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# 6,6′-Dihydroxy-3,3′-dithiodibenzoic acid

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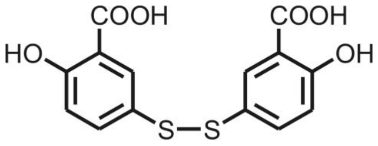
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.045; $wR$ factor = 0.103; data-to-parameter ratio = 11.9.

In the title compound, $C_{14}H_{10}O_6S_2$, the dihedral angle between the planes of the two phenylene rings is 55.9 (1)°. Both hydroxy groups form intramolecular hydrogen bonds; however, one of them also engages in intermolecular hydrogen bonding. In the crystal, molecules are connected into helical chains by O—H···O hydrogen bonds. The crystal studied was an inversion twin with a domain ratio of 0.51 (13):0.49 (13).

## Related literature

For hydrogen bonds and $\pi$–$\pi$ stacking interactions in aromatic compounds, see: Janiak (2000); Hunter & Sanders (1990); Orr *et al.* (1999); Kaafarani *et al.* (2001). For a comparison of bond dimensions for disulfide compounds, see: Kaitner & Pavlovic (1997); Korp & Bernal (1984); Ni *et al.* (2004); Sacerdoti *et al.* (1975).



## Experimental

### *Crystal data*

$C_{14}H_{10}O_6S_2$
$M_r$ = 338.34
Orthorhombic, $P2_12_12_1$
$a$ = 5.3065 (6) Å
$b$ = 11.1657 (13) Å
$c$ = 23.906 (2) Å
$V$ = 1416.5 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.40 mm$^{-1}$
$T$ = 298 K
0.24 × 0.15 × 0.14 mm

### *Data collection*

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\min}$ = 0.910, $T_{\max}$ = 0.946
6436 measured reflections
2502 independent reflections
2060 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.043

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.103
$S$ = 1.09
2502 reflections
211 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ = 0.40 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.28 e Å$^{-3}$
Absolute structure: Flack (1983), 1007 Friedel pairs
Flack parameter: 0.49 (13)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O5$^{\rm i}$ | 0.85 (3) | 1.90 (3) | 2.739 (4) | 171 (4) |
| O3—H3···O1 | 0.84 (4) | 1.91 (5) | 2.616 (4) | 142 (5) |
| O3—H3···O6$^{\rm ii}$ | 0.84 (4) | 2.52 (4) | 3.063 (5) | 123 (4) |
| O4—H4···O1$^{\rm iii}$ | 0.85 (4) | 1.79 (4) | 2.636 (4) | 175 (4) |
| O6—H6···O5 | 0.85 (4) | 1.90 (4) | 2.642 (4) | 146 (5) |

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We are grateful to Professor Da-QI Wang, Liaocheng University, for the X-ray structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2599).

## References

Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hunter, C. A. & Sanders, J. K. (1990). *J. Am. Chem. Soc.* **112**, 5525–5534.
Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.
Kaafarani, B. R., Pinkerton, A. A. & Neckers, D. C. (2001). *Tetrahedron Lett.* **42**, 8137–8139.
Kaitner, B. & Pavlovic, G. (1997). *Acta Cryst.* C**53**, 1103–1105.
Korp, J. D. & Bernal, I. (1984). *J. Mol. Struct.* **118**, 157–164.
Ni, Q.-L., Wang, X.-J., Zeng, J.-Q. & Jian, H.-X. (2004). *Acta Cryst.* E**60**, o2318–o2320.
Orr, G. W., Barbour, L. J. & Atwood, J. L. (1999). *Science*, **285**, 1049–1052.
Sacerdoti, M., Gilli, G. & Domiano, P. (1975). *Acta Cryst.* B**31**, 327–329.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2009). E**65**, o1701    [doi:10.1107/S1600536809023757]

## 6,6′-Dihydroxy-3,3′-dithiodibenzoic acid

**Shu-Wen Sun, Fu-Lin Zhou, Gao-Feng Wang and Gui-Hua Cui**

### S1. Comment

Hydrogen bonds and *π–π* stacking interactions play an important role in the self-assembly and recognition of aromatic compounds((Janiak, 2000; Hunter & Sanders, 1990) as an auxiliary stabilizing short contact (Orr *et al.*, 1999; Kaafarani *et al.*, 2001).

