The structure of the title salt (systematic name: oxodiphenyl-\(\lambda^5\)-iodanylium 4-methylbenzenesulfonate dihydrate), \(\text{C}_{12}\text{H}_{10}\text{IO}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-\cdot2\text{H}_2\text{O}\), at 150 K, has monoclinic (\(P2_1/c\)) symmetry. The molecular structure features an angular (phenyliodosyl)benzene cation, the geometry of which was hitherto undescribed in the literature: in the cation, both I—C bonds are approximately normal to the I—O bond, forming a C—I—C angle of 95.36 (4)°. The crystal structure displays O—H⋯O, O—H⋯I and O—H⋯S hydrogen bonding.

Structure description

The crystal structure of (phenyliodosyl)benzene tosylate dihydrate (I) is shown in Fig. 1. A partial packing structure is shown in Fig. 2. The title compound I crystallizes from water via slow cooling to 293 K to the monoclinic crystal system with space group \(P2_1/c\). This iodosyl salt arose from the reaction of iodoxybenzene with sodium hydroxide (Fig. 3). The intermediate formed was captured with \(p\)-toluene sulfonic acid, generating I.

In compound I there are two phenyl rings connected to the iodine centre, C1—I1—C7, with a bond angle of 95.36 (4)°. The bond lengths of C1—I1 and C7—I1 are 2.1289 (11) and 2.1370 (12) Å, respectively. These values are comparable to the sum of the van der Waals radii (2.05 Å; Bondi, 1964). These bond lengths are comparable to those found in 1,1,1-triacetoxy1,1-dihydro-1,2-benziodoxol-3(1H)-one, i.e. the Dess–Martin periodinane, with a C—I bond length between the phenyl and iodine of 2.1025 (16) Å (Schröckeneder et al., 2012). A secondary bonding interaction with the \(p\)-toluene sulfonate anion, O4⋯I1 [2.7076 (10) Å], resides nearly perpendicular at 77.55 (4)° to the I1—O1 bond. This bond length is shorter than the sum (3.05 Å) of the covalent radii, and this is analogous to secondary bonding that was observed by Rentzeperis in his bis(di-phenyliodonium I-oxide) diacetate trihydrate, between the acetate anion and the iodo-
I–O single bond length was shorter (1.91 Å) than the computed distance (1.96 Å) in his seminal work on hydroxy(tosyloxy)iodobenzene. Additionally, in I, secondary coordination of the iodonium I–oxide centre with neighbouring water molecules indicates a close contact via the I1···O2 and I1···O3 with bond distances of 2.5674 (10) and 2.8118 (10) Å, respectively.

The title compound forms a distorted octahedral geometry in accordance with comparison to a VSEPR model. The O1—I1—O2 bond angle of 175.27 (4)°, the C7—I1—O3 angle of 176.33 (4)°, the O1—I1—O4 angle of 77.55 (4)° with the coordinating tosylate anion and the C1—I1—C7 angle of 95.36 (4)° complete the distorted octahedral geometry. The accompanying tosylate anion and water molecules occupy apical and equatorial positions to stabilize the monomeric complex. Bis(diphenyliodonium I–oxide) diacetate trihydrate also adopted a distorted octahedral geometry, albeit via a dimeric coordinating structure (Bozopoulos & Rentzeperis, 1987). In this complex, the asymmetric units form distorted trigonal–pyramidal arrangements, where the iodine atoms occupy the apices, resembling the IO5– iodate anion. Secondary I···O interactions complete the distorted octahedral geometry around each individual iodine atom. The title complex I does not dimerize like the Rentzeperis compound, most likely due to the bulky nature of the coordinating tosylate anion, along with additional hydrogen bonding of the sulfone O atoms and water O atoms with neighbouring water molecules.

Examination of the molecular packing as illustrated in Fig. 2 shows O3···H2A and O6···H3B contacts, with O···H distances of 1.92 (2) and 1.99 (2) Å, respectively, as viewed down the a axis (Fig. 2 and Table 1). These two coordinations inhibit aggregation of the iodonium centres as seen in bis(diphenyliodonium I–oxide) diacetate trihydrate (Bozopoulos & Rentzeperis, 1987).

