Isoquinolin-1(2H)-one

Rosica Petrova,[a]* Rositsa Titorenkova[b] and Boris Shivachev[b]

[a]Department of Advanced Materials Science and Engineering, Faculty of Engineering, Yamaguchi University, 2-16-1 Tokiwadai, Ube 755-8611, Japan, and [b]Bulgarian Academy of Sciences, Central Laboratory of Mineralogy and Crystallography, Academician G. Bonchev Street Building 107, 1113 Sofia, Bulgaria

Correspondence e-mail: rosica@yamaguchi-u.ac.jp

The molecule of the title compound, C_9H_7NO, is nearly planar, with an r.m.s. deviation of 0.018 (7) Å. In the crystal structure, two molecules form an $R_2^2(8)$ centrosymmetric dimer through N—H⋯O hydrogen bonds. The three-dimensional packing is additionally stabilized through weak C—H⋯O interactions.

Related literature

For related literature, see: Bernan *et al.* (1994); Bernstein *et al.* (1995); Ferrer *et al.* (2002); Jayaraman *et al.* (2000); Kolev *et al.* (2007); Koleva *et al.* (1998); Parveen *et al.* (1999); Petrova *et al.* (2005); Zhang *et al.* (1997).
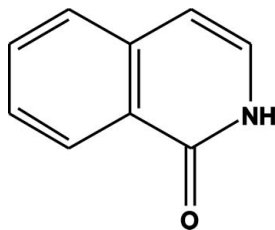
Experimental

Crystal data

C_9H_7NO
$M_r = 145.16$
Monoclinic, $P2_1/n$
$a = 11.6138$ (17) Å
$b = 5.2965$ (9) Å
$c = 12.2946$ (9) Å
$\beta = 111.745$ (9)°

$V = 702.46$ (17) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 290$ (2) K
$0.36 \times 0.36 \times 0.34$ mm

Data collection

Enraf–Nonius CAD4 diffractometer
Absorption correction: none
3292 measured reflections
1678 independent reflections

1053 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
3 standard reflections
 frequency: 120 min
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.123$
$S = 1.01$
1678 reflections

101 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N—H1N⋯O[i]	0.86	1.96	2.818 (2)	172
C8—H8⋯O[ii]	0.93	2.66	3.243 (2)	121
C9—H9⋯O[ii]	0.93	2.65	3.230 (2)	121

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2239).

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supplementary materials

Isoquinolin-1(2*H*)-one

R. Petrova, R. Titorenkova and B. Shivachev

Comment

Isoquinolines are important from both technological and applied points of view as a part of a significant class of compounds with a variety of pharmacological applications in anticancer, retroviral infections, rheumatoid arthritis and diabets treatment (Jayaraman *et al.*, 2000; Zhang *et al.*, 1997; Bernan *et al.*, 1994; Koleva *et al.*, 1998).

As part of our research on isoquinoline derivatives the structures of (3RS,4RS)-3-(2-furyl)-2-phenethyl-4-(pyrrolidin-1-ylcarbonyl)-3,4- dihydroisoquinolin-1(2*H*)-one (Petrova *et al.*, 2005) and 1,2,3,4-tetrahydroisoquinolinium hydrogensquarate (Kolev *et al.*, 2007) were reported. The title compound,(I), was investigated in order to provide relevant information on the changes observed upon substitution.

In the asymmetric unit of (I), only one independent molecule is present (Fig. 1). The fused ring system is nearly planar with an r.m.s. deviation of 0.018 (7) Å. The molecules are coupled through bicyclic N—H1···O^i [symmetry code (i): $-x + 1, -y + 2, -z + 1$] hydrogen bonds and build $R^2_2(8)$ dimers (Fig. 2) (Bernstein *et al.*, 1995). The three-dimensional packing is stabilized through weak C8—H8···O^{ii} and C9—H9···O^{ii} interactions [symmetry code (ii): $1/2 + x, 3/2 - y, 1/2 + z$].