The two phenyl rings of the title compound are bonded with two S atoms at a distance of 1.781 (4)Å (S2—C13) and 1.793 (4) Å (S1—C6), and the C—C distances of two phenyl groups range from 1.371 (5) to 1.407 (6) Å (Figure. 1 and Table 1). Interestingly, there are intermolecular S···S interactions in the crystal structures, which are not common in diphenyl disulfide derivaties (Korp & Bernal, 1984; Kaitner & Pavlovic 1997; Ni *et al.*, 2004; Sacerdoti *et al.*, 1975). The intermolecular S···S interactions distance is 3.414 (2) Å, whereas the shorter intramolecular S—S distance is 2.051 (2) Å. The dihedral angle of these two phenyl rings is 55.9 (1)°, which is different from other molecules such as 4, 4′-dithiodiphenol (48.1 (2)°) (Ni *et al.*, 2004) and diphenyl disulfide (76.7 (3)°) (Sacerdoti *et al.*, 1975).

The crystal structure of 5, 5′-dithiodisalicylic acid demonstrates the self-assembly of molecules into three dimensional networks *via* hydrogen bonds(Table 2) and intermolecular S···S interactions.

### S2. Experimental

The title compound (I) was prepared as follows: To a solution of 5-(chlorosulfonyl)-2-hydroxybenzoic acid(19 mmol, 4.5 g) in conc. HCl (30 ml) cooled to 0 °C in an ice bath, Sn(118 mmol, 14.0 g) was added. The reaction mixture was stirred for 12 h and then refluxed for 6 h. The precipitate was separated and dissolved in $Et_2O$. After filtration the organic layer was concentrated under reduced pressure to afford a solid that was subsequently purified by recrystallization using a mixture of EtOH and $H_2O$. Yellow needle crystals of (I) were obtained by slow evaporation from EtOH/acetone/DMSO/DMF(5:1:3:3) after five months. Analysis calculated for $C_{14}H_{10}O_6S_2$: C 49.70, H 2.98%; found: C 49.18, H 2.75%.

### S3. Refinement

All H atoms were placed in calculated positions and treated as riding, with C—H in the range 0.93–0.98 Å and with $U_{iso}(H)=1.2–1.5U_{eq}(C)$.

