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# 2,3-[(3,6-Dioxaoctane-1,8-diyl)bis(sulfanediylmethylene)]-6,7-bis(methylsulfanyl)-1,4,5,8-tetrathiafulvalene

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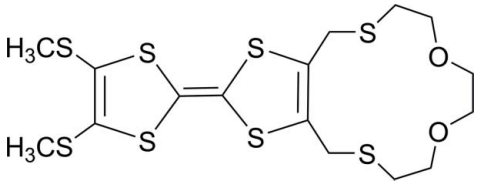
Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.042; $wR$ factor = 0.128; data-to-parameter ratio = 16.7.

In the title molecule, $C_{16}H_{22}S_8O_2$, two S atoms, two O atoms and ten C atoms form a 14-membered ring with a boat conformation. In the crystal, C—H···O hydrogen bonds link the molecules into dimers which are further connected into a chain along the *a* axis by C—H···S hydrogen bonds.

## Related literature

Over the past three decades, chemical groups such as crown ethers have been extensively modified on the tetrathiafulvalene (TTF) skeleton, see: Jeppesen & Becher (2003). For details of the synthesis, see: Chen *et al.* (2005). For a related structure, see: Hou *et al.* (2009).



## Experimental

### Crystal data

$C_{16}H_{22}O_2S_8$
$M_r$ = 502.82
Triclinic, $P\overline{1}$
$a$ = 9.1748 (18) Å
$b$ = 10.177 (2) Å
$c$ = 14.273 (3) Å
$\alpha$ = 98.49 (3)°
$\beta$ = 105.58 (3)°
$\gamma$ = 113.33 (3)°
$V$ = 1129.1 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.80 mm$^{-1}$
$T$ = 291 K
0.14 × 0.12 × 0.12 mm

### Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.896, $T_{max}$ = 0.910
8752 measured reflections
3948 independent reflections
3345 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
$S$ = 1.17
3948 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$A$···S5$^{i}$ | 0.97 | 2.94 | 3.762 (5) | 143 |
| C1—H1$C$···O2$^{ii}$ | 0.96 | 2.49 | 3.379 (6) | 154 |

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2569).

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# supporting information

*Acta Cryst.* (2009). E**65**, o2783 [https://doi.org/10.1107/S1600536809041804]

## 2,3-[(3,6-Dioxaoctane-1,8-diyl)bis(sulfanediylmethylene)]-6,7-bis(methylsulfanyl)-1,4,5,8-tetrathiafulvalene

**Rui-Bin Hou, Bao Li, Tie Chen, Bing-Zhu Yin and Li-Xin Wu**

### S1. Comment

Over the past three decades, chemical groups such as crown ethers have been extensively modified on the tetrathiafulvalene (TTF) skeleton (Jeppesen *et al.*, 2003). A series of different type and different ring size TTF crown ether derivatives (containing nitrogen, sulfur and thia-aza atoms), aiming at molecular sensors, switches and wires in which TTF was used as an organic redox-active unit in host–guest system and crown ether was used as the choice of ligand system suitable as an "antenna". In order to get a novel and promising ion sensor, we have designed and synthesized the TTF - crown ether title compound, (I).

In the structure (I) (Fig. 1) all bond lengths and angles are normal and comparable with those reported for the related structure (Hou *et al.*, 2009). In the crystal lattice, two molecules form a dimer by C—H···O hydrogen bonds, involving one O atom of the crown ether as acceptors, and the methylene C—H groups as donors (Table 1). The intermolecular C—H···S hydrogen bonds link the dimers into one-dimensional chain along the *a* axis.

### S2. Experimental

The title compound, (I), was prepared according to literature (Chen *et al.*, 2005) and single crystals suitable for X-ray diffraction were prepared by slow evaporation a mixture of dichloromethane and petroleum (60–90°C) at room temperature.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.96-0.97Å) and were included in the refinement in the riding model with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C).

