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2-Oxo-*N*-phenylthiazolidine-3-carboxamide

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The title compound, $C_{10}H_{10}N_2O_2S$, was prepared from a condensation reaction of phenyl isocyanate and thiazolidin-2-one. There are two independent molecules in the asymmetric unit, showing similar conformations. The C—N single bonds linked to the phenyl ring have lengths 1.408 (3) and 1.414 (3) Å, and are longer than the C—N bonds to the carbonyl groups [1.342 (3)–1.370 (3) Å].

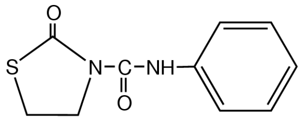
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.108
Data-to-parameter ratio = 8.9

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

Comment

Thiazolidinone derivatives have a high potential for biological activity and have been widely used in pesticides and fungicides (Haga *et al.*, 1986). In order to investigate the structure–activity relationship of thiazolidinone derivatives, a series of new thiazolidinone derivatives has been synthesized in our laboratory. We have obtained a colourless crystalline compound, (I), which was the product of the condensation reaction of phenyl isocyanate and thiazolidin-2-one. The structure of (I) is reported here as an early result in our study of this new series of compounds.



(I)

The asymmetric unit of (I) contains two molecules (Fig. 1 and Table 1). There are three different C—N single bonds of the acylamine group. The C4—N1 or C14—N3 bond length is longer than the other two C—N bond lengths to the carbonyl groups, and is also appreciably longer than the C—N single-bond length of a typical acylamine group, which ranges from 1.327 (10) to 1.352 (6) Å (Ganis *et al.*, 1971).

In the structure of (I), there are intramolecular N—H···O hydrogen bonds (Table 2).

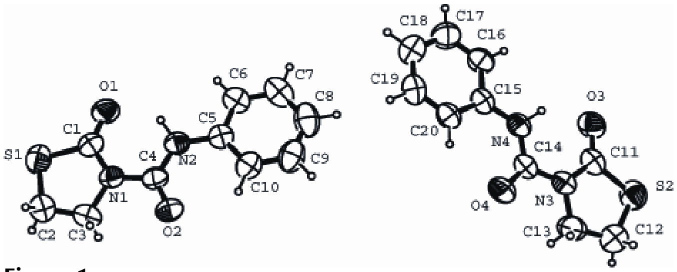


Figure 1
The structure of the asymmetric unit of (I), showing the atom-numbering scheme for the two independent molecules. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

Experimental

Thiazolidin-2-one (0.52 g, 5 mmol), prepared according to the procedure of Crawhall & Elliott (1952), was dissolved in dichloromethane (10 ml) with stirring. Phenyl isocyanate (0.66 g, 5.5 mmol) was added dropwise to the solution in an ice bath. The mixture was stirred at 273 K for 5 h and then dried *in vacuo* to give a solid (1.02 g, yield 91.8%), which was then recrystallized from acetone to give colourless chunks of (I) (m.p. 396–397 K).

Crystal data

$C_{10}H_{10}N_2O_2S$
$M_r = 222.27$
Monoclinic, $P2_1/c$
$a = 22.201$ (1) Å
$b = 8.1176$ (3) Å
$c = 11.8485$ (5) Å
$\beta = 104.480$ (1)°
$V = 2067.49$ (15) Å^3
$Z = 8$

$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 002 reflections
$\theta = 2.3$–27.5°
$\mu = 0.29$ mm^{-1}
$T = 293$ (1) K
Chunk, colourless
0.29 × 0.25 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.826$, $T_{\max} = 0.932$
16 794 measured reflections

4736 independent reflections
2564 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 27.5°$
$h = -28 \rightarrow 28$
$k = -10 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.108$
$S = 1.00$
4736 reflections
291 parameters

H-atom parameters constrained
$w = 4F_o^2/[0.0017F_o^2 + \sigma(F_o^2)]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}

Table 1
Selected interatomic distances (Å).

S1—C1	1.761 (2)	N1—C3	1.458 (3)
S1—C2	1.789 (4)	N1—C4	1.414 (3)
S2—C11	1.754 (3)	N2—C4	1.344 (3)
S2—C12	1.789 (4)	N2—C5	1.413 (3)
O1—C1	1.209 (3)	N3—C11	1.369 (3)
O2—C4	1.212 (3)	N3—C13	1.468 (4)
O3—C11	1.216 (3)	N3—C14	1.408 (3)
O4—C14	1.212 (3)	N4—C14	1.342 (3)
N1—C1	1.370 (3)	N4—C15	1.411 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O1	0.96	1.88	2.663 (3)	137
N4—H2···O3	0.96	1.89	2.668 (2)	137

All H atoms were placed in idealized positions and allowed to ride on their parent atoms (N—H = 0.96 Å and C—H = 0.96 Å), with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(parent atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1993); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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