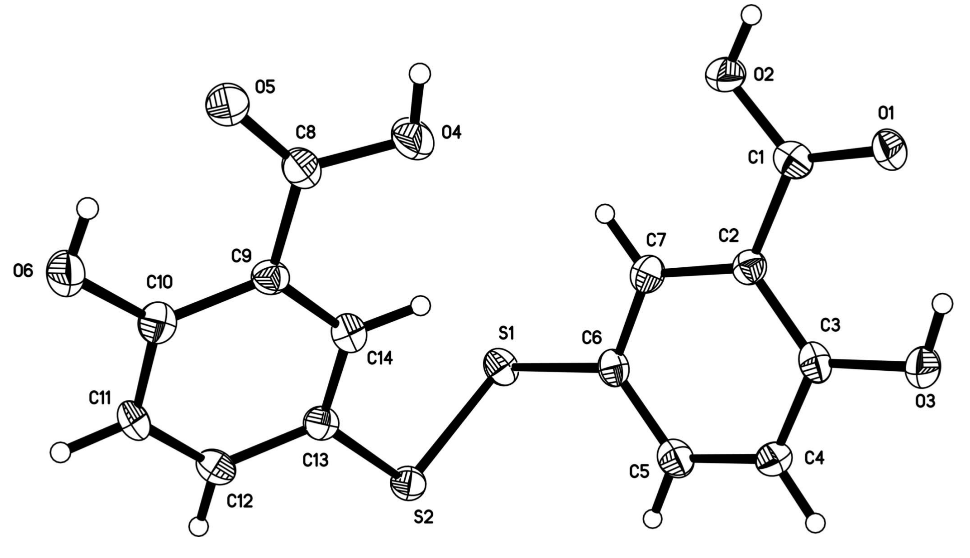


**Figure 1**

The molecular structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

### 6,6′-Dihydroxy-3,3′-dithiodibenzoic acid

*Crystal data*

$C_{14}H_{10}O_6S_2$
$M_r = 338.34$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.3065$ (6) Å
$b = 11.1657$ (13) Å
$c = 23.906$ (2) Å
$V = 1416.5$ (3) Å$^3$
$Z = 4$
$F(000) = 696$
$D_x = 1.587$ Mg m$^{-3}$
Melting point: 523 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2489 reflections
$\theta = 2.5$–$25.5°$
$\mu = 0.40$ mm$^{-1}$
$T = 298$ K
Needle, yellow
$0.24 \times 0.15 \times 0.14$ mm

*Data collection*

Bruker SMART area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.910$, $T_{\max} = 0.946$
6436 measured reflections
2502 independent reflections
2060 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.043$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 1.7°$
$h = -6 \rightarrow 6$
$k = -13 \rightarrow 13$
$l = -28 \rightarrow 12$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.103$
$S = 1.09$
2502 reflections
211 parameters
4 restraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.9484P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å$^{-3}$
$\Delta\rho_{min} = -0.28$ e Å$^{-3}$
Absolute structure: Flack (1983), 1007 Friedel pairs
Absolute structure parameter: 0.49 (13)

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | −0.4934 (6) | 0.8216 (2) | 0.21892 (11) | 0.0439 (7) |
| O2 | −0.6036 (6) | 0.6399 (3) | 0.18732 (11) | 0.0439 (8) |
| H2 | −0.717 (6) | 0.643 (4) | 0.2123 (14) | 0.066* |
| O3 | −0.1299 (6) | 0.9391 (3) | 0.16941 (13) | 0.0519 (8) |
| H3 | −0.254 (6) | 0.934 (5) | 0.1911 (17) | 0.078* |
| O4 | −0.1551 (7) | 0.3528 (3) | 0.20456 (12) | 0.0505 (8) |
| H4 | −0.269 (7) | 0.338 (4) | 0.2286 (15) | 0.076* |
| O5 | −0.0215 (6) | 0.1743 (3) | 0.23556 (11) | 0.0438 (7) |
| O6 | 0.3765 (6) | 0.0759 (3) | 0.18767 (12) | 0.0503 (8) |
| H6 | 0.252 (6) | 0.080 (5) | 0.2099 (17) | 0.075* |
| S1 | −0.0244 (2) | 0.52404 (9) | 0.01641 (4) | 0.0370 (3) |
| S2 | 0.34345 (19) | 0.46809 (9) | 0.01989 (4) | 0.0360 (2) |
| C1 | −0.4622 (8) | 0.7376 (4) | 0.18627 (14) | 0.0343 (9) |
| C2 | −0.2645 (7) | 0.7386 (3) | 0.14288 (15) | 0.0303 (9) |
| C3 | −0.1095 (8) | 0.8396 (3) | 0.13723 (15) | 0.0360 (10) |
| C4 | 0.0804 (8) | 0.8402 (4) | 0.09698 (16) | 0.0391 (10) |
| H4A | 0.1880 | 0.9057 | 0.0942 | 0.047* |
| C5 | 0.1095 (8) | 0.7447 (3) | 0.06154 (16) | 0.0391 (10) |
| H5 | 0.2337 | 0.7470 | 0.0341 | 0.047* |
| C6 | −0.0443 (8) | 0.6441 (3) | 0.06607 (15) | 0.0324 (9) |
| C7 | −0.2280 (8) | 0.6406 (3) | 0.10693 (15) | 0.0339 (9) |
| H7 | −0.3285 | 0.5729 | 0.1107 | 0.041* |
| C8 | −0.0058 (8) | 0.2582 (4) | 0.20199 (16) | 0.0367 (9) |
| C9 | 0.1795 (7) | 0.2604 (3) | 0.15645 (15) | 0.0314 (9) |
| C10 | 0.3593 (8) | 0.1685 (3) | 0.15118 (15) | 0.0356 (9) |
| C11 | 0.5317 (8) | 0.1726 (3) | 0.10729 (16) | 0.0404 (10) |
| H11 | 0.6534 | 0.1130 | 0.1041 | 0.048* |
| C12 | 0.5236 (8) | 0.2640 (3) | 0.06854 (16) | 0.0387 (9) |
| H12 | 0.6396 | 0.2651 | 0.0394 | 0.046* |
| C13 | 0.3440 (8) | 0.3550 (3) | 0.07246 (14) | 0.0312 (9) |
| C14 | 0.1790 (8) | 0.3533 (3) | 0.11681 (15) | 0.0350 (9) |