Synthesis and crystallization

(Phenyliodosyl)benzene tosylate dihydrate was synthesized according to a modified procedure by Chen (2007) and is illustrated in Fig. 3. Iodobenzene (2.04 g, 10 mmol) was added to a water solution (20 ml) of sodium metaperiodate (4.7 g, 22 mmol) with a small amount of toluene (0.3 ml) to minimize steam distillation. The reaction was heated to reflux for 18 h.
and then cooled to room temperature. To the cooled reaction flask were added 50 ml of ice-cold water, and the white crystals that formed were filtered, washed with cold water (20 ml), cold chloroform (10 ml), and air-dried in a dark room until a constant weight was found (2.08 g, 8.81 mmol, 88% yield). The crude material was used in the next step without further purification. The iodoxybenzene (2.08 g, 8.81 mmol) was added to a stirred solution of 1 N NaOH (18.7 ml) pre-cooled to 277 K. The reaction was stirred for 1 h maintaining the temperature of the reaction below 281 K. The NaIO3 that formed was filtered off. The filtrate was poured into a round-bottomed flask equipped with a magnetic stir bar and cooled to 277 K. The white crystals that formed were filtered, washed with cold water (20 ml), cold chloroform (10 ml), and vacuum-dried in a dark room until a constant weight was found (2.08 g, 8.81 mmol, 88% yield). The product (1.75 g, 15.08 mmol) was added to the cooled filtrate and a white precipitate formed. The suspension was allowed to stand for 4 days to return to room temperature. After additional cooling in a thermal bath, insuring that the temperature took at least two days to return to room temperature, the crystals that formed were suitable for X-ray analysis.

Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2.

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Table 2
Experimental details.

| Crystal data | Chemical formula | C_{12}H_{10}IO^+·C_{7}H_{7}O_{3}S^-·2H_{2}O |
|---------------|-----------------|---------------------------------------------|
|               | M_r            | 504.32                                      |
| Crystal system, space group | Monoclinic, P2_1/c |
| Temperature (K) | 150          |
| a, b, c (Å) | 6.1823 (3), 24.9509 (11), 12.7606 (6) |
| β (°) | 100.257 (2) |
| V (Å³) | 1936.92 (16) |
| Z | 4 |
| Radiation type | Mo Kα |
| μ (mm⁻¹) | 1.79 |
| Crystal size (mm) | 0.23 × 0.18 × 0.15 |

Data collection
Diffractometer
Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD).

Absorption correction
Multi-scan (SADABS; Bruker, 2021).

Rint
0.033

R Values
R-I^2 > 2σ(I), 841 reflections,
R[I^2 > 2σ(I)], 3811 reflections,
S = 6815

H-atom treatment
H atoms treated by a mixture of independent and constrained refinement.

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *Mercury* (Macrae et al., 2020) and *publCIF* (Westrip, 2010).

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full crystallographic data

*IUCrData* (2022). 7, x220522  [https://doi.org/10.1107/S2414314622005223]

*(Phenyliodosyl)benzene tosylate dihydrate*

Timothy J. Smith, Gerald Koser, Yi Chen, Matthias Zeller, Rocco Iacino and Nichole Selzer

Oxodiphenyl-$\lambda^5$-iodanylium 4-methylbenzenesulfonate dihydrate

**Crystal data**

$\text{C}_{12}\text{H}_{10}\text{IO}^+\cdot\text{C}_7\text{H}_7\text{O}_3\text{S}^-\cdot2\text{H}_2\text{O}$

$M_r = 504.32$

Monoclinic, $P2_1/c$

$a = 6.1823$ (3) Å

$b = 24.9509$ (11) Å

$c = 12.7606$ (6) Å

$\beta = 100.257$ (2)$^\circ$

$V = 1936.92$ (16) Å$^3$

$Z = 4$

$F(000) = 1008$

$D_\lambda = 1.729$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9659 reflections

