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(*E*)-*N*-(1,3-Oxazolidin-2-ylidene)-benzamide

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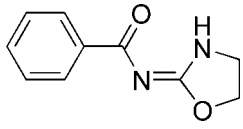
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.122; data-to-parameter ratio = 14.5.

The aryl and oxazolidine rings in the title compound, $C_{10}H_{10}N_2O_2$, are essentially coplanar [dihedral angle = 3.8 (6)°]. The crystal structure involves intra- and intermolecular N—H···O hydrogen bonds.

Related literature

For related literature, see: Allen (2002); Jiang *et al.* (2006); Lorente *et al.* (1995); Zhang *et al.* (2003).



Experimental

Crystal data

$C_{10}H_{10}N_2O_2$
M_r = 190.20
Orthorhombic, *Pccn*
a = 11.4194 (18) Å
b = 20.590 (3) Å
c = 8.0325 (13) Å
V = 1888.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.25 × 0.23 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.973, T_{max} = 0.988
9475 measured reflections
1850 independent reflections
1091 reflections with $I > 2\sigma(I)$
R_{int} = 0.095

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.122
S = 0.91
1850 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O1	0.86	2.17	2.696 (2)	119
N1—H11···O1^{i}	0.86	2.17	2.8944 (19)	142

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2168).

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supplementary materials

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(*E*)-*N*-(1,3-Oxazolidin-2-ylidene)benzamide

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Comment

The X-ray crystallographic structure of the title compound, (I) (Fig. 1), has not been published previously, although the deprotonated molecule has been reported in two metal complexes, namely, *trans*-bis(2-benzamido)oxazoline metal(II) where *M* = Ni (Jiang *et al.*, 2006) and *M* = Cu (Zhang *et al.*, 2004).

The bond lengths and angles have the usual values found for structurally similar molecules in the Cambridge Structural Database (CSD Version 5.24; Allen, 2002). Because of the existence of a conjugated system, the N1—C8 [1.314 (2) Å] and N2—C8 [1.301 (2) Å] bond distances are significantly shorter than the typical Csp^2—N bond distance (1.426 Å; Lorente *et al.*, 1995). The dihedral angle between the aryl rings and the oxazolidine ring is 2.856 (3)° and the C4—C7—N2—C8 torsion angle is 175.45 (2)°.

An intramolecular N1—H11···O1 hydrogen bond is found and centrosymmetrically related molecules are connected *via* N—H···O hydrogen bonds involving the same atoms (Table 1).

Experimental

N-Benzoyl-*N*'-(2-hydroxy-ethyl)thiourea was reacted with dicyclohexylcarbodiimide under weakly basic conditions in CH_3CN to give (I) in 90% yield. Single crystals suitable for the X-ray diffraction study were obtained by slow evaporation of an acetone/water solution of (I).

Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(carrier atom).

Figures

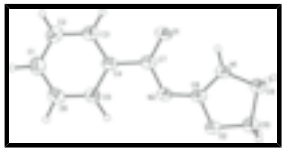

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids.

(*E*)—*N*-(1,3-Oxazolidin-2-ylidene)benzamide

Crystal data

$C_{10}H_{10}N_2O_2$ $D_x = 1.338$ Mg m^{-3}

M_r = 190.20	Melting point: 411-412 K
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 1672 reflections
a = 11.4194 (18) Å	θ = 3.3–22.3º
b = 20.590 (3) Å	μ = 0.10 mm^{-1}
c = 8.0325 (13) Å	*T* = 293 (2) K
V = 1888.7 (5) $Å^3$	Block, colorless
Z = 8	0.25 × 0.23 × 0.18 mm
F_{000} = 800	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	1850 independent reflections
Radiation source: sealed tube	1091 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.095
T = 293(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	*h* = −8→14
T_{min} = 0.973, T_{max} = 0.988	*k* = −25→25
9475 measured reflections	*l* = −9→9