| | | | | |
|---|---|---|---|---|
| H14 | 0.0637 | 0.4155 | 0.1207 | 0.042* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0515 (18) | 0.0345 (16) | 0.0456 (15) | 0.0031 (16) | 0.0185 (17) | −0.0067 (13) |
| O2 | 0.047 (2) | 0.0394 (16) | 0.0449 (16) | −0.0082 (15) | 0.0179 (15) | −0.0035 (14) |
| O3 | 0.057 (2) | 0.0356 (16) | 0.063 (2) | −0.0068 (15) | 0.0226 (17) | −0.0158 (15) |
| O4 | 0.0540 (19) | 0.0474 (18) | 0.0502 (18) | 0.0124 (17) | 0.0237 (16) | 0.0074 (15) |
| O5 | 0.0474 (18) | 0.0416 (17) | 0.0423 (16) | 0.0038 (16) | 0.0113 (16) | 0.0068 (13) |
| O6 | 0.050 (2) | 0.0404 (17) | 0.0605 (19) | 0.0127 (16) | 0.0138 (17) | 0.0138 (16) |
| S1 | 0.0372 (6) | 0.0428 (5) | 0.0311 (5) | 0.0055 (5) | −0.0017 (5) | −0.0050 (5) |
| S2 | 0.0371 (5) | 0.0370 (5) | 0.0340 (5) | 0.0005 (5) | 0.0064 (5) | 0.0011 (5) |
| C1 | 0.034 (2) | 0.040 (2) | 0.0291 (19) | 0.005 (2) | 0.0003 (19) | 0.0052 (18) |
| C2 | 0.031 (2) | 0.0292 (19) | 0.031 (2) | 0.0008 (18) | −0.0014 (18) | 0.0029 (17) |
| C3 | 0.040 (2) | 0.032 (2) | 0.036 (2) | 0.0092 (19) | 0.002 (2) | −0.0012 (18) |
| C4 | 0.036 (3) | 0.033 (2) | 0.049 (2) | −0.0035 (19) | 0.006 (2) | 0.004 (2) |
| C5 | 0.044 (3) | 0.040 (2) | 0.033 (2) | 0.007 (2) | 0.009 (2) | 0.009 (2) |
| C6 | 0.036 (2) | 0.031 (2) | 0.0302 (19) | 0.0064 (19) | −0.0022 (19) | 0.0001 (16) |
| C7 | 0.039 (2) | 0.031 (2) | 0.032 (2) | 0.0007 (19) | −0.0032 (19) | 0.0034 (17) |
| C8 | 0.032 (2) | 0.038 (2) | 0.040 (2) | 0.003 (2) | −0.001 (2) | −0.0059 (19) |
| C9 | 0.031 (2) | 0.034 (2) | 0.0297 (19) | −0.0025 (18) | 0.0036 (18) | −0.0039 (17) |
| C10 | 0.041 (2) | 0.034 (2) | 0.032 (2) | 0.000 (2) | −0.002 (2) | −0.0023 (17) |
| C11 | 0.034 (2) | 0.034 (2) | 0.052 (2) | 0.011 (2) | 0.009 (2) | −0.0032 (19) |
| C12 | 0.033 (2) | 0.045 (2) | 0.038 (2) | 0.003 (2) | 0.008 (2) | −0.0022 (19) |
| C13 | 0.031 (2) | 0.033 (2) | 0.0293 (19) | −0.0027 (19) | 0.0005 (19) | −0.0065 (17) |
| C14 | 0.035 (2) | 0.035 (2) | 0.035 (2) | 0.0044 (19) | −0.0009 (19) | −0.0021 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.231 (4) | C4—C5 | 1.371 (5) |
| O2—C1 | 1.324 (5) | C4—H4A | 0.9300 |
| O2—H2 | 0.848 (10) | C5—C6 | 1.393 (5) |
| O3—C3 | 1.356 (5) | C5—H5 | 0.9300 |
| O3—H3 | 0.842 (10) | C6—C7 | 1.380 (5) |
| O4—C8 | 1.322 (5) | C7—H7 | 0.9300 |
| O4—H4 | 0.848 (10) | C8—C9 | 1.467 (5) |
| O5—C8 | 1.236 (5) | C9—C14 | 1.405 (5) |
| O6—C10 | 1.356 (4) | C9—C10 | 1.407 (6) |
| O6—H6 | 0.849 (10) | C10—C11 | 1.393 (5) |
| S1—C6 | 1.793 (4) | C11—C12 | 1.380 (5) |
| S1—S2 | 2.0511 (15) | C11—H11 | 0.9300 |
| S2—C13 | 1.781 (4) | C12—C13 | 1.396 (5) |
| C1—C2 | 1.476 (5) | C12—H12 | 0.9300 |
| C2—C3 | 1.402 (5) | C13—C14 | 1.375 (5) |
| C2—C7 | 1.404 (5) | C14—H14 | 0.9300 |
| C3—C4 | 1.394 (5) | | |