Experimental

Compound (I) was synthesized in a manner similar to the procedure described by Ferrer *et al.* (2002) and Parveen *et al.* (1999). Isocoumarin (996 mg, 6.8 mmol) in 2-methoxyethanol (30 ml) was saturated with ammonia for 3 h, after which the mixture was boiled under reflux for 18 h. Subsequent evaporation and recrystallization from ethylacetate yielded the title compound (815 mg, yield 82%). Crystals suitable for *x*-ray diffraction have been obtained by slow evaporation from hydrazine/water mixture (4:1) at room temperature. IR (KBr pellet, ν, cm^{-1}): The most intensive band in the IR spectrum is located at 1656 cm^{-1} and is characteristic for ν$_{C=O}$ stretching mode. Skeletal stretching of aromatic ring, ν$_{C\cdots C}$, are detected at 1605, 1549, 1475, 1346 and 1230 cm^{-1}. The ν$_{C—H}$ of the phenyl group appears at 551, 669 and 797 cm^{-1}(*m*), and in the 2855–3160 cm^{-1} (w) region. The weak broad band at 3290 cm^{-1} is associated with the N—H group.

Refinement

All H atoms were placed in idealized positions (C—H = 0.93 and N—H = 0.86 Å) and were constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C or N).
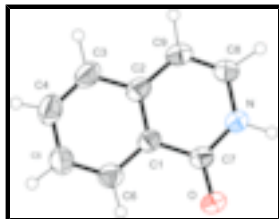
supplementary materials

Figures

Fig. 1. View of the molecule and the atom-numbering scheme of (I), showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.
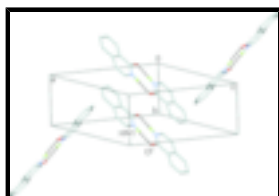

Fig. 2. A view of the molecular packing in (I). All H atoms not involved in hydrogen bonds have been omitted for clarity [symmetry code: (i) $-x$, $1 - y$, $-z$].

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Crystal data

C_9H_7NO	$F_{000} = 304$
$M_r = 145.16$	$D_x = 1.373$ Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: not measured K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.6138$ (17) Å	Cell parameters from 22 reflections
$b = 5.2965$ (9) Å	$\theta = 18.0–19.2°$
$c = 12.2946$ (9) Å	$\mu = 0.09$ mm^{-1}
$\beta = 111.745$ (9)°	$T = 290$ (2) K
$V = 702.46$ (17) Å^3	Prism, pale orange
$Z = 4$	$0.36 \times 0.36 \times 0.34$ mm

Data collection

Enraf–Nonius CAD4 diffractometer	$R_{int} = 0.044$
Radiation source: fine-focus sealed tube	$\theta_{max} = 28.0°$
Monochromator: graphite	$\theta_{min} = 2.1°$
$T = 290(2)$ K	$h = 0\rightarrow15$
$\omega/2\theta$ scans	$k = -6\rightarrow6$
Absorption correction: none	$l = -16\rightarrow15$
3292 measured reflections	3 standard reflections
1678 independent reflections	every 120 min
1053 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o{}^2) + (0.0535P)^2 + 0.0424P]$ where $P = (F_o{}^2 + 2F_c{}^2)/3$
$wR(F^2) = 0.123$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
1678 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
101 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.033 (5)
Secondary atom site location: difference Fourier map	

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	0.67389 (14)	0.5067 (3)	0.44839 (13)	0.0362 (4)
C2	0.79688 (14)	0.4736 (3)	0.52641 (13)	0.0418 (4)
C3	0.86794 (17)	0.2858 (4)	0.50006 (17)	0.0534 (5)
H3	0.9499	0.2615	0.5497	0.064*
C4	0.81862 (18)	0.1389 (4)	0.40290 (17)	0.0581 (5)
H4	0.8675	0.0161	0.3870	0.070*
C5	0.69666 (18)	0.1697 (4)	0.32727 (16)	0.0525 (5)
H5	0.6636	0.0666	0.2617	0.063*
C6	0.62517 (15)	0.3528 (3)	0.34971 (14)	0.0447 (4)
H6	0.5435	0.3747	0.2988	0.054*
C7	0.59723 (14)	0.7040 (3)	0.46979 (13)	0.0380 (4)
C8	0.77064 (15)	0.8060 (3)	0.64655 (14)	0.0457 (4)
H8	0.8011	0.9065	0.7132	0.055*
C9	0.84330 (15)	0.6297 (4)	0.62860 (15)	0.0485 (5)
H9	0.9238	0.6080	0.6821	0.058*
N	0.65169 (12)	0.8423 (3)	0.56868 (11)	0.0428 (4)