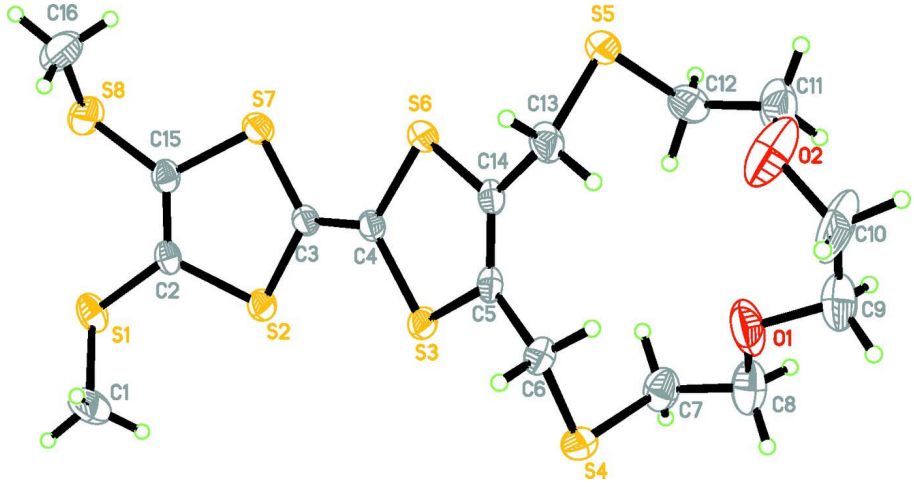


**Figure 1**

The asymmetric of title compound, with the atom numbering. Displacement ellipsoids of non-H atoms are drawn at the 30% probability level.

**2,3-[(3,6-Dioxaoctane-1,8-diyl)bis(sulfanediylmethylene)]-6,7- bis(methylsulfanyl)-1,4,5,8-tetrathiafulvalene**

*Crystal data*

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$\gamma = 113.33\ (3)°$
$V = 1129.1\ (4)$ Å$^3$
$Z = 2$
$F(000) = 524$
$D_x = 1.479$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9031 reflections
$\theta = 3.1–27.5°$
$\mu = 0.80$ mm$^{-1}$
$T = 291$ K
Block, yellow
0.14 × 0.12 × 0.12 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.896$, $T_{max} = 0.910$
8752 measured reflections
3948 independent reflections
3345 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -10\rightarrow10$
$k = -12\rightarrow12$
$l = -16\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.128$
$S = 1.17$
3948 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 0.3957P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.011$

$\Delta\rho_{max} = 0.89$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ e Å$^{-3}$

*Special details*

**Experimental**. (See detailed section in the paper)

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 1.3188 (5) | 1.3283 (5) | 1.4807 (3) | 0.0753 (11) |
| H1A | 1.3746 | 1.2709 | 1.4639 | 0.113* |
| H1B | 1.3938 | 1.4078 | 1.5421 | 0.113* |
| H1C | 1.2897 | 1.3696 | 1.4264 | 0.113* |
| C2 | 1.0102 (4) | 1.0784 (3) | 1.3801 (2) | 0.0407 (6) |
| C3 | 0.9324 (3) | 0.8957 (3) | 1.2084 (2) | 0.0391 (6) |
| C4 | 0.9441 (3) | 0.8476 (3) | 1.1199 (2) | 0.0385 (6) |
| C5 | 1.0573 (4) | 0.8202 (3) | 0.9740 (2) | 0.0390 (6) |
| C6 | 1.1888 (4) | 0.8549 (3) | 0.9252 (2) | 0.0468 (7) |
| H6A | 1.2329 | 0.9591 | 0.9262 | 0.056* |
| H6B | 1.1347 | 0.7950 | 0.8548 | 0.056* |
| C7 | 1.2681 (5) | 0.6217 (4) | 0.9544 (3) | 0.0651 (9) |
| H7A | 1.3327 | 0.5927 | 1.0056 | 0.078* |
| H7B | 1.1542 | 0.5855 | 0.9562 | 0.078* |
| C8 | 1.2573 (7) | 0.5487 (5) | 0.8545 (4) | 0.0880 (13) |
| H8A | 1.3674 | 0.5934 | 0.8475 | 0.106* |
| H8B | 1.2227 | 0.4433 | 0.8467 | 0.106* |
| C9 | 1.0860 (8) | 0.4660 (7) | 0.6849 (4) | 0.1128 (19) |
| H9A | 1.1787 | 0.4945 | 0.6595 | 0.135* |
| H9B | 1.0565 | 0.3662 | 0.6920 | 0.135* |
| C10 | 0.9459 (9) | 0.4676 (9) | 0.6175 (4) | 0.131 (3) |
| H10A | 0.8974 | 0.3828 | 0.5580 | 0.157* |
| H10B | 0.9870 | 0.5570 | 0.5958 | 0.157* |
| C11 | 0.7180 (7) | 0.3431 (5) | 0.6827 (4) | 0.0914 (14) |
| H11A | 0.7741 | 0.2801 | 0.6902 | 0.110* |
| H11B | 0.6044 | 0.2836 | 0.6321 | 0.110* |
| C12 | 0.7074 (4) | 0.4011 (4) | 0.7818 (3) | 0.0623 (9) |
| H12A | 0.8214 | 0.4560 | 0.8325 | 0.075* |
| H12B | 0.6441 | 0.3173 | 0.8033 | 0.075* |
| C13 | 0.7897 (4) | 0.7058 (4) | 0.8160 (2) | 0.0529 (7) |
| H13A | 0.8643 | 0.7022 | 0.7798 | 0.063* |