| | | | |
|---|---|---|---|
| C1—O2—H2 | 113 (3) | C6—C7—C2 | 120.6 (4) |
| C3—O3—H3 | 111 (4) | C6—C7—H7 | 119.7 |
| C8—O4—H4 | 108 (4) | C2—C7—H7 | 119.7 |
| C10—O6—H6 | 108 (4) | O5—C8—O4 | 122.4 (4) |
| C6—S1—S2 | 104.89 (14) | O5—C8—C9 | 122.7 (4) |
| C13—S2—S1 | 104.24 (14) | O4—C8—C9 | 115.0 (4) |
| O1—C1—O2 | 122.6 (4) | C14—C9—C10 | 118.6 (3) |
| O1—C1—C2 | 122.4 (4) | C14—C9—C8 | 120.8 (4) |
| O2—C1—C2 | 115.0 (3) | C10—C9—C8 | 120.6 (3) |
| C3—C2—C7 | 119.1 (3) | O6—C10—C11 | 117.7 (4) |
| C3—C2—C1 | 119.4 (3) | O6—C10—C9 | 123.0 (3) |
| C7—C2—C1 | 121.5 (3) | C11—C10—C9 | 119.3 (4) |
| O3—C3—C4 | 116.4 (4) | C12—C11—C10 | 120.6 (4) |
| O3—C3—C2 | 123.9 (4) | C12—C11—H11 | 119.7 |
| C4—C3—C2 | 119.6 (4) | C10—C11—H11 | 119.7 |
| C5—C4—C3 | 120.3 (4) | C11—C12—C13 | 121.0 (4) |
| C5—C4—H4A | 119.9 | C11—C12—H12 | 119.5 |
| C3—C4—H4A | 119.9 | C13—C12—H12 | 119.5 |
| C4—C5—C6 | 120.9 (4) | C14—C13—C12 | 118.4 (4) |
| C4—C5—H5 | 119.6 | C14—C13—S2 | 123.6 (3) |
| C6—C5—H5 | 119.6 | C12—C13—S2 | 118.0 (3) |
| C7—C6—C5 | 119.4 (3) | C13—C14—C9 | 121.9 (4) |
| C7—C6—S1 | 119.3 (3) | C13—C14—H14 | 119.0 |
| C5—C6—S1 | 121.1 (3) | C9—C14—H14 | 119.0 |