$\theta = 3.4$–$33.2^\circ$

$\mu = 1.79$ mm$^{-1}$

$T = 150$ K

Fragment, colourless

$0.23 \times 0.18 \times 0.15$ mm

**Data collection**

Bruker AXS D8 Quest
diffractometer with PhotonII charge-integrating pixel array detector (CPAD)

Absorption correction: multi-scan

(SADABS; Bruker, 2021)

$T_{\text{min}} = 0.644$, $T_{\text{max}} = 0.747$

55248 measured reflections

7429 independent reflections

6815 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\text{max}} = 33.3^\circ$, $\theta_{\text{min}} = 2.9^\circ$

$h = -9$→$9$

$k = -38$→$38$

$l = -19$→$19$

**Refinement**

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.042$

$S = 1.09$

7429 reflections

258 parameters

0 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F^2) + (0.0115P)^2 + 1.2666P]$

where $P = (F^2 + 2F_c^2)/3$

$(\Delta\sigma)_{\text{max}} = 0.004$

$\Delta\rho_{\text{max}} = 0.49$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -0.39$ e Å$^{-3}$

Extinction correction: SHELXL2018/3 (Sheldrick, 2015b),

$F_c^\infty = kF_c[1+0.001x F_c^\lambda \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00186 (16)
Special details

Refinement. H atoms attached to carbon were positioned geometrically and constrained to ride on their parent atoms. C—H bond distances were constrained to 0.95 Å for aromatic CH moieties, and to 0.98 Å for the CH3 group, respectively. Water H atom positions were freely refined. Uiso(H) values were set to a multiple of Ueq(carrier C/O), with 1.5 for CH3 and OH, and 1.2 for CH units, respectively.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|    | x      | y      | z      | Ueq         |
|----|--------|--------|--------|-------------|
| I1 | 0.6878 (2) | 0.46909 (2) | 0.68867 (2) | 0.01154 (3) |
| S1 | 0.78701 (5) | 0.36098 (2) | 0.47914 (2) | 0.01522 (5) |
| O1 | 0.97764 (14) | 0.46950 (4) | 0.74614 (8) | 0.01780 (17) |
| O2 | 0.27627 (16) | 0.47673 (4) | 0.61133 (8) | 0.01981 (18) |
| H2A | 0.242 (3) | 0.4622 (8) | 0.5495 (17) | 0.030* |
| H2B | 0.173 (3) | 0.4724 (8) | 0.6458 (17) | 0.030* |
| O3 | 0.75786 (17) | 0.56665 (4) | 0.58959 (8) | 0.01987 (18) |
| H3A | 0.665 (3) | 0.5916 (8) | 0.5781 (16) | 0.030* |
| H3B | 0.869 (4) | 0.5829 (8) | 0.6024 (16) | 0.030* |
| O4 | 0.86090 (18) | 0.40372 (4) | 0.55568 (8) | 0.02297 (19) |
| O5 | 0.55011 (16) | 0.35301 (5) | 0.46211 (10) | 0.0294 (2) |
| O6 | 0.87304 (16) | 0.36783 (4) | 0.38086 (7) | 0.02007 (18) |
| C1 | 0.5945 (2) | 0.51811 (5) | 0.80971 (9) | 0.0142 (2) |
| C2 | 0.7369 (2) | 0.51635 (6) | 0.90699 (11) | 0.0212 (2) |
| H2 | 0.862288 | 0.493668 | 0.917364 | 0.025* |
| C3 | 0.6902 (3) | 0.54883 (6) | 0.98885 (11) | 0.0249 (3) |
| H3 | 0.783620 | 0.548237 | 1.056562 | 0.030* |
| C4 | 0.5077 (3) | 0.58201 (6) | 0.97162 (11) | 0.0236 (3) |
| H4 | 0.477050 | 0.604223 | 1.027645 | 0.028* |
| C5 | 0.3694 (2) | 0.58310 (6) | 0.87349 (12) | 0.0229 (3) |
| H5 | 0.244730 | 0.606019 | 0.862871 | 0.027* |
| C6 | 0.4115 (2) | 0.55088 (5) | 0.79013 (10) | 0.0182 (2) |
| H6 | 0.317967 | 0.551429 | 0.722456 | 0.022* |
| C7 | 0.6142 (2) | 0.39479 (5) | 0.75784 (9) | 0.0139 (2) |
| C8 | 0.7930 (2) | 0.37027 (5) | 0.82033 (10) | 0.0187 (2) |
| H8 | 0.934473 | 0.386350 | 0.830739 | 0.022* |
| C9 | 0.7592 (3) | 0.32126 (6) | 0.86755 (11) | 0.0235 (3) |
| H9 | 0.878788 | 0.303693 | 0.911211 | 0.028* |
| C10 | 0.5521 (3) | 0.29802 (5) | 0.85114 (11) | 0.0231 (3) |
| H10 | 0.530416 | 0.264622 | 0.883500 | 0.028* |
| C11 | 0.3762 (2) | 0.32346 (5) | 0.78748 (11) | 0.0217 (2) |
| H11 | 0.234867 | 0.307259 | 0.776581 | 0.026* |
| C12 | 0.4048 (2) | 0.37264 (5) | 0.73933 (10) | 0.0178 (2) |
| H12 | 0.285534 | 0.390249 | 0.695560 | 0.021* |
| C13 | 0.90551 (19) | 0.30148 (5) | 0.53950 (9) | 0.0143 (2) |
| C14 | 1.1068 (2) | 0.28329 (5) | 0.51879 (10) | 0.0166 (2) |
| H14 | 1.177697 | 0.301415 | 0.468824 | 0.020* |
| C15 | 1.2027 (2) | 0.23823 (5) | 0.57228 (10) | 0.0180 (2) |
| H15 | 1.339293 | 0.225549 | 0.557827 | 0.022* |
### Atomic displacement parameters (Å²)