| | | | | |
|---|---|---|---|---|
| H13B | 0.7503 | 0.7771 | 0.7975 | 0.063* |
| C14 | 0.8897 (4) | 0.7596 (3) | 0.9285 (2) | 0.0396 (6) |
| C15 | 0.8397 (4) | 1.0198 (3) | 1.3351 (2) | 0.0443 (6) |
| C16 | 0.5893 (6) | 1.1099 (6) | 1.2868 (4) | 0.0912 (14) |
| H16A | 0.6654 | 1.1911 | 1.2698 | 0.137* |
| H16B | 0.5123 | 1.1380 | 1.3080 | 0.137* |
| H16C | 0.5258 | 1.0238 | 1.2283 | 0.137* |
| O1 | 1.1364 (5) | 0.5674 (4) | 0.7799 (2) | 0.0980 (10) |
| O2 | 0.8095 (6) | 0.4633 (5) | 0.6516 (3) | 0.1180 (14) |
| S1 | 1.12983 (11) | 1.21034 (9) | 1.49854 (6) | 0.0562 (2) |
| S2 | 1.10990 (9) | 0.99321 (8) | 1.32208 (5) | 0.0452 (2) |
| S3 | 1.13813 (9) | 0.87356 (9) | 1.10784 (5) | 0.0456 (2) |
| S4 | 1.36459 (10) | 0.82043 (9) | 0.98642 (7) | 0.0545 (2) |
| S5 | 0.60655 (10) | 0.52141 (11) | 0.77587 (7) | 0.0664 (3) |
| S6 | 0.76769 (9) | 0.74362 (8) | 1.00707 (5) | 0.0456 (2) |
| S7 | 0.74108 (9) | 0.86596 (9) | 1.22600 (6) | 0.0486 (2) |
| S8 | 0.71029 (12) | 1.06618 (12) | 1.38866 (7) | 0.0675 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.062 (2) | 0.072 (3) | 0.051 (2) | 0.0072 (19) | 0.0037 (16) | −0.0007 (18) |
| C2 | 0.0527 (16) | 0.0355 (14) | 0.0323 (14) | 0.0190 (12) | 0.0161 (12) | 0.0072 (11) |
| C3 | 0.0420 (14) | 0.0340 (14) | 0.0362 (14) | 0.0157 (12) | 0.0118 (11) | 0.0049 (11) |
| C4 | 0.0411 (14) | 0.0338 (14) | 0.0360 (14) | 0.0174 (11) | 0.0103 (11) | 0.0037 (11) |
| C5 | 0.0522 (16) | 0.0361 (14) | 0.0335 (14) | 0.0279 (13) | 0.0129 (12) | 0.0057 (11) |
| C6 | 0.0524 (16) | 0.0505 (17) | 0.0488 (17) | 0.0315 (14) | 0.0221 (13) | 0.0149 (14) |
| C7 | 0.082 (2) | 0.054 (2) | 0.076 (2) | 0.0400 (19) | 0.037 (2) | 0.0251 (18) |
| C8 | 0.121 (4) | 0.068 (3) | 0.091 (3) | 0.057 (3) | 0.046 (3) | 0.013 (2) |
| C9 | 0.122 (4) | 0.122 (4) | 0.080 (3) | 0.051 (4) | 0.046 (3) | −0.016 (3) |
| C10 | 0.187 (6) | 0.230 (8) | 0.069 (3) | 0.164 (6) | 0.076 (4) | 0.046 (4) |
| C11 | 0.117 (4) | 0.077 (3) | 0.089 (3) | 0.063 (3) | 0.030 (3) | 0.008 (2) |
| C12 | 0.0570 (19) | 0.054 (2) | 0.062 (2) | 0.0141 (16) | 0.0183 (16) | 0.0165 (17) |
| C13 | 0.0618 (18) | 0.0575 (19) | 0.0353 (16) | 0.0327 (16) | 0.0074 (13) | 0.0055 (14) |
| C14 | 0.0506 (15) | 0.0340 (14) | 0.0346 (14) | 0.0240 (12) | 0.0116 (12) | 0.0046 (11) |
| C15 | 0.0539 (16) | 0.0419 (16) | 0.0398 (15) | 0.0208 (13) | 0.0233 (13) | 0.0099 (12) |
| C16 | 0.073 (3) | 0.117 (4) | 0.094 (3) | 0.062 (3) | 0.026 (2) | 0.014 (3) |
| O1 | 0.123 (3) | 0.077 (2) | 0.0679 (19) | 0.0270 (19) | 0.0434 (18) | −0.0154 (15) |
| O2 | 0.174 (4) | 0.173 (4) | 0.125 (3) | 0.139 (3) | 0.107 (3) | 0.092 (3) |
| S1 | 0.0735 (5) | 0.0488 (5) | 0.0330 (4) | 0.0198 (4) | 0.0176 (4) | 0.0014 (3) |
