C13	−55.3 (3)
O2—C2—C3—C8	10.9 (3)	C11—C12—C13—C14	53.3 (4)

C1—C2—C3—C8	−168.0 (2)	N1—C9—C14—C13	178.8 (2)
C8—C3—C4—C5	0.0 (4)	C10—C9—C14—C13	55.6 (3)
C2—C3—C4—C5	176.7 (2)	C12—C13—C14—C9	−53.3 (3)
C3—C4—C5—C6	0.9 (5)	O1—C1—N1—C9	−3.0 (4)
C4—C5—C6—C7	−0.9 (6)	C2—C1—N1—C9	178.6 (2)
C5—C6—C7—C8	−0.1 (6)	C10—C9—N1—C1	−125.1 (2)
C4—C3—C8—C7	−1.1 (4)	C14—C9—N1—C1	111.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.02	2.863 (2)	159

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