|    | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$   | $U^{23}$   |
|----|------------|------------|------------|------------|------------|------------|
| I1 | 0.00981 (3) | 0.01211 (4) | 0.01291 (4) | $-0.00066$ (2) | 0.00260 (2) | $-0.00161$ (2) |
| S1 | 0.01308 (12) | 0.01470 (12) | 0.01821 (13) | 0.00026 (10) | 0.00368 (10) | 0.00096 (10) |
| O1 | 0.0086 (3) | 0.0232 (4) | 0.0211 (4) | $-0.0009$ (3) | 0.0013 (3) | $-0.0040$ (3) |
| O2 | 0.0141 (4) | 0.0254 (5) | 0.0199 (4) | $-0.0026$ (4) | 0.0030 (3) | $-0.0025$ (4) |
| O3 | 0.0179 (4) | 0.0171 (4) | 0.0250 (5) | $-0.0021$ (4) | 0.0049 (4) | 0.0001 (3) |
| O4 | 0.0158 (4) | 0.0245 (5) | 0.0055 (4) | 0.0104 (4) | $-0.0040$ (4) |
| O5 | 0.0127 (4) | 0.0304 (6) | 0.0064 (6) | 0.0024 (4) | 0.0130 (5) |
| O6 | 0.0234 (4) | 0.0212 (4) | 0.0160 (4) | 0.0045 (3) | 0.0021 (3) |
| C1 | 0.0147 (5) | 0.0131 (5) | 0.0153 (5) | $-0.0004$ (4) | 0.0040 (4) | $-0.0032$ (4) |
| C2 | 0.0196 (6) | 0.0242 (6) | 0.0186 (6) | 0.0043 (5) | 0.0000 (4) | $-0.0052$ (5) |
| C3 | 0.0286 (7) | 0.0280 (7) | 0.0170 (6) | 0.0019 (6) | 0.0013 (5) | $-0.0069$ (5) |
| C4 | 0.0305 (7) | 0.0209 (6) | 0.0216 (6) | 0.0003 (5) | 0.0108 (5) | $-0.0067$ (5) |
| C5 | 0.0238 (6) | 0.0192 (6) | 0.0270 (6) | 0.0055 (5) | 0.0080 (5) | $-0.0035$ (5) |
| C6 | 0.0177 (5) | 0.0174 (5) | 0.0192 (5) | 0.0029 (4) | 0.0026 (4) | $-0.0014$ (4) |
| C7 | 0.0162 (5) | 0.0127 (5) | 0.0132 (5) | 0.0003 (4) | 0.0036 (4) | $-0.0007$ (4) |
| C8 | 0.0184 (5) | 0.0180 (5) | 0.0194 (6) | 0.0027 (4) | 0.0027 (4) | 0.0006 (4) |
| C9 | 0.0288 (7) | 0.0201 (6) | 0.0214 (6) | 0.0073 (5) | 0.0037 (5) | 0.0040 (5) |
| C10 | 0.0350 (7) | 0.0162 (5) | 0.0204 (6) | 0.0015 (5) | 0.0110 (5) | 0.0022 (4) |
| C11 | 0.0252 (6) | 0.0170 (6) | 0.0242 (6) | $-0.0047$ (5) | 0.0084 (5) | $-0.0009$ (5) |
| C12 | 0.0174 (5) | 0.0161 (5) | 0.0199 (5) | $-0.0015$ (4) | 0.0033 (4) | 0.0000 (4) |
| C13 | 0.0140 (5) | 0.0130 (5) | 0.0160 (5) | $-0.0011$ (4) | 0.0028 (4) | $-0.0010$ (4) |
| C14 | 0.0152 (5) | 0.0169 (5) | 0.0187 (5) | $-0.0009$ (4) | 0.0055 (4) | 0.0002 (4) |
| C15 | 0.0150 (5) | 0.0193 (6) | 0.0201 (6) | 0.0022 (4) | 0.0046 (4) | $-0.0005$ (4) |
| C16 | 0.0208 (6) | 0.0152 (5) | 0.0181 (5) | 0.0013 (4) | 0.0037 (4) | $-0.0003$ (4) |
| C17 | 0.0225 (6) | 0.0170 (5) | 0.0208 (6) | $-0.0004$ (5) | 0.0092 (5) | 0.0010 (4) |
| C18 | 0.0159 (5) | 0.0168 (5) | 0.0203 (5) | $-0.0001$ (4) | 0.0069 (4) | 0.0001 (4) |
| C19 | 0.0334 (8) | 0.0234 (7) | 0.0292 (7) | 0.0094 (6) | 0.0090 (6) | 0.0083 (5) |

