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3-Phenyloxazolidin-2-one

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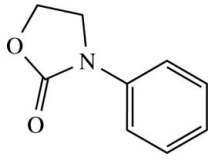
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 13.4.

In the title compound, $C_9H_9NO_2$, amide–π-system conjugation results in an almost coplanar arrangement of the phenyl ring and the almost planar heterocycle. In the crystal structure, π-stacked dimers [perpendicular distance 3.563 (2) Å] interact with neighbouring dimers *via* C—H$\cdots\pi$ interactions.

Related literature

For related literature, see: Shibuya *et al.* (1998); List (2000).



Experimental

Crystal data

$C_9H_9NO_2$
M_r = 163.17
Monoclinic, $P2_1/c$
a = 8.9290 (4) Å
b = 8.1865 (4) Å
c = 10.7583 (4) Å
β = 104.127 (3)°
V = 762.62 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 200 (2) K
0.32 × 0.29 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
4808 measured reflections
1484 independent reflections
1205 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.06
1484 reflections
111 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

Cg is the centroid of the phenyl group.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H31$\cdots Cg^{i}$	0.99	2.72	3.3854 (16)	125

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

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); 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: HK2376).

References

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supplementary materials

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3-Phenyloxazolidin-2-one

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Comment

The title compound, (I), was unintentionally prepared upon the attempted synthesis of 2,2'-spirobi[3-phenyl-1,3-oxazolone].

In the molecule of (I) a five-membered heterocycle is bonded to a phenyl moiety as an exocyclic substituent on the N atom (Fig. 1). Since (I) is an amide, the N atom binds essentially planarly. The phenyl group and the heterocycle are not in perfect co-planarity, yet the torsional angle between the two planes is found to be smaller than 9°. The heterocycle adopts a *twist* conformation; however, puckering is small, the amplitude being only 0.085 (2) Å. Bond lengths and angles are normal (List, 2000).

In the crystal structure, pairs of molecules are oriented parallel to each other with the aromatic moieties facing the heterocyclic rings (Fig. 2). The perpendicular distance of the dimer's mean planes is 3.563 (2) Å. The π-stacked dimers interact with neighbouring dimers *via* C–H/π interactions: for C3–H31···*Cg*, the H···*Cg* distance is 2.72 Å (*Cg* is the centroid of the phenyl ring at 2_645).

Experimental

The title compound was accidentially obtained as the product upon the attempted synthesis of 2,2'-spirobi[3-phenyl-1,3-oxazolone] according to a published procedure (Shibuya *et al.*, 1998) by reacting 2-anilinoethanol with carbon disulfide in acetonitrile in the presence of triethylamine and silver nitrate. Crystals suitable for X-ray analysis were obtained directly from the crystallized reaction product.

Refinement

H atoms were located in a difference map and refined as riding on their parent atoms with C—H = 0.95 and 0.99 Å, for aromatic and methylene H atoms. One common isotropic displacement parameter for all H atoms was refined to U_{iso}(H) = 0.0444 (15) Å^2.

Figures

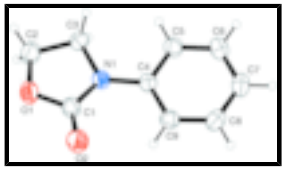

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

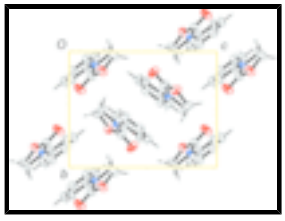

Fig. 2. A packing diagram of (I), viewed along [−1 0 0].

3-Phenyloxazolidin-2-one

Crystal data

$C_9H_9NO_2$	F_{000} = 344
M_r = 163.17	D_x = 1.421 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6001 reflections
a = 8.9290 (4) Å	θ = 3.1–26.0º
b = 8.1865 (4) Å	μ = 0.10 mm^{-1}
c = 10.7583 (4) Å	T = 200 (2) K
β = 104.127 (3)º	Platelet, colorless
V = 762.62 (6) Å^3	0.32 × 0.29 × 0.06 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1205 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	R_{int} = 0.052
Monochromator: MONTEL, graded multilayered X-ray optics	θ_{max} = 26.0º
T = 200(2) K	θ_{min} = 3.2º
CCD; rotation images; thick slices scans	h = −11→11
Absorption correction: none	k = −9→10
4808 measured reflections	l = −13→13
1484 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	Only H-atom displacement parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.1977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.106	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
1484 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
111 parameters	Extinction correction: SHELXL

