STRUCTURAL CHEMISTRY

ISSN: 2053-2296
journals.iucr.org/c

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Acta Cryst. (2012). C**68**, o332–o334

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

An optically resolved crystal of thiomalate: (*S*)-1-phenylethanaminium (*R*)-thiomalate

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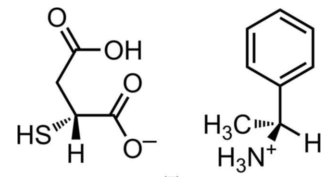
Received 19 June 2012
Accepted 20 July 2012
Online 1 August 2012

The asymmetric unit of the optically resolved title salt, $C_8H_{12}N^+\cdot C_4H_5O_4S^-$, contains a 1-phenylethanaminium monocation and a thiomalate (3-carboxy-2-sulfanylpropanoate) monoanion. The absolute configurations of the cation and the anion are determined to be *S* and *R*, respectively. In the crystal, cation–anion N—H···O hydrogen bonds, together with anion–anion O—H···O and S—H···O hydrogen bonds, construct a two-dimensional supramolecular sheet parallel to the *ab* plane. The two-dimensional sheet is linked with the upper and lower sheets through C—H···π interactions to stack along the *c* axis.

Comment

Thiomalic acid (2-mercaptosuccinic acid, H_3msa) is one of the simplest chiral thiol-containing dicarboxylic acids and has been widely employed as a raw material for sulfur-containing organic materials. Because commercially available H_3msa is a racemic mixture of the *S* and *R* enantiomers, the preparation of enantiopure H_3msa has been intensively investigated, prompted by the finding of efficient antirheumatic activity in a gold(I) adduct of the thiomalate ion, *viz.* $\{Na_2[Au(msa)]\cdot 1.75H_2O\}_n$, by Nomiya *et al.* (1995). For example, LeBlanc *et al.* (1997) reported the asymmetric synthesis of pure (*R*)-thiomalic acid from L-aspartic acid in three steps, while Shiraiwa *et al.* (1998) reported the optical resolution of the racemic H_3msa with the use of (*S*)-pea (pea = 1-phenylethanamine), which led to the preferential crystallization of the title compound, $[(S)\text{-Hpea}]^+\cdot[(R)\text{-}H_2\text{msa}]^-$, (I). The latter method is undoubtedly superior to the former, but the resulting salt, (I), has not been crystallographically characterized.

As part of our studies on the rational construction of coordination systems based on chiral thiol-containing multidentate ligands (Konno, 2004; Igashira-Kamiyama & Konno, 2011), we started to investigate the coordination system derived from H_3msa. In the course of this investigation, we obtained an optically active single crystal of (I) from the reaction of racemic H_3msa and (*S*)-pea, and its structure was determined by X-ray crystallography. The optical activity of the compound was confirmed by circular dichroism spectroscopy.



(I)

The asymmetric unit of (I) contains an $[(S)\text{-Hpea}]^+$ cation and an $[(R)\text{-}H_2\text{msa}]^-$ anion. The absolute configurations of cation and anion, which were confirmed by the Flack (1983) parameter, are consistent with the previous prediction made by optical rotation measurements (Shiraiwa *et al.*, 1998). In (I), the amine group of pea is protonated to form a $[\text{Hpea}]^+$ cation, while one of the two carboxy groups of thiomalic acid (C3, O1 and O2) is protonated and the other (C4, O3 and O4) is deprotonated to form a $[H_2\text{msa}]^-$ anion (Fig. 1). Reflecting the protonation of the O1 atom, the C3—O1 bond length [1.297 (3) Å] is obviously longer than that of C3—O2 [1.213 (3) Å]. On the other hand, the difference between the C4—O3 [1.276 (2) Å] and C4—O4 [1.237 (3) Å] bond lengths is smaller, which is consistent with the deprotonated form of the COO^- group. The other bond lengths and angles of the cation and the anion are in the ranges normally observed for related compounds.