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.064P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.122	$(\Delta/\sigma)_{max} < 0.001$
S = 0.91	$\Delta\rho_{max}$ = 0.15 e $Å^{-3}$
1850 reflections	$\Delta\rho_{min}$ = −0.13 e $Å^{-3}$
128 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0047 (12)
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	0.34177 (19)	0.35640 (11)	0.2998 (3)	0.0796 (7)
H1	0.3107	0.3467	0.1958	0.096*
C2	0.33903 (19)	0.41901 (11)	0.3592 (3)	0.0792 (7)
H2	0.3060	0.4518	0.2948	0.095*
C3	0.38492 (17)	0.43353 (9)	0.5133 (2)	0.0652 (5)
H3	0.3824	0.4760	0.5523	0.078*
C4	0.43460 (15)	0.38564 (8)	0.6105 (2)	0.0518 (5)
C5	0.43765 (17)	0.32282 (9)	0.5492 (2)	0.0606 (5)
H5	0.4716	0.2900	0.6123	0.073*
C6	0.3907 (2)	0.30858 (10)	0.3953 (3)	0.0734 (6)
H6	0.3923	0.2661	0.3561	0.088*
C7	0.48292 (16)	0.40198 (8)	0.7777 (2)	0.0539 (5)
C8	0.58435 (15)	0.35996 (8)	1.0000 (2)	0.0514 (5)
C9	0.6620 (2)	0.39852 (9)	1.2444 (2)	0.0701 (6)
H9A	0.6106	0.4059	1.3387	0.084*
H9B	0.7325	0.4243	1.2574	0.084*
C10	0.69031 (19)	0.32699 (9)	1.2239 (2)	0.0709 (6)
H10A	0.7742	0.3204	1.2149	0.085*
H10B	0.6611	0.3021	1.3177	0.085*
N1	0.60390 (14)	0.41239 (7)	1.08905 (18)	0.0630 (5)
H11	0.5746	0.4494	1.0618	0.076*
N2	0.53248 (13)	0.35040 (7)	0.85798 (18)	0.0557 (4)
O1	0.47644 (13)	0.45792 (6)	0.83169 (16)	0.0782 (5)
O2	0.63240 (12)	0.30804 (6)	1.07298 (15)	0.0702 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0837 (16)	0.0822 (17)	0.0728 (14)	0.0054 (13)	−0.0193 (12)	−0.0120 (12)
C2	0.0868 (16)	0.0684 (15)	0.0823 (15)	0.0118 (12)	−0.0207 (13)	0.0051 (12)
C3	0.0741 (13)	0.0489 (11)	0.0725 (12)	0.0070 (10)	−0.0089 (11)	−0.0020 (10)
C4	0.0559 (11)	0.0425 (10)	0.0568 (10)	0.0018 (8)	0.0024 (9)	−0.0010 (8)
C5	0.0740 (13)	0.0465 (11)	0.0613 (11)	0.0053 (9)	−0.0016 (10)	−0.0052 (9)
C6	0.0869 (15)	0.0582 (13)	0.0749 (13)	0.0031 (11)	−0.0054 (12)	−0.0148 (10)
C7	0.0604 (12)	0.0413 (10)	0.0601 (11)	0.0024 (8)	0.0036 (9)	−0.0008 (8)
C8	0.0566 (11)	0.0381 (10)	0.0595 (11)	0.0041 (8)	0.0055 (9)	−0.0014 (8)
C9	0.0838 (15)	0.0544 (12)	0.0723 (13)	0.0090 (10)	−0.0162 (11)	−0.0075 (10)
C10	0.0814 (14)	0.0557 (12)	0.0756 (13)	0.0105 (10)	−0.0195 (11)	−0.0054 (10)
N1	0.0832 (12)	0.0403 (9)	0.0655 (9)	0.0110 (8)	−0.0120 (9)	−0.0057 (7)

N2	0.0694 (10)	0.0404 (9)	0.0572 (9)	0.0036 (7)	−0.0051 (8)	−0.0042 (7)
O1	0.1163 (12)	0.0400 (8)	0.0782 (9)	0.0130 (8)	−0.0197 (8)	−0.0105 (6)
O2	0.0925 (10)	0.0420 (7)	0.0760 (9)	0.0129 (6)	−0.0233 (8)	−0.0034 (6)

Geometric parameters (Å, °)

C1—C6	1.367 (3)	C7—N2	1.365 (2)
C1—C2	1.375 (3)	C8—N2	1.301 (2)
C1—H1	0.9300	C8—N1	1.314 (2)
C2—C3	1.377 (3)	C8—O2	1.3368 (19)
C2—H2	0.9300	C9—N1	1.442 (2)
C3—C4	1.380 (2)	C9—C10	1.517 (2)
C3—H3	0.9300	C9—H9A	0.9700
C4—C5	1.384 (2)	C9—H9B	0.9700
C4—C7	1.491 (2)	C10—O2	1.435 (2)
C5—C6	1.379 (2)	C10—H10A	0.9700
C5—H5	0.9300	C10—H10B	0.9700
C6—H6	0.9300	N1—H11	0.8599
C7—O1	1.2328 (19)		
C6—C1—C2	119.4 (2)	N2—C8—N1	132.76 (16)
C6—C1—H1	120.3	N2—C8—O2	116.77 (15)
C2—C1—H1	120.3	N1—C8—O2	110.42 (16)
C1—C2—C3	120.44 (19)	N1—C9—C10	101.33 (15)
C1—C2—H2	119.8	N1—C9—H9A	111.5
C3—C2—H2	119.8	C10—C9—H9A	111.5
C2—C3—C4	120.66 (18)	N1—C9—H9B	111.5
C2—C3—H3	119.7	C10—C9—H9B	111.5
C4—C3—H3	119.7	H9A—C9—H9B	109.3
C3—C4—C5	118.47 (17)	O2—C10—C9	104.92 (14)
C3—C4—C7	120.05 (16)	O2—C10—H10A	110.8
C5—C4—C7	121.48 (16)	C9—C10—H10A	110.8
C6—C5—C4	120.52 (17)	O2—C10—H10B	110.8
C6—C5—H5	119.7	C9—C10—H10B	110.8
C4—C5—H5	119.7	H10A—C10—H10B	108.8
C1—C6—C5	120.6 (2)	C8—N1—C9	112.72 (15)
C1—C6—H6	119.7	C8—N1—H11	121.5
C5—C6—H6	119.7	C9—N1—H11	125.1
O1—C7—N2	125.85 (17)	C8—N2—C7	119.04 (14)
O1—C7—C4	120.36 (16)	C8—O2—C10	109.99 (14)
N2—C7—C4	113.79 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H11···O1	0.86	2.17	2.696 (2)	119
N1—H11···O1^{i}	0.86	2.17	2.8944 (19)	142

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

Fig. 1