| H1N | 0.6088 | 0.9604 | 0.5835 | 0.051* |
| O | 0.48896 (10) | 0.7471 (2) | 0.40287 (10) | 0.0481 (4) |

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0357 (8)	0.0373 (8)	0.0359 (7)	0.0028 (7)	0.0135 (6)	0.0052 (7)
C2	0.0382 (9)	0.0438 (10)	0.0421 (9)	0.0064 (7)	0.0135 (7)	0.0079 (7)
C3	0.0428 (10)	0.0582 (12)	0.0558 (10)	0.0179 (9)	0.0142 (8)	0.0076 (9)
C4	0.0640 (12)	0.0518 (11)	0.0627 (12)	0.0208 (9)	0.0282 (10)	0.0026 (9)
C5	0.0618 (11)	0.0486 (10)	0.0492 (10)	0.0042 (9)	0.0229 (9)	−0.0052 (8)
C6	0.0429 (9)	0.0477 (10)	0.0411 (9)	0.0019 (8)	0.0128 (7)	0.0018 (7)
C7	0.0357 (8)	0.0403 (9)	0.0357 (8)	0.0020 (7)	0.0108 (7)	0.0032 (7)
C8	0.0413 (9)	0.0498 (10)	0.0376 (8)	0.0020 (8)	0.0049 (7)	−0.0031 (7)
C9	0.0356 (9)	0.0563 (11)	0.0449 (9)	0.0069 (8)	0.0048 (7)	0.0035 (8)
N	0.0379 (7)	0.0452 (8)	0.0408 (7)	0.0091 (6)	0.0094 (6)	−0.0024 (6)
O	0.0344 (6)	0.0548 (8)	0.0457 (6)	0.0113 (5)	0.0039 (5)	−0.0026 (5)

Geometric parameters (Å, °)

C1—C6	1.396 (2)	C5—H5	0.9300
C1—C2	1.406 (2)	C6—H6	0.9300
C1—C7	1.458 (2)	C7—O	1.2423 (18)
C2—C3	1.405 (2)	C7—N	1.358 (2)
C2—C9	1.432 (2)	C8—C9	1.331 (2)
C3—C4	1.362 (3)	C8—N	1.3718 (19)
C3—H3	0.9300	C8—H8	0.9300
C4—C5	1.386 (3)	C9—H9	0.9300
C4—H4	0.9300	N—H1N	0.8600
C5—C6	1.370 (2)		
C6—C1—C2	120.15 (15)	C5—C6—C1	120.53 (16)
C6—C1—C7	119.82 (14)	C5—C6—H6	119.7
C2—C1—C7	120.02 (14)	C1—C6—H6	119.7
C3—C2—C1	117.80 (15)	O—C7—N	121.01 (14)
C3—C2—C9	123.28 (15)	O—C7—C1	123.22 (14)
C1—C2—C9	118.92 (15)	N—C7—C1	115.77 (13)
C4—C3—C2	120.99 (17)	C9—C8—N	121.28 (15)
C4—C3—H3	119.5	C9—C8—H8	119.4
C2—C3—H3	119.5	N—C8—H8	119.4
C3—C4—C5	120.97 (17)	C8—C9—C2	119.67 (15)
C3—C4—H4	119.5	C8—C9—H9	120.2
C5—C4—H4	119.5	C2—C9—H9	120.2
C6—C5—C4	119.54 (17)	C7—N—C8	124.31 (14)
C6—C5—H5	120.2	C7—N—H1N	117.8
C4—C5—H5	120.2	C8—N—H1N	117.8
C6—C1—C2—C3	1.2 (2)	C6—C1—C7—O	−1.1 (2)
C7—C1—C2—C3	−178.18 (14)	C2—C1—C7—O	178.23 (15)
C6—C1—C2—C9	−178.33 (16)	C6—C1—C7—N	179.14 (14)

C7—C1—C2—C9	2.3 (2)	C2—C1—C7—N	−1.5 (2)
C1—C2—C3—C4	−0.8 (3)	N—C8—C9—C2	−0.2 (3)
C9—C2—C3—C4	178.67 (18)	C3—C2—C9—C8	179.07 (17)
C2—C3—C4—C5	−0.2 (3)	C1—C2—C9—C8	−1.4 (3)
C3—C4—C5—C6	0.9 (3)	O—C7—N—C8	−179.94 (15)
C4—C5—C6—C1	−0.5 (3)	C1—C7—N—C8	−0.2 (2)
C2—C1—C6—C5	−0.5 (2)	C9—C8—N—C7	1.1 (3)
C7—C1—C6—C5	178.83 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H1N···O^i	0.86	1.96	2.818 (2)	172
C8—H8···O^{ii}	0.93	2.66	3.243 (2)	121
C9—H9···O^{ii}	0.93	2.65	3.230 (2)	121

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

Fig. 1

Fig. 2