In the crystal, the protonated carboxy group of each $[(R)\text{-}H_2\text{msa}]^-$ anion acts as a hydrogen-bond donor, forming an intermolecular O—H···O hydrogen bond with a deprotonated carboxylate group of a neighbouring anion [$O1\cdots O3^{ii}$ = 2.501 (2) Å; symmetry code: (ii) $-x, y - \frac{1}{2}, -z + 1$]. In addition, its protonated carboxy group acts as a hydrogen-bond acceptor, forming an intermolecular S—H···O hydrogen

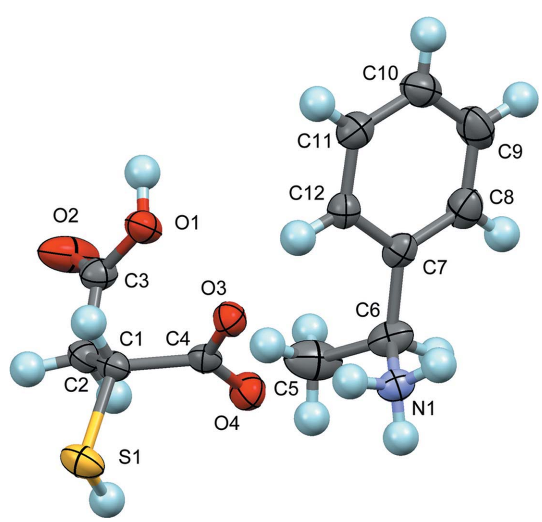


Figure 1
A view of the asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

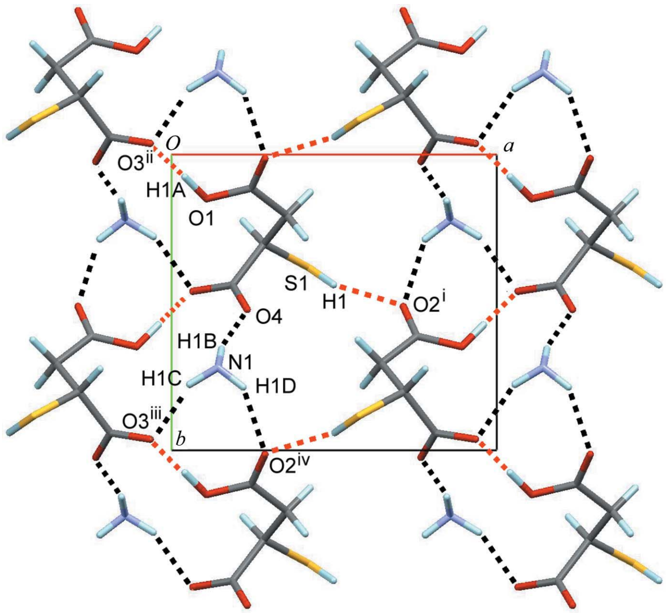


Figure 2
The two-dimensional grid network of [(*R*)-H_2msa]$^-$ anions which incorporates ammonium groups of [(*S*)-Hpea]$^+$ cations in (I), viewed parallel to the crystallographic *c* axis. [(*S*)-Hpea]$^+$ cations, except for their NH_3^+ groups, have been omitted for clarity. The grey dashed lines (red in the electronic version of the paper) show the hydrogen bonds between anions and the black broken lines show the hydrogen bonds between anions and cations. [Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+1$; (ii) $-x, y-\frac{1}{2}, -z+1$; (iii) $-x, y+\frac{1}{2}, -z+1$; (iv) $x, y+1, z$.]

bond with a thiol group of another neighbouring anion [S1$\cdots$O2^{i} = 3.2741 (19) Å; symmetry code: (i) $-x+1, y+\frac{1}{2}, -z+1$]. Based on these two kinds of hydrogen bonds, [(*R*)-H_2msa]$^-$ anions construct a two-dimensional grid network having rectangular cavities surrounded by four anions parallel to the *ab* plane (Fig. 2). It is noted that each rectangular cavity accommodates an ammonium group of an [(*S*)-Hpea]$^+$ cation through three N—H$\cdots$O hydrogen bonds [N1$\cdots$O4 = 2.751 (3) Å, N1$\cdots$O3^{iii} = 2.797 (2) Å and N1$\cdots$O2^{iv} = 2.845 (3) Å; symmetry codes: (iii) $-x, y+\frac{1}{2}, -z+1$; (iv) $x, y+1, z$]. Besides these hydrogen-bonding interactions, two kinds of C—H$\cdots\pi$ interactions exist in the crystal; one is a contact between a methine group of an [(*R*)-H_2msa]$^-$ anion and a phenyl group of an [(*S*)-Hpea]$^+$ cation [H1*E*$\cdots$*Cg*^{ii} = 2.62 Å; *Cg* is the centroid of the C6–C12 ring; symmetry code: (ii) $-x, y-\frac{1}{2}, -z+1$], and the other is between a methine group of an [(*S*)-Hpea]$^+$ cation and a phenyl group of a neighbouring cation [H6$\cdots$*Cg*^{v} = 2.85 Å; symmetry code: (v) $-x, y+\frac{1}{2}, -z$] (Fig. 3). The latter interaction connects the two-dimensional grids along the *c* axis, giving a three-dimensional structure in (I).

