organic papers

3-Benzoyl-1,3-oxazolidin-2-one

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Key indicators

Single-crystal X-ray study
$T = 296$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.075
Data-to-parameter ratio = 16.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The non-planar title compound, $C_{10}H_9NO_3$, prepared from a condensation reaction of benzoyl chloride and oxazolidin-2-one, has longer than usual C—N bond lengths compared with typical acylamine groups.

Comment

Oxazolidinone derivatives have a high potential for biological activity, *e.g.* they have been widely used as pesticides and fungicides (Edwin & Bing, 1963). As a continuation of our work on the structure–activity relationship of thiazolidinone derivatives, the structure of a colourless crystalline compound, (I), which was the product of the condensation reaction between benzoyl chloride and 2-oxazolidinone, was determined.

(I)
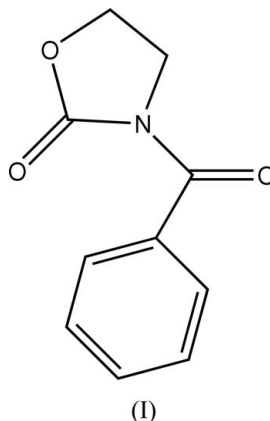
The molecular structure of (I) (Fig. 1 and Table 1) establishes the molecular connectivity. The molecule is non-planar, as seen in the C1—N1—C4—C5 and N1—C4—C5—C6 torsion angles of −30.23 (15) and −50.48 (13)°, respectively. The most notable feature of (I) is that the average (O═C)—N bond length of 1.4211 (16) Å is greater than the C—N single-bond length (1.33–1.35 Å) of a typical acylamine group.

Experimental

2-Oxazolidinone (0.44 g, 5 mmol), prepared according to the procedure of Homeyer (1946), and triethylamine (0.72 g, 7 mmol) were dissolved in dichloromethane (20 ml) with stirring. Benzoyl chloride (0.85 g, 6 mmol) was added dropwise to the mixture in an ice bath. The mixture was stirred at 273 K for 10 h, washed with water three times and then dried *in vacuo* to give a solid (yield 90.1%, 0.86 g), which was then recrystallized from ethanol to give colourless blocks (m.p. 447–448 K).
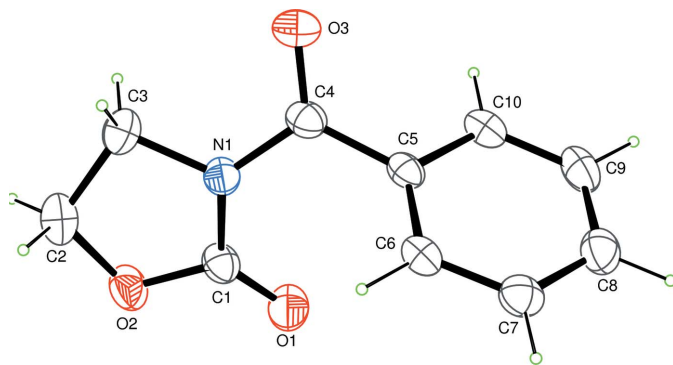
Figure 1
The structure of (I), showing 30% probability displacement ellipsoids.

Crystal data

$C_{10}H_9NO_3$	$D_x = 1.418$ Mg m^{-3}
$M_r = 191.19$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6957
$a = 13.305$ (7) Å	reflections
$b = 5.676$ (4) Å	$\theta = 3.2$–$27.5°$
$c = 12.455$ (6) Å	$\mu = 0.11$ mm^{-1}
$\beta = 107.784$ (16)°	$T = 296$ (1) K
$V = 895.7$ (9) Å^3	Block, colourless
$Z = 4$	$0.24 \times 0.23 \times 0.15$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2051 independent reflections
	1403 reflections with $F^2 > 2\sigma(F^2)$
ω scans	$R_{int} = 0.026$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{max} = 27.5°$
	$h = -16 \rightarrow 17$
$T_{min} = 0.952$, $T_{max} = 0.984$	$k = -7 \rightarrow 7$
8404 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[0.0002F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.075$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.14$ e Å^{-3}
2051 reflections	Extinction correction: Larson
126 parameters	(1970), equation 22
H-atom parameters constrained	Extinction coefficient: 195 (15)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.1958 (15)	C4—C5	1.4835 (17)
O2—C1	1.3377 (15)	C5—C6	1.3845 (16)
O2—C2	1.4472 (15)	C5—C10	1.3882 (16)
O3—C4	1.2156 (15)	C6—C7	1.3783 (18)
N1—C1	1.3888 (14)	C7—C8	1.3793 (18)
N1—C3	1.4600 (16)	C8—C9	1.3726 (19)
N1—C4	1.3822 (16)	C9—C10	1.3844 (19)
C2—C3	1.5044 (19)		
C1—O2—C2	110.45 (9)	O2—C1—N1	108.66 (9)
C1—N1—C3	110.92 (9)	O2—C2—C3	105.64 (10)
C1—N1—C4	126.00 (9)	N1—C3—C2	101.05 (9)
C3—N1—C4	120.51 (9)	O3—C4—N1	118.74 (12)
O1—C1—O2	123.06 (10)	O3—C4—C5	121.77 (11)
O1—C1—N1	128.25 (11)	N1—C4—C5	119.36 (10)

H atoms were included in the riding-model approximation, with C—H = 0.97 and 0.98 Å for methylene and aromatic H atoms, respectively, and with U_{iso}(H) = 1.2U_{eq}(C) of the parent atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku & Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *CrystalStructure*.

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