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction coefficient: 0.042 (6)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.90188 (11)	0.16725 (14)	0.22618 (10)	0.0422 (3)
O2	0.75635 (13)	0.32281 (15)	0.07287 (11)	0.0517 (4)
N1	0.64862 (13)	0.12175 (14)	0.17631 (11)	0.0295 (3)
C1	0.76398 (17)	0.21333 (19)	0.14944 (14)	0.0340 (4)
C2	0.88041 (19)	0.0318 (2)	0.30567 (16)	0.0429 (4)
H21	0.9276	0.0556	0.3971	0.0444 (15)*
H22	0.9282	−0.0685	0.2812	0.0444 (15)*
C3	0.70748 (17)	0.01065 (18)	0.28320 (13)	0.0322 (4)
H31	0.6760	−0.1035	0.2599	0.0444 (15)*
H32	0.6714	0.0425	0.3598	0.0444 (15)*
C4	0.48820 (16)	0.13842 (16)	0.12138 (12)	0.0276 (3)
C5	0.38575 (16)	0.04866 (19)	0.17378 (14)	0.0343 (4)
H5	0.4245	−0.0220	0.2444	0.0444 (15)*
C6	0.22804 (18)	0.0620 (2)	0.12354 (15)	0.0402 (4)
H6	0.1593	−0.0001	0.1597	0.0444 (15)*
C7	0.16968 (17)	0.1646 (2)	0.02150 (15)	0.0403 (4)
H7	0.0613	0.1742	−0.0122	0.0444 (15)*
C8	0.27030 (18)	0.2529 (2)	−0.03092 (14)	0.0378 (4)
H8	0.2304	0.3233	−0.1014	0.0444 (15)*
C9	0.42905 (17)	0.24101 (18)	0.01742 (13)	0.0328 (4)
H9	0.4970	0.3024	−0.0201	0.0444 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0282 (6)	0.0456 (7)	0.0504 (7)	−0.0038 (5)	0.0048 (5)	0.0089 (5)
O2	0.0416 (7)	0.0524 (8)	0.0590 (8)	−0.0089 (5)	0.0085 (5)	0.0224 (6)
N1	0.0279 (6)	0.0284 (7)	0.0326 (6)	0.0004 (5)	0.0080 (5)	0.0032 (5)
C1	0.0309 (8)	0.0324 (8)	0.0390 (8)	−0.0019 (6)	0.0092 (6)	0.0019 (7)
C2	0.0343 (9)	0.0429 (10)	0.0480 (9)	0.0000 (7)	0.0033 (7)	0.0096 (7)
C3	0.0340 (8)	0.0311 (8)	0.0307 (7)	0.0017 (6)	0.0062 (6)	0.0034 (6)
C4	0.0282 (7)	0.0260 (7)	0.0288 (7)	0.0007 (6)	0.0074 (5)	−0.0047 (6)
C5	0.0325 (8)	0.0330 (8)	0.0376 (8)	−0.0009 (6)	0.0087 (6)	0.0032 (6)
C6	0.0314 (8)	0.0423 (10)	0.0476 (9)	−0.0056 (7)	0.0112 (7)	−0.0011 (7)
C7	0.0289 (8)	0.0445 (10)	0.0441 (9)	0.0015 (7)	0.0023 (6)	−0.0071 (7)
C8	0.0392 (9)	0.0397 (9)	0.0313 (7)	0.0069 (7)	0.0025 (6)	−0.0013 (7)
C9	0.0350 (8)	0.0334 (8)	0.0315 (7)	0.0020 (6)	0.0106 (6)	0.0000 (6)

Geometric parameters (Å, °)

O1—C1	1.3579 (18)	C4—C5	1.395 (2)
O1—C2	1.4414 (19)	C4—C9	1.395 (2)