From these structural features, it is likely that [(*S*)-Hpea]$^+$ selects the *R* isomer of [H_2msa]$^-$ such that each [(*S*)-Hpea]$^+$ ammonium group forms multiple hydrogen bonds with three [H_2msa]$^-$ carboxy groups and that each [(*S*)-Hpea]$^+$ phenyl group forms a C—H$\cdots\pi$ interaction with a [H_2msa]$^-$ methine group, leading to the excellent optical resolution of the racemic H_3msa with the use of (*S*)-pea.

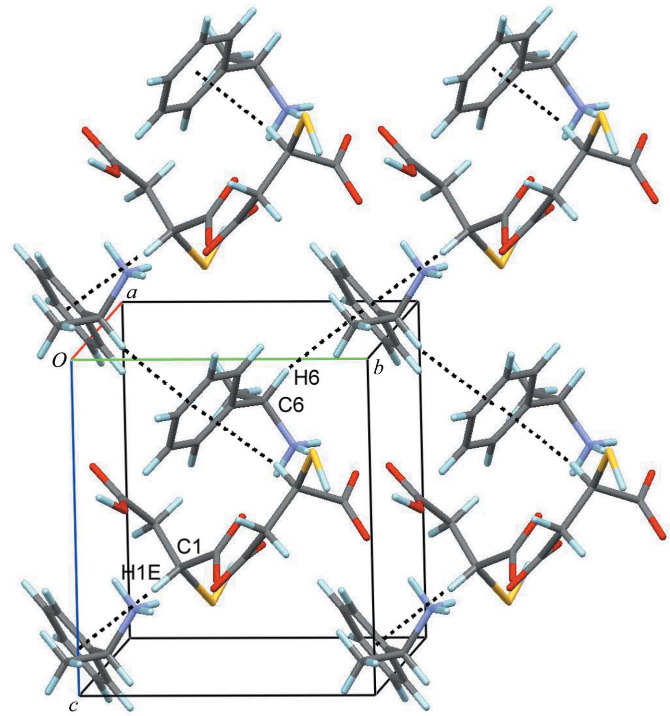


Figure 3
A view of the C—H$\cdots\pi$ interaction network in (I). Dashed lines indicate the C—H$\cdots\pi$ interactions.

Experimental

Compound (I) was prepared according to the method of Shiraiwa *et al.* (1998). (*RS*)-H_3msa (5.0 g, 33 mmol) and (*S*)-pea (4.0 g, 33 mmol) were dissolved in propan-1-ol (27 ml). After allowing the mixture to stand in a freezer for one week, the crude product of (I) (4.6 g) was collected by filtration. This product was dissolved in propan-1-ol at 353 K to give a colourless solution. The solution was cooled slowly to room temperature and colourless plate-shaped crystals of (I) appeared after several hours.

Crystal data

$C_8H_{12}N^+\cdot C_4H_5O_4S^-$
M_r = 271.33
Monoclinic, $P2_1$
a = 9.0547 (7) Å
b = 8.2304 (5) Å
c = 9.3016 (7) Å
β = 92.760 (2)°
V = 692.39 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 200 K
0.30 × 0.15 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min} = 0.788, T_{max} = 0.988
6800 measured reflections
3100 independent reflections
2723 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.107
S = 1.12
3100 reflections
179 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1408 Friedel pairs
Flack parameter: 0.07 (8)

Table 1
Selected bond lengths (Å).

S1—C1	1.817 (2)	O3—C4	1.276 (2)
O1—C3	1.297 (3)	O4—C4	1.237 (3)
O2—C3	1.213 (3)		

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

Cg is the centroid of the C6–C12 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
S1—H1$\cdots$O2^{i}	1.24 (3)	2.16 (3)	3.2741 (19)	148.0 (19)
O1—H1$A\cdots$O3^{ii}	0.96 (3)	1.54 (3)	2.501 (2)	177 (3)
N1—H1$B\cdots$O4	0.94 (2)	1.84 (2)	2.751 (3)	162 (3)
N1—H1$C\cdots$O3^{iii}	0.92 (2)	1.94 (2)	2.797 (2)	154 (3)
N1—H1$D\cdots$O2^{iv}	0.89 (2)	2.10 (2)	2.845 (3)	141 (3)
C1—H1$E\cdots Cg^{ii}$	1.00	2.62	3.56	156
C6—H6$\cdots Cg^{v}$	1.00	2.85	3.83	166