### Geometric parameters (Å, °)

|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| I1—O1 | 1.8108 (9) | C7—C8 | 1.3849 (17) |
| I1—C1 | 2.1289 (11) | C7—C12 | 1.3883 (17) |
| I1—C7 | 2.1370 (12) | C8—C9 | 1.3954 (19) |
| I1—O2 | 2.5674 (10) | C8—H8 | 0.9500 |
| I1—O4 | 2.7076 (10) | C9—C10 | 1.387 (2) |
| Bond (Angstroms) |  
|-----------------|  
| I1—O3          | 2.8118 (10)  
| S1—O5          | 1.4555 (10)  
| S1—O6          | 1.4568 (10)  
| S1—O4          | 1.4631 (10)  
| S1—C13         | 1.7702 (12)  
| O2—H2A         | 0.86 (2)     
| O2—H2B         | 0.85 (2)     
| O3—H3A         | 0.84 (2)     
| O3—H3B         | 0.79 (2)     
| C1—C6          | 1.3819 (17)  
| C1—C2          | 1.3888 (18)  
| C2—C3          | 1.3923 (19)  
| C2—H2          | 0.9500       
| C3—C4          | 1.385 (2)    
| C3—H3          | 0.9500       
| C4—C5          | 1.385 (2)    
| C4—H4          | 0.9500       
| C5—C6          | 1.3942 (18)  
| C5—H5          | 0.9500       
| C6—H6          | 0.9500       
| O1—I1—C1       | 94.57 (4)    
| O1—I1—C7       | 96.08 (5)    
| C1—I1—C7       | 95.36 (4)    
| O1—I1—O2       | 175.27 (4)   
| C1—I1—O2       | 81.83 (4)    
| C7—I1—O2       | 87.34 (4)    
| O1—I1—O4       | 77.55 (4)    
| C1—I1—O4       | 171.59 (4)   
| C7—I1—O4       | 82.72 (4)    
| O2—I1—O4       | 106.19 (3)   
| O1—I1—O3       | 87.53 (4)    
| C1—I1—O3       | 84.96 (4)    
| C7—I1—O3       | 176.33 (4)   
| O2—I1—O3       | 89.09 (3)    
| O4—I1—O3       | 97.47 (3)    
| O5—S1—O6       | 113.54 (7)   
| O5—S1—O4       | 112.68 (7)   
| O6—S1—O4       | 111.76 (6)   
| O5—S1—C13      | 106.12 (6)   
| O6—S1—C13      | 106.66 (6)   
| O4—S1—C13      | 105.37 (6)   
| I1—O2—H2A      | 112.9 (14)   
| I1—O2—H2B      | 125.5 (14)   
| H2A—O2—H2B     | 110 (2)      
| I1—O3—H3A      | 124.2 (14)   
| I1—O3—H3B      | 123.4 (15)   
| H3A—O3—H3B     | 101.5 (19)   