O2—C1	1.2079 (18)	C5—C6	1.384 (2)
N1—C1	1.3608 (19)	C5—H5	0.9500
N1—C4	1.4164 (18)	C6—C7	1.380 (2)
N1—C3	1.4598 (17)	C6—H6	0.9500
C2—C3	1.513 (2)	C7—C8	1.377 (2)
C2—H21	0.9900	C7—H7	0.9500
C2—H22	0.9900	C8—C9	1.389 (2)
C3—H31	0.9900	C8—H8	0.9500
C3—H32	0.9900	C9—H9	0.9500
C1—O1—C2	110.01 (11)	C5—C4—C9	118.92 (13)
C1—N1—C4	126.80 (12)	C5—C4—N1	118.47 (12)
C1—N1—C3	111.40 (12)	C9—C4—N1	122.60 (13)
C4—N1—C3	121.44 (11)	C6—C5—C4	120.38 (14)
O2—C1—O1	120.84 (13)	C6—C5—H5	119.8
O2—C1—N1	129.34 (14)	C4—C5—H5	119.8
O1—C1—N1	109.81 (12)	C7—C6—C5	120.63 (15)
O1—C2—C3	105.75 (12)	C7—C6—H6	119.7
O1—C2—H21	110.6	C5—C6—H6	119.7
C3—C2—H21	110.6	C8—C7—C6	119.23 (14)
O1—C2—H22	110.6	C8—C7—H7	120.4
C3—C2—H22	110.6	C6—C7—H7	120.4
H21—C2—H22	108.7	C7—C8—C9	121.21 (14)
N1—C3—C2	102.22 (12)	C7—C8—H8	119.4
N1—C3—H31	111.3	C9—C8—H8	119.4
C2—C3—H31	111.3	C8—C9—C4	119.63 (14)
N1—C3—H32	111.3	C8—C9—H9	120.2
C2—C3—H32	111.3	C4—C9—H9	120.2
H31—C3—H32	109.2		
C2—O1—C1—O2	−178.30 (15)	C3—N1—C4—C5	1.54 (19)
C2—O1—C1—N1	2.78 (17)	C1—N1—C4—C9	8.8 (2)
C4—N1—C1—O2	−2.2 (3)	C3—N1—C4—C9	−178.57 (13)
C3—N1—C1—O2	−175.42 (15)	C9—C4—C5—C6	−0.3 (2)
C4—N1—C1—O1	176.62 (12)	N1—C4—C5—C6	179.63 (13)
C3—N1—C1—O1	3.37 (17)	C4—C5—C6—C7	−0.3 (2)
C1—O1—C2—C3	−7.44 (17)	C5—C6—C7—C8	0.6 (2)
C1—N1—C3—C2	−7.58 (16)	C6—C7—C8—C9	−0.3 (2)
C4—N1—C3—C2	178.76 (12)	C7—C8—C9—C4	−0.3 (2)
O1—C2—C3—N1	8.73 (16)	C5—C4—C9—C8	0.6 (2)
C1—N1—C4—C5	−171.09 (14)	N1—C4—C9—C8	−179.31 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H31···Cg^{i}	0.99	2.72	3.3854 (16)	125

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

Fig. 1

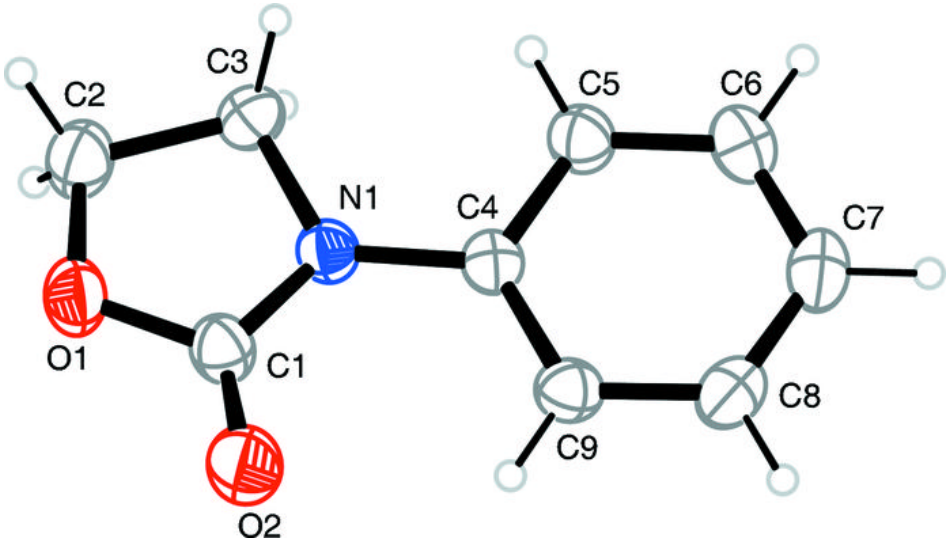

Fig. 2