| | | | |
|---|---|---|---|
| C6—S1—S2—C13 | 89.96 (17) | O5—C8—C9—C14 | 175.4 (4) |
| O1—C1—C2—C3 | −1.7 (5) | O4—C8—C9—C14 | −4.7 (5) |
| O2—C1—C2—C3 | 178.1 (3) | O5—C8—C9—C10 | −3.8 (6) |
| O1—C1—C2—C7 | 178.4 (4) | O4—C8—C9—C10 | 176.1 (4) |
| O2—C1—C2—C7 | −1.7 (5) | C14—C9—C10—O6 | 179.2 (4) |
| C7—C2—C3—O3 | 179.5 (3) | C8—C9—C10—O6 | −1.6 (6) |
| C1—C2—C3—O3 | −0.3 (6) | C14—C9—C10—C11 | 0.4 (6) |
| C7—C2—C3—C4 | −1.3 (6) | C8—C9—C10—C11 | 179.5 (4) |
| C1—C2—C3—C4 | 178.9 (3) | O6—C10—C11—C12 | 179.7 (4) |
| O3—C3—C4—C5 | −178.1 (4) | C9—C10—C11—C12 | −1.4 (6) |
| C2—C3—C4—C5 | 2.7 (6) | C10—C11—C12—C13 | 0.4 (6) |
| C3—C4—C5—C6 | −1.9 (6) | C11—C12—C13—C14 | 1.8 (6) |
| C4—C5—C6—C7 | −0.2 (6) | C11—C12—C13—S2 | −178.8 (3) |
| C4—C5—C6—S1 | 174.9 (3) | S1—S2—C13—C14 | −29.0 (3) |
| S2—S1—C6—C7 | −127.2 (3) | S1—S2—C13—C12 | 151.6 (3) |
| S2—S1—C6—C5 | 57.7 (3) | C12—C13—C14—C9 | −2.9 (6) |
| C5—C6—C7—C2 | 1.5 (6) | S2—C13—C14—C9 | 177.8 (3) |
| S1—C6—C7—C2 | −173.7 (3) | C10—C9—C14—C13 | 1.8 (6) |
| C3—C2—C7—C6 | −0.8 (6) | C8—C9—C14—C13 | −177.4 (4) |
| C1—C2—C7—C6 | 179.0 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O5$^{i}$ | 0.85 (3) | 1.90 (3) | 2.739 (4) | 171 (4) |
| O3—H3···O1 | 0.84 (4) | 1.91 (5) | 2.616 (4) | 142 (5) |
| O3—H3···O6$^{ii}$ | 0.84 (4) | 2.52 (4) | 3.063 (5) | 123 (4) |
| O4—H4···O1$^{iii}$ | 0.85 (4) | 1.79 (4) | 2.636 (4) | 175 (4) |
| O6—H6···O5 | 0.85 (4) | 1.90 (4) | 2.642 (4) | 146 (5) |

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