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Redetermination of 1,3-thiazolidine-2,4-dione

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.031
wR factor = 0.083
Data-to-parameter ratio = 14.5

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

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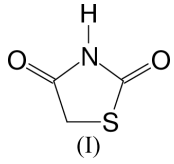
The structure of the title compound, $C_3H_3NO_2S$, comprises flat molecules that associate *via* a single N—H···O interaction and a C—H···O close contact to the second O atom. Furthermore, 10% of the molecules have S and CH_2 interchanged, generating disorder.

Comment

The structure of the title compound, (I), is known with the room-temperature structure being refined to R = 0.069 (Form *et al.*, 1975). Refinement on data collected at 150 K yielded R = 0.066 but left C5 as non-positive-definite, with significant electron density close to this atom. Further refinement of the disorder revealed that 10% of the molecules have S and CH_2 interchanged, with the O═C—NH—C═O sites being in common. The molecule was consequently split into two separate partial-occupancy fragments and refined in both configurations with bond distances (for the major fragment) allowed to vary while the displacement parameters and ring geometry were restrained to be equal in each portion.



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis.

Crystal data

$C_3H_3NO_2S$
M_r = 117.12
Orthorhombic, *Pbca*
a = 7.2926 (2) Å
b = 9.3642 (3) Å
c = 13.1208 (5) Å
V = 896.01 (5) Å^3
Z = 8
D_x = 1.736 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3675 reflections
θ = 1.0–27.5°
μ = 0.58 mm^{-1}
T = 150 (2) K
Plate, colourless
0.50 × 0.30 × 0.07 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.759, T_{max} = 0.960
5895 measured reflections
1018 independent reflections
919 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.44P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.031$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.083$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.29$ e Å^{-3}
1018 reflections	
70 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N3A—H3A···O21A^{i}	0.88	1.97	2.8465 (16)	178
C5A—H52A···O41A^{ii}	0.99	2.50	3.453 (3)	161

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $-\frac{1}{2}-x, y-\frac{1}{2}, z$.

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.88 (N—H) and 0.99 Å (CH_2).

Data collection, cell refinement and data reduction: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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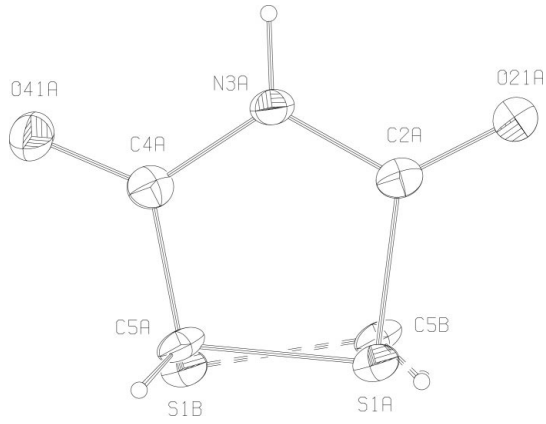

Figure 1
The molecular configuration and atom numbering scheme for (I), showing 50% probability displacement ellipsoids.

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