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

H atoms bound to C atoms were placed at calculated positions [C—H = 0.98 (CH_3), 0.99 (CH_2) and 1.00 Å (CH)] and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ for CH_2 and CH groups, and $1.5U_{eq}(C)$ for methyl groups (rotating group model). H atoms bound to O and S atoms were located in a difference Fourier map and were refined with constrained displacement parameters [$U_{iso}(H) = 1.2U_{eq}(O,S)$]. H atoms bound to N atoms were located in a difference Fourier map and refined with distance restraints and constrained displacement parameters [N—H = 0.89 (2) Å and $U_{iso}(H) = 1.5U_{eq}(N)$].

Data collection: *RAPID-AUTO* (Rigaku, 2000); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Yadokari-XG 2009* (Kabuto *et al.*, 2009); software used to prepare material for publication: *Yadokari-XG 2009*.

This work was supported by a Grant-in-Aid for Science Research (grant No. 23350026) from the Ministry of Education, Culture, Sports, Science and Technology of Japan, and by Izumi Science and Technology Foundation.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: UK3047). Services for accessing these data are described at the back of the journal.

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supplementary materials

Acta Cryst. (2012). C**68**, o332–o334   [doi:10.1107/S0108270112032933]

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Crystal data

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$M_r = 271.33$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 9.0547$ (7) Å
$b = 8.2304$ (5) Å
$c = 9.3016$ (7) Å
$\beta = 92.760$ (2)°
$V = 692.39$ (9) Å^3
$Z = 2$
$F(000) = 288$
$D_x = 1.301$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 4466 reflections
$\theta = 3.1$–27.5°
$\mu = 0.24$ mm^{-1}
$T = 200$ K
Platelet, colourless
0.30 × 0.15 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotating-anode X-ray tube
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Rigaku, 1995)
$T_{min} = 0.788$, $T_{max} = 0.988$
6800 measured reflections
3100 independent reflections
2723 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.107$
$S = 1.12$
3100 reflections
179 parameters
4 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 0.051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Absolute structure: Flack (1983), 1408 Friedel pairs
Flack parameter: 0.07 (8)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.42305 (6)	0.38313 (8)	0.79560 (6)	0.04537 (17)
H1	0.498 (3)	0.440 (3)	0.700 (3)	0.054*
O1	0.10777 (16)	0.1497 (2)	0.46721 (18)	0.0386 (4)
H1A	0.041 (3)	0.076 (4)	0.418 (3)	0.046*
O2	0.28726 (19)	0.0139 (3)	0.3674 (3)	0.0688 (7)