| S2 | 0.0465 (4) | 0.0487 (4) | 0.0353 (4) | 0.0234 (3) | 0.0099 (3) | 0.0029 (3) |
| S3 | 0.0433 (4) | 0.0557 (5) | 0.0351 (4) | 0.0277 (3) | 0.0082 (3) | 0.0015 (3) |
| S4 | 0.0418 (4) | 0.0531 (5) | 0.0658 (5) | 0.0231 (4) | 0.0160 (4) | 0.0109 (4) |
| S5 | 0.0432 (4) | 0.0805 (6) | 0.0507 (5) | 0.0237 (4) | 0.0052 (3) | −0.0148 (4) |
| S6 | 0.0404 (4) | 0.0461 (4) | 0.0384 (4) | 0.0164 (3) | 0.0089 (3) | −0.0005 (3) |
| S7 | 0.0433 (4) | 0.0459 (4) | 0.0454 (4) | 0.0121 (3) | 0.0176 (3) | 0.0029 (3) |
| S8 | 0.0690 (5) | 0.0832 (7) | 0.0609 (6) | 0.0388 (5) | 0.0379 (4) | 0.0115 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—S1 | 1.786 (4) | C9—C10 | 1.391 (8) |
| C1—H1A | 0.9600 | C9—O1 | 1.410 (5) |
| C1—H1B | 0.9600 | C9—H9A | 0.9700 |
| C1—H1C | 0.9600 | C9—H9B | 0.9700 |
| C2—C15 | 1.351 (4) | C10—O2 | 1.448 (6) |
| C2—S1 | 1.741 (3) | C10—H10A | 0.9700 |
| C2—S2 | 1.760 (3) | C10—H10B | 0.9700 |
| C3—C4 | 1.335 (4) | C11—O2 | 1.394 (6) |
| C3—S7 | 1.753 (3) | C11—C12 | 1.493 (6) |
| C3—S2 | 1.759 (3) | C11—H11A | 0.9700 |
| C4—S6 | 1.753 (3) | C11—H11B | 0.9700 |
| C4—S3 | 1.753 (3) | C12—S5 | 1.802 (4) |
| C5—C14 | 1.327 (4) | C12—H12A | 0.9700 |
| C5—C6 | 1.500 (4) | C12—H12B | 0.9700 |
| C5—S3 | 1.763 (3) | C13—C14 | 1.506 (4) |
| C6—S4 | 1.809 (3) | C13—S5 | 1.828 (4) |
| C6—H6A | 0.9700 | C13—H13A | 0.9700 |
| C6—H6B | 0.9700 | C13—H13B | 0.9700 |
| C7—C8 | 1.465 (6) | C14—S6 | 1.767 (3) |
| C7—S4 | 1.782 (4) | C15—S8 | 1.744 (3) |
| C7—H7A | 0.9700 | C15—S7 | 1.760 (3) |
| C7—H7B | 0.9700 | C16—S8 | 1.806 (5) |
| C8—O1 | 1.411 (6) | C16—H16A | 0.9600 |
| C8—H8A | 0.9700 | C16—H16B | 0.9600 |
| C8—H8B | 0.9700 | C16—H16C | 0.9600 |
| | | | |
| S1—C1—H1A | 109.5 | O2—C10—H10A | 107.7 |
| S1—C1—H1B | 109.5 | C9—C10—H10B | 107.7 |
| H1A—C1—H1B | 109.5 | O2—C10—H10B | 107.7 |
| S1—C1—H1C | 109.5 | H10A—C10—H10B | 107.1 |
| H1A—C1—H1C | 109.5 | O2—C11—C12 | 109.1 (4) |
| H1B—C1—H1C | 109.5 | O2—C11—H11A | 109.9 |
| C15—C2—S1 | 124.6 (2) | C12—C11—H11A | 109.9 |
| C15—C2—S2 | 116.2 (2) | O2—C11—H11B | 109.9 |
| S1—C2—S2 | 118.48 (17) | C12—C11—H11B | 109.9 |
| C4—C3—S7 | 124.5 (2) | H11A—C11—H11B | 108.3 |
| C4—C3—S2 | 123.0 (2) | C11—C12—S5 | 113.1 (3) |
| S7—C3—S2 | 112.44 (15) | C11—C12—H12A | 109.0 |
| C3—C4—S6 | 123.6 (2) | S5—C12—H12A | 108.9 |
| C3—C4—S3 | 122.6 (2) | C11—C12—H12B | 108.9 |
| S6—C4—S3 | 113.75 (15) | S5—C12—H12B | 109.0 |
| C14—C5—C6 | 127.7 (3) | H12A—C12—H12B | 107.8 |
| C14—C5—S3 | 116.9 (2) | C14—C13—S5 | 113.2 (2) |
| C6—C5—S3 | 115.3 (2) | C14—C13—H13A | 108.9 |
| C5—C6—S4 | 113.8 (2) | S5—C13—H13A | 108.9 |
| C5—C6—H6A | 108.8 | C14—C13—H13B | 108.9 |

