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3,3'-(Ethane-1,2-diyl)bis(2-thioxo-1,3-oxazolidin-4-one)

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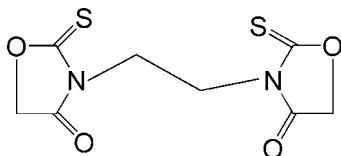
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.043; wR factor = 0.127; data-to-parameter ratio = 13.9.

The asymmetric unit of the title compound, $\text{C}_8\text{H}_8\text{N}_2\text{O}_4\text{S}_2$, contains one half of a centrosymmetric molecule. A short $\text{C}\cdots\text{O}$ distance of 3.012 (4) Å between the carbonyl groups of neighbouring molecules indicates the presence of dipole-dipole interactions. The crystal packing exhibits also weak intermolecular $\text{O}\cdots\text{S}$ [3.239 (3) Å] and $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

For general background, see: Gupta *et al.* (1981); Cutshall *et al.* (2005). For details of the synthesis, see: Doğan *et al.* (1992);



Experimental

Crystal data

 $\text{C}_8\text{H}_8\text{N}_2\text{O}_4\text{S}_2$ $M_r = 260.28$ Monoclinic, $P2_1/c$ $a = 6.2845$ (12) Å $b = 12.3252$ (19) Å $c = 7.080$ (2) Å $\beta = 105.22$ (2)° $V = 529.2$ (2) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.50$ mm⁻¹ $T = 293$ (2) K

0.20 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 2001)

 $T_{\min} = 0.908$, $T_{\max} = 0.955$

1390 measured reflections

1012 independent reflections

761 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.028$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.043$ $wR(F^2) = 0.127$ $S = 1.02$

1012 reflections

73 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3A}\cdots\text{O2}^i$	0.97	2.56	3.215 (4)	125
$\text{C3}-\text{H3B}\cdots\text{O2}^{ii}$	0.97	2.57	3.325 (4)	135

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); 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: CV2350).

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supporting information

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3,3'-(Ethane-1,2-diyl)bis(2-thioxo-1,3-oxazolidin-4-one)

Chunhua Ge, Ya'nan Guo, Xiangdong Zhang, Xiaoyan Zhang and Qitao Liu

S1. Comment

The research on *N*-substitution 2-thioxooxazolidin-4-one compounds have been mushroomed for their interesting biological and spectral properties (Cutshall *et al.*, 2005; Gupta *et al.*, 1981).

The title compound is composed of two functional groups of 2-thioxooxazolidin-4-one which are bridged by ethane group (Fig.1). In the crystal, C1—C4, O1—O2, N1 and S1 atoms are almost coplanar with a highest deviation of 0.0440 Å for O2. As a derivative of ethane, the molecule has a perfect *anti*-linear conformation. Dihedral angle of N1—C1—C1A—N1A is -180.00 (19)°. The crystal packing exhibits weak intermolecular C—H···O hydrogen bonds (Table 1), O···S interaction (S1···O2ⁱⁱⁱ 3.239 (3) Å [symmetry code: (iii) -1 + x, y, -1 + z]), and strong dipole-dipole interactions proved by short C···O distance of 3.012 (4) Å between the carbonyl groups of neighbouring molecules.

S2. Experimental

The title compound was prepared according to the method of Doğan *et al.* (1992). Colourless block-shape crystal of (I) suitable for X-ray diffraction was obtained from ethanol/water (V: V = 4: 1).

S3. Refinement

H atoms were found in difference map, placed in idealized positions (C—H 0.97 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

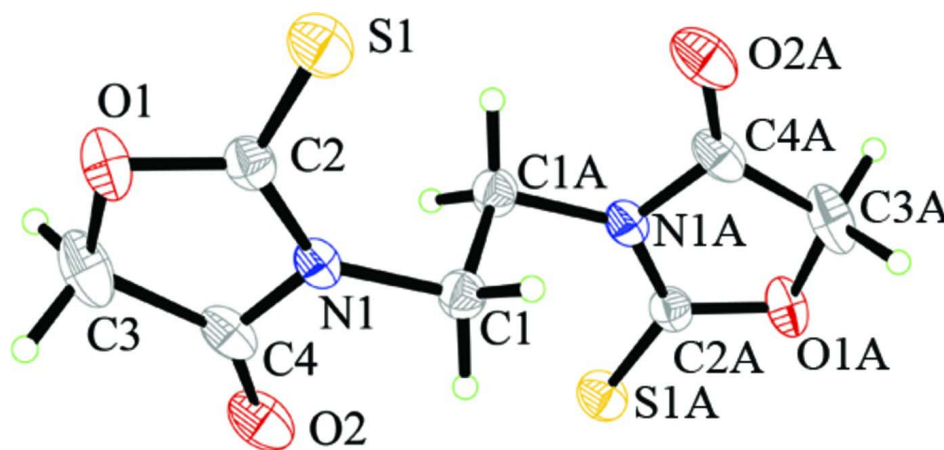


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level and atomix numbering [symmetry code: (A) 1 - x, 1 - y, 1 - z].