O3	0.06554 (15)	0.46249 (17)	0.66908 (16)	0.0358 (3)
O4	0.23275 (17)	0.5239 (2)	0.50889 (17)	0.0421 (4)
N1	0.1426 (2)	0.7201 (2)	0.2819 (2)	0.0361 (4)
H1B	0.154 (3)	0.658 (3)	0.367 (2)	0.054*
H1C	0.056 (2)	0.777 (3)	0.284 (3)	0.054*
H1D	0.220 (2)	0.786 (3)	0.287 (3)	0.054*
C1	0.2845 (2)	0.3014 (3)	0.6675 (2)	0.0320 (4)
H1E	0.2202	0.2255	0.7206	0.038*
C2	0.3547 (2)	0.2056 (3)	0.5492 (3)	0.0374 (5)
H2	0.4108	0.2815	0.4898	0.045*
H2A	0.4261	0.1273	0.5940	0.045*
C3	0.2457 (2)	0.1138 (3)	0.4524 (2)	0.0363 (5)
C4	0.1875 (2)	0.4410 (2)	0.6086 (2)	0.0310 (4)
C5	0.2609 (3)	0.5042 (4)	0.1466 (4)	0.0635 (8)
H5	0.2557	0.4299	0.2286	0.095*
H5A	0.3537	0.5654	0.1548	0.095*
H5B	0.2568	0.4416	0.0569	0.095*
C6	0.1313 (3)	0.6215 (3)	0.1460 (2)	0.0422 (5)
H6	0.1394	0.6971	0.0626	0.051*
C7	−0.0189 (2)	0.5413 (2)	0.1337 (2)	0.0339 (4)
C8	−0.1179 (3)	0.5811 (3)	0.0209 (3)	0.0444 (5)
H8	−0.0892	0.6555	−0.0507	0.053*
C9	−0.2589 (3)	0.5132 (4)	0.0114 (3)	0.0526 (6)
H9	−0.3263	0.5426	−0.0657	0.063*
C10	−0.3007 (2)	0.4033 (3)	0.1138 (3)	0.0470 (6)
H10	−0.3970	0.3574	0.1077	0.056*
C11	−0.2021 (2)	0.3603 (3)	0.2254 (3)	0.0420 (5)
H11	−0.2308	0.2844	0.2957	0.050*
C12	−0.0616 (2)	0.4273 (2)	0.2353 (2)	0.0354 (5)
H12	0.0060	0.3956	0.3114	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0360 (3)	0.0627 (4)	0.0367 (3)	−0.0065 (3)	−0.0065 (2)	−0.0025 (3)
O1	0.0312 (7)	0.0395 (8)	0.0447 (9)	0.0006 (6)	−0.0028 (6)	−0.0084 (7)
O2	0.0384 (9)	0.0769 (14)	0.0922 (16)	−0.0091 (10)	0.0151 (9)	−0.0504 (13)
O3	0.0322 (7)	0.0350 (7)	0.0402 (8)	0.0034 (6)	0.0029 (6)	0.0012 (7)
O4	0.0401 (8)	0.0445 (8)	0.0420 (9)	0.0004 (7)	0.0040 (7)	0.0079 (7)
N1	0.0380 (10)	0.0339 (9)	0.0367 (10)	−0.0040 (8)	0.0042 (8)	−0.0038 (8)
C1	0.0273 (9)	0.0361 (10)	0.0322 (10)	−0.0032 (8)	−0.0010 (8)	−0.0001 (9)
C2	0.0267 (9)	0.0402 (11)	0.0451 (12)	0.0009 (8)	−0.0003 (9)	−0.0031 (10)
C3	0.0324 (10)	0.0357 (11)	0.0410 (12)	−0.0029 (8)	0.0055 (9)	−0.0045 (9)
C4	0.0304 (9)	0.0319 (9)	0.0302 (10)	−0.0035 (8)	−0.0039 (8)	−0.0038 (8)
C5	0.0436 (13)	0.0740 (19)	0.0746 (19)	−0.0067 (14)	0.0206 (13)	−0.0354 (17)
C6	0.0494 (13)	0.0451 (13)	0.0331 (11)	−0.0123 (11)	0.0117 (9)	−0.0058 (10)
C7	0.0421 (11)	0.0303 (10)	0.0294 (10)	0.0003 (9)	0.0036 (8)	−0.0044 (8)
C8	0.0616 (14)	0.0388 (12)	0.0322 (11)	−0.0003 (11)	−0.0033 (10)	−0.0002 (9)
C9	0.0566 (15)	0.0544 (14)	0.0449 (13)	0.0085 (12)	−0.0177 (11)	−0.0060 (13)
C10	0.0379 (11)	0.0470 (14)	0.0559 (13)	−0.0016 (11)	−0.0021 (9)	−0.0098 (13)
C11	0.0437 (11)	0.0369 (11)	0.0457 (12)	−0.0023 (10)	0.0072 (9)	−0.0007 (11)
C12	0.0382 (10)	0.0341 (11)	0.0339 (10)	0.0032 (8)	0.0008 (8)	0.0014 (8)

Geometric parameters (Å, º)

