organic papers

3-Benzoylthiazolidin-2-one

Delong Shen, Jianquan Weng,* Chengxia Tan and Aishu Tang

College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China

Correspondence e-mail: wengjianquan@163.net

Key indicators

Single-crystal X-ray study
$T = 297$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.093
Data-to-parameter ratio = 10.6

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

The title compound, $C_{10}H_9NO_2S$, was prepared from a condensation reaction of benzoyl chloride and thiazolidin-2-one. The average C—N bond length to carbonyl groups is 1.393 (2) Å, which is longer then the C—N bond length of a typical acylamine group.

Comment

Thiazolidinone derivatives have a high potential for biological activity, and these derivatives have been widely used in pesticides and fungicides (Kusatsu *et al.*, 1986). In a continuation of our work on the structure–activity relationship of thiazolidinone derivatives, we have obtained a colourless crystalline compound that was the product of the condensation reaction of benzoyl chloride and thiazolidin-2-one. The structural identity of our product, (I), was resolved using single-crystal X-ray diffraction.

(I)
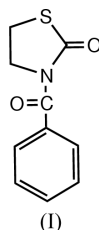
The molecular structure of (I) is illustrated in Fig. 1. Selected bond lengths and angles are listed in Table 1. The asymmetric unit contains two molecules. In (I), the average C—N bond length to carbonyl groups in the two molecules is 1.393 (2) Å. The C—N bond length is longer than the C—N single-bond length of a typical acylamine group, which is 1.327–1.352 Å (Ganis *et al.*, 1971).

Experimental

Thiazolidin-2-one (0.52 g, 5 mmol), prepared according to the procedure of Crawhall & Elliott (1952), and triethylamine (0.72 g, 7 mmol) were dissolved in dichloromethane (10 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 and washed with water three times and then dried *in vacuo* to give a solid (0.90 g, yield 86.1%), which was then recrystallized from ethanol to give colourless chunks (m.p. 394–395 K).

Crystal data

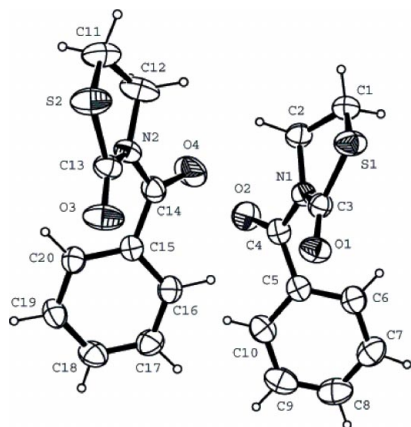|	
$C_{10}H_9NO_2S$	$D_x = 1.414$ Mg m^{-3}
$M_r = 207.25$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 12 657
$a = 11.2818$ (5) Å	reflections
$b = 12.4987$ (6) Å	$\theta = 1.5$–$27.4°$
$c = 13.8074$ (5) Å	$\mu = 0.30$ mm^{-1}
$\beta = 91.209$ (1)°	$T = 297.1$ K
$V = 1946.52$ (15) Å^3	Chunk, colourless
$Z = 8$	$0.38 \times 0.35 \times 0.20$ mm

Figure 1
The structure of the asymmetric unit of (I), shown with 30% probability displacement ellipsoids.

Data collection

Rigaku R-AXIS RAPID diffractometer	4451 independent reflections
ω scans	2873 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan ($ABSCOR$; Higashi, 1995)	$R_{int} = 0.026$
$T_{min} = 0.857$, $T_{max} = 0.941$	$\theta_{max} = 27.4°$
37 290 measured reflections	$h = -14 \rightarrow 12$
	$k = -16 \rightarrow 16$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[0.0013F_o^2 + 1.05\sigma(F_o^2)]/(4F_o^2)$
$wR(F^2) = 0.093$	
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4451 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.803 (2)	N1—C2	1.468 (2)
S1—C3	1.766 (2)	N1—C3	1.395 (2)
O1—C3	1.202 (2)	N1—C4	1.391 (2)
O2—C4	1.213 (2)		
C1—S1—C3	92.52 (9)	C2—N1—C4	119.6 (1)
C2—N1—C3	113.4 (1)	C3—N1—C4	124.3 (1)

All H atoms were placed in calculated in idealized positions and refined (C—H = 0.96 Å) as riding on their parent atoms. H atoms were given isotropic displacement parameters equal to 1.2 times the equivalent isotropic displacement parameters of their parent atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

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