| Angle (Degree) |  
|----------------|  
| C9—H9          | 0.9500       
| C10—C11        | 1.390 (2)    
| C10—H10        | 0.9500       
| C11—C12        | 1.3975 (18)  
| C11—H11        | 0.9500       
| C12—H12        | 0.9500       
| C13—C18        | 1.3931 (17)  
| C13—C14        | 1.3935 (17)  
| C14—C15        | 1.3919 (18)  
| C14—H14        | 0.9500       
| C15—C16        | 1.3973 (18)  
| C15—H15        | 0.9500       
| C15—C19        | 1.5037 (19)  
| C16—C17        | 1.3970 (18)  
| C16—C19        | 1.3888 (18)  
| C17—C18        | 0.9500       
| C17—H17        | 0.9500       
| C18—H18        | 0.9500       
| C19—C13        | 0.9800       
| C19—H19A       | 0.9800       
| C19—H19B       | 0.9800       
| C19—H19C       | 0.9800       
| C1—C6—H6       | 121.3        
| C5—C6—H6       | 121.3        
| C8—C7—C12      | 123.12 (12)  
| C8—C7—I1       | 114.46 (9)   
| C12—C7—I1      | 122.41 (9)   
| C7—C8—C9       | 118.05 (12)  
| C7—C8—H8       | 121.0        
| C9—C8—H8       | 121.0        
| C10—C9—C8      | 120.41 (13)  
| C10—C9—H9      | 119.8        
| C8—C9—H9       | 119.8        
| C9—C10—C11     | 120.17 (13)  
| C9—C10—H10     | 119.9        
| C11—C10—H10    | 119.9        
| C10—C11—C12    | 120.71 (13)  
| C10—C11—H11    | 119.6        
| C12—C11—H11    | 119.6        
| C7—C12—C11     | 117.53 (12)  
| C7—C12—H12     | 121.2        
| C7—C12—H12     | 121.2        
| C11—C12—H12    | 120.4        
| C18—C13—C14    | 120.40 (11)  
| C18—C13—S1     | 119.17 (9)   
| C14—C13—S1     | 120.33 (9)   
| C15—C14—C13    | 119.13 (11)  
| C15—C14—H14    | 120.4        
| C15—C14—H14    | 120.4        
| C13—C14—H14    | 121.38 (12)  