S1—C1	1.817 (2)	C5—C6	1.519 (4)
S1—H1	1.24 (3)	C5—H5	0.9800
O1—C3	1.297 (3)	C5—H5A	0.9800
O1—H1A	0.96 (3)	C5—H5B	0.9800
O2—C3	1.213 (3)	C6—C7	1.511 (3)
O3—C4	1.276 (2)	C6—H6	1.0000
O4—C4	1.237 (3)	C7—C8	1.386 (3)
N1—C6	1.501 (3)	C7—C12	1.399 (3)
N1—H1B	0.943 (17)	C8—C9	1.392 (4)
N1—H1C	0.917 (17)	C8—H8	0.9500
N1—H1D	0.886 (17)	C9—C10	1.380 (4)
C1—C2	1.518 (3)	C9—H9	0.9500
C1—C4	1.531 (3)	C10—C11	1.382 (3)
C1—H1E	1.0000	C10—H10	0.9500
C2—C3	1.507 (3)	C11—C12	1.385 (3)
C2—H2	0.9900	C11—H11	0.9500
C2—H2A	0.9900	C12—H12	0.9500
C1—S1—H1	93.1 (13)	H5—C5—H5A	109.5
C3—O1—H1A	113.0 (16)	C6—C5—H5B	109.5
C6—N1—H1B	114.3 (18)	H5—C5—H5B	109.5
C6—N1—H1C	105.7 (18)	H5A—C5—H5B	109.5
H1B—N1—H1C	109 (2)	N1—C6—C7	108.94 (18)
C6—N1—H1D	113.3 (19)	N1—C6—C5	108.6 (2)
H1B—N1—H1D	103 (2)	C7—C6—C5	114.5 (2)
H1C—N1—H1D	111 (3)	N1—C6—H6	108.2

C2—C1—C4	112.52 (18)	C7—C6—H6	108.2
C2—C1—S1	111.56 (14)	C5—C6—H6	108.2
C4—C1—S1	108.82 (14)	C8—C7—C12	118.7 (2)
C2—C1—H1E	107.9	C8—C7—C6	120.0 (2)
C4—C1—H1E	107.9	C12—C7—C6	121.3 (2)
S1—C1—H1E	107.9	C7—C8—C9	120.7 (2)
C3—C2—C1	114.12 (17)	C7—C8—H8	119.6
C3—C2—H2	108.7	C9—C8—H8	119.6
C1—C2—H2	108.7	C10—C9—C8	120.0 (2)
C3—C2—H2A	108.7	C10—C9—H9	120.0
C1—C2—H2A	108.7	C8—C9—H9	120.0
H2—C2—H2A	107.6	C9—C10—C11	119.9 (2)
O2—C3—O1	123.7 (2)	C9—C10—H10	120.1
O2—C3—C2	121.0 (2)	C11—C10—H10	120.1
O1—C3—C2	115.36 (19)	C10—C11—C12	120.4 (2)
O4—C4—O3	125.38 (19)	C10—C11—H11	119.8
O4—C4—C1	118.54 (18)	C12—C11—H11	119.8
O3—C4—C1	116.08 (18)	C11—C12—C7	120.3 (2)
C6—C5—H5	109.5	C11—C12—H12	119.8
C6—C5—H5A	109.5	C7—C12—H12	119.8

C4—C1—C2—C3	−66.1 (2)	N1—C6—C7—C12	−63.2 (3)
S1—C1—C2—C3	171.31 (16)	C5—C6—C7—C12	58.6 (3)
C1—C2—C3—O2	−169.0 (2)	C12—C7—C8—C9	2.1 (3)
C1—C2—C3—O1	11.0 (3)	C6—C7—C8—C9	−177.3 (2)
C2—C1—C4—O4	−41.8 (2)	C7—C8—C9—C10	−0.9 (4)
S1—C1—C4—O4	82.4 (2)	C8—C9—C10—C11	−0.3 (4)
C2—C1—C4—O3	138.90 (18)	C9—C10—C11—C12	0.2 (4)
S1—C1—C4—O3	−96.94 (18)	C10—C11—C12—C7	1.1 (3)
N1—C6—C7—C8	116.3 (2)	C8—C7—C12—C11	−2.2 (3)
C5—C6—C7—C8	−121.9 (3)	C6—C7—C12—C11	177.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
S1—H1···O2^{i}	1.24 (3)	2.16 (3)	3.2741 (19)	148.0 (19)
O1—H1*A*···O3^{ii}	0.96 (3)	1.54 (3)	2.501 (2)	177 (3)
N1—H1*B*···O4	0.94 (2)	1.84 (2)	2.751 (3)	162 (3)
N1—H1*C*···O3^{iii}	0.92 (2)	1.94 (2)	2.797 (2)	154 (3)
N1—H1*D*···O2^{iv}	0.89 (2)	2.10 (2)	2.845 (3)	141 (3)
C1—H1*E*···*Cg*^{ii}	1.00	2.62	3.56	156
C6—H6···*Cg*^{v}	1.00	2.85	3.83	166

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1; (ii) −*x*, *y*−1/2, −*z*+1; (iii) −*x*, *y*+1/2, −*z*+1; (iv) *x*, *y*+1, *z*; (v) −*x*, *y*+1/2, −*z*.