| | | | |
|---|---|---|---|
| S4—C6—H6A | 108.8 | S5—C13—H13B | 108.9 |
| C5—C6—H6B | 108.8 | H13A—C13—H13B | 107.7 |
| S4—C6—H6B | 108.8 | C5—C14—C13 | 127.3 (3) |
| H6A—C6—H6B | 107.7 | C5—C14—S6 | 117.3 (2) |
| C8—C7—S4 | 114.3 (3) | C13—C14—S6 | 115.4 (2) |
| C8—C7—H7A | 108.7 | C2—C15—S8 | 124.2 (2) |
| S4—C7—H7A | 108.7 | C2—C15—S7 | 116.8 (2) |
| C8—C7—H7B | 108.7 | S8—C15—S7 | 118.15 (17) |
| S4—C7—H7B | 108.7 | S8—C16—H16A | 109.5 |
| H7A—C7—H7B | 107.6 | S8—C16—H16B | 109.5 |
| O1—C8—C7 | 108.0 (3) | H16A—C16—H16B | 109.5 |
| O1—C8—H8A | 110.1 | S8—C16—H16C | 109.5 |
| C7—C8—H8A | 110.1 | H16A—C16—H16C | 109.5 |
| O1—C8—H8B | 110.1 | H16B—C16—H16C | 109.5 |
| C7—C8—H8B | 110.1 | C9—O1—C8 | 110.0 (4) |
| H8A—C8—H8B | 108.4 | C11—O2—C10 | 121.3 (4) |
| C10—C9—O1 | 108.7 (5) | C2—S1—C1 | 102.60 (16) |
| C10—C9—H9A | 109.9 | C3—S2—C2 | 94.09 (13) |
| O1—C9—H9A | 109.9 | C4—S3—C5 | 94.92 (13) |
| C10—C9—H9B | 109.9 | C7—S4—C6 | 102.45 (18) |
| O1—C9—H9B | 109.9 | C12—S5—C13 | 101.68 (16) |
| H9A—C9—H9B | 108.3 | C4—S6—C14 | 94.74 (13) |
| C9—C10—O2 | 118.5 (4) | C3—S7—C15 | 93.90 (14) |
| C9—C10—H10A | 107.7 | C15—S8—C16 | 101.88 (18) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*A*···S5$^{i}$ | 0.97 | 2.94 | 3.762 (5) | 143 |
| C1—H1*C*···O2$^{ii}$ | 0.96 | 2.49 | 3.379 (6) | 154 |

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