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S1—O4—I1 138.26 (6) C14—C15—H15 119.3
C6—C1—C2 123.26 (11) C16—C15—H15 119.3
C6—C1—I1 121.86 (9) C17—C16—C15 118.41 (12)
C2—C1—I1 114.81 (9) C17—C16—C19 120.65 (12)
C1—C2—C3 117.98 (13) C15—C16—C19 120.93 (12)
C1—C2—H2 121.0 C18—C17—C16 120.94 (12)
C3—C2—H2 121.0 C18—C17—H17 119.5
C4—C3—C2 120.03 (13) C16—C17—H17 119.5
C4—C3—H3 120.0 C17—C18—C13 119.73 (12)
C2—C3—H3 120.0 C17—C18—H18 120.1
C5—C4—C3 120.63 (12) C16—C19—C19B 109.5
C6—C5—C4 120.63 (13) H19A—C19—H19B 109.5
C4—C5—H5 119.7 C16—C19—H19C 109.5
C3—C4—H4 119.7 C19A—C19—H19C 109.5
C6—C5—H5 119.7 C19B—C19—H19C 109.5
C1—C6—C5 117.46 (12) C19C—C19—H19C 109.5

O5—S1—O4—I1 5.82 (11) C10—C11—C12—C7 −0.16 (19)
O6—S1—O4—I1 135.08 (8) O5—S1—C13—C18 −36.61 (12)
C13—S1—O4—I1 −109.46 (9) O6—S1—C13—C18 −157.97 (10)
C6—C1—C2—C3 0.8 (2) O4—S1—C13—C14 83.11 (11)
C1—C2—C3—C4 −0.7 (2) O5—S1—C13—C14 147.06 (11)
C2—C3—C4—C5 0.3 (2) O6—S1—C13—C14 25.70 (12)
C3—C4—C5—C6 −0.1 (2) O4—S1—C13—C14 −93.22 (11)
C2—C1—C6—C5 −0.6 (2) S1—C13—C14—C15 176.11 (10)
C1—C1—C6—C5 177.39 (10) C13—C14—C15—C16 −0.6 (2)
C4—C5—C6—C1 0.2 (2) C14—C15—C16—C17 1.0 (2)
C12—C7—C8—C9 −0.70 (19) C14—C15—C16—C19 −177.83 (13)
C1—C7—C8—C9 −179.34 (10) C15—C16—C17—C18 −0.7 (2)
C7—C8—C9—C10 0.4 (2) C15—C16—C17—C19 178.17 (13)
C8—C9—C10—C11 −0.1 (2) C16—C17—C18—C13 −0.1 (2)
C9—C10—C11—C12 −0.1 (2) C14—C13—C18—C17 0.51 (19)
C8—C7—C12—C11 0.56 (19) S1—C13—C14—C15 −175.82 (10)
C1—C7—C12—C11 179.10 (9)

Hydrogen-bond geometry (Å, °)

| D—H···A     | D—H | H···A | D···A  | D—H···A |
|------------|-----|-------|-------|---------|
| O2—H2A···O3 | 0.86 (2) | 1.92 (2) | 2.7563 (14) | 165 (2) |
| O2—H2B···O1 | 0.85 (2) | 3.14 (2) | 3.9397 (10) | 158.1 (18) |
| O2—H2B···O1 | 0.85 (2) | 1.91 (2) | 2.7443 (14) | 169 (2) |
| O3—H3A···S1 | 0.84 (2) | 3.00 (2) | 3.7847 (11) | 155.7 (17) |
| O3—H3A···O5 | 0.84 (2) | 1.92 (2) | 2.7625 (15) | 174.6 (19) |
| O3—H3B···O1 | 0.79 (2) | 2.89 (2) | 3.5812 (10) | 147.5 (18) |
| O3—H3B···O6 | 0.79 (2) | 1.99 (2) | 2.7776 (14) | 171 (2) |
| C2—H2···O1 | 0.95 | 2.49 | 2.9805 (16) | 112 |
|          | d   | r   | E   | ı   |
|----------|-----|-----|-----|-----|
| C6—H6···O2 | 0.95 | 2.33 | 2.9408 (17) | 122 |
| C6—H6···O6ı | 0.95 | 2.58 | 3.2562 (16) | 129 |
| C8—H8···O1 | 0.95 | 2.38 | 2.9521 (17) | 119 |
| C12—H12···O2 | 0.95 | 2.41 | 3.0957 (17) | 129 |
| C14—H14···O5ıv | 0.95 | 2.65 | 3.4301 (16) | 139 |

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