3,3'-(Ethane-1,2-diyl)bis(2-thioxo-1,3-oxazolidin-4-one)*Crystal data*C₈H₈N₂O₄S₂ $M_r = 260.28$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 6.2845$ (12) Å $b = 12.3252$ (19) Å $c = 7.080$ (2) Å $\beta = 105.22$ (2)° $V = 529.2$ (2) Å³ $Z = 2$ $F(000) = 268$ $D_x = 1.634$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 554 reflections

 $\theta = 2.7$ – 22.1 ° $\mu = 0.50$ mm⁻¹ $T = 293$ K

Block, colourless

 $0.20 \times 0.15 \times 0.11$ mm*Data collection*Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ϕ and ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2001) $T_{\min} = 0.908$, $T_{\max} = 0.955$

1390 measured reflections

1012 independent reflections

761 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.028$ $\theta_{\text{max}} = 26.0$ °, $\theta_{\text{min}} = 3.3$ ° $h = -7 \rightarrow 7$ $k = -15 \rightarrow 1$ $l = -8 \rightarrow 1$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.043$ $wR(F^2) = 0.127$ $S = 1.02$

1012 reflections

73 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0798P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} < 0.001$ $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³*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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.33868 (11)	0.36411 (6)	0.00385 (12)	0.0506 (3)
O1	0.7149 (3)	0.33522 (16)	0.0792 (3)	0.0486 (6)
C2	0.5626 (4)	0.36727 (18)	0.1543 (4)	0.0373 (6)
N1	0.6306 (3)	0.40084 (16)	0.3674 (3)	0.0350 (5)

C1	0.5096 (4)	0.4388 (2)	0.5081 (4)	0.0389 (6)
H1A	0.5884	0.4182	0.6401	0.047*
H1B	0.3641	0.4063	0.4781	0.047*
O2	0.9269 (3)	0.40856 (17)	0.6269 (4)	0.0600 (7)
C4	0.8323 (4)	0.3902 (2)	0.4422 (5)	0.0442 (7)
C3	0.8954 (4)	0.3505 (3)	0.2477 (6)	0.0605 (9)
H3A	0.9950	0.4034	0.2159	0.073*
H3B	0.9752	0.2826	0.2764	0.073*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0373 (4)	0.0552 (5)	0.0535 (5)	-0.0042 (3)	0.0018 (3)	-0.0021 (3)
O1	0.0338 (10)	0.0488 (11)	0.0634 (13)	0.0019 (8)	0.0132 (9)	-0.0174 (10)
C2	0.0359 (13)	0.0282 (12)	0.0484 (16)	-0.0001 (10)	0.0118 (12)	0.0005 (11)
N1	0.0300 (10)	0.0300 (10)	0.0440 (14)	0.0011 (8)	0.0077 (9)	-0.0010 (9)
C1	0.0397 (13)	0.0354 (13)	0.0432 (15)	0.0007 (11)	0.0137 (11)	-0.0002 (12)
O2	0.0412 (11)	0.0528 (12)	0.0730 (16)	-0.0003 (9)	-0.0083 (10)	-0.0046 (11)
C4	0.0337 (13)	0.0307 (13)	0.0613 (19)	0.0023 (10)	0.0000 (13)	-0.0036 (12)
C3	0.0315 (14)	0.0564 (18)	0.090 (3)	0.0008 (12)	0.0094 (15)	-0.0195 (18)

Geometric parameters (Å, °)

S1—C2	1.526 (3)	C1—H1A	0.9700
O1—C2	1.274 (3)	C1—H1B	0.9700
O1—C3	1.427 (4)	O2—C4	1.307 (4)
C2—N1	1.514 (4)	C4—C3	1.606 (5)
N1—C4	1.246 (3)	C3—H3A	0.9700
N1—C1	1.479 (3)	C3—H3B	0.9700
C1—C1 ⁱ	1.514 (5)		
C2—O1—C3	97.4 (2)	C1 ⁱ —C1—H1B	110.1
O1—C2—N1	117.0 (2)	H1A—C1—H1B	108.4
O1—C2—S1	110.9 (2)	N1—C4—O2	123.5 (3)
N1—C2—S1	132.0 (2)	N1—C4—C3	96.9 (3)
C4—N1—C1	113.1 (2)	O2—C4—C3	139.6 (3)
C4—N1—C2	112.6 (2)	O1—C3—C4	115.9 (2)
C1—N1—C2	134.2 (2)	O1—C3—H3A	108.3
N1—C1—C1 ⁱ	108.0 (3)	C4—C3—H3A	108.3
N1—C1—H1A	110.1	O1—C3—H3B	108.3
C1 ⁱ —C1—H1A	110.1	C4—C3—H3B	108.3
N1—C1—H1B	110.1	H3A—C3—H3B	107.4

Symmetry code: (i) $-x+1, -y+1, -z+1$.*Hydrogen-bond geometry (Å, °)*

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3A \cdots O2 ⁱⁱ	0.97	2.56	3.215 (4)	125

C3—H3B···O2 ⁱⁱⁱ	0.97	2.57	3.325 (4)	135
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Symmetry codes: (ii) $-x+2, -y+1, -z+1$; (iii) $x, -y+1/2, z-1/2$.