

Monoclinic polymorph of 2,5-dideoxy-2,5-epithio-1,3:4,6-bis-O-[(*R*)-phenylmethylene]-L-iditol¹

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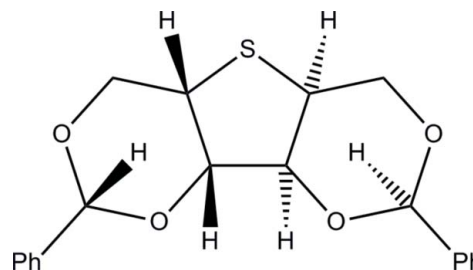
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Key indicators: single-crystal X-ray study; $T = 100$ K, $P = 0.0$ kPa; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 27.4.

The title compound $\text{C}_{20}\text{H}_{20}\text{O}_4\text{S}$, is polymorphic. In the tetragonal form, the molecule lies on a crystallographic twofold axis, while the monoclinic form has only approximate C_2 molecular symmetry. The greatest excursion from C_2 symmetry is in the orientation of the two phenyl rings; at 100 K, one of the rings is rotated -37.2 (3)° and the other by 46.9 (3)° from their symmetric (tetragonal) positions. There are only minor differences in the three-ring nucleus; the best molecular fit of the tetragonal and monoclinic forms, both at 100 K and excluding phenyl rings and H atoms, shows an r.m.s. deviation of 0.066 Å. Both forms have the same absolute configuration.

Related literature

For details of the synthesis, see: Rao *et al.* (1988). For the structure of the tetragonal form at 295 K (CCDC refcode WAMRAD), see: Rao *et al.* (1993); and at 100 K (CCDC refcode 851380), see: Gibson *et al.* (2011). For a preliminary report of the structures of both polymorphs at room temperature, see: Fronczek *et al.* (2002). For a description of the Cambridge Structural Database, see: Allen (2002). For the determination of the absolute configuration from Bijvoet pairs, see: Hooft *et al.* (2008); Flack (1983). For details of the molecular mechanics software used, see: Cambridgesoft (2010); Winn & Goodman (2001).



Experimental

Crystal data

$\text{C}_{20}\text{H}_{20}\text{O}_4\text{S}$	$V = 870.6$ (3) Å ³
$M_r = 356.42$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 6.158$ (1) Å	$\mu = 0.21$ mm ⁻¹
$b = 9.223$ (2) Å	$T = 100$ K
$c = 15.407$ (4) Å	$0.25 \times 0.22 \times 0.10$ mm
$\beta = 95.785$ (8)°	

Data collection

Nonius KappaCCD diffractometer	6225 measured reflections
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)	6225 independent reflections
$T_{\min} = 0.950$, $T_{\max} = 0.980$	5648 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.088$	$\Delta\rho_{\max} = 0.29$ e Å ⁻³
$S = 1.05$	$\Delta\rho_{\min} = -0.23$ e Å ⁻³
6225 reflections	Absolute structure: Flack (1983),
227 parameters	2730 Bijvoet pairs
1 restraint	Flack parameter: 0.02 (5)

Data collection: COLLECT (Nonius, 2000); cell refinement: DENZO and SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO and SCALEPACK; program(s) used to solve structure: SHELXS86 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999) and IDEAL (Gould *et al.*, 1988).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2079).

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supporting information

Acta Cryst. (2012). E68, o2668–o2669 [doi:10.1107/S1600536812034514]

Monoclinic polymorph of 2,5-dideoxy-2,5-epithio-1,3:4,6-bis-*O*-[(*R*)-phenyl-methylene]-*L*-iditol

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S1. Comment

The tetragonal form of the title compound (**I**), C₂₀H₂₀O₄S, was determined at 295 K (Rao *et al.*, 1993, hereinafter P4₂₉₅). We re-examined the tetragonal form at 100 K in our laboratory (hereinafter P4₁₀₀) and determined the absolute configuration. These data are deposited at the Cambridge Crystallographic Data Centre (Allen, 2002), CCDC 851380 (Gibson *et al.*, 2011). There is a 2.8% volume decrease upon lowering the temperature from 295 K to 100 K but the molecular symmetry is C₂ at both temperatures and there is no significant change in molecular structure. The best molecular fit (Gould *et al.*, 1988) of all non-H atoms in P4₂₉₅ and P4₁₀₀ yields $\delta_{\text{r.m.s.}} = 0.022$ Å, while excluding the phenyl groups yields $\delta_{\text{r.m.s.}} = 0.011$ Å.

In the monoclinic form at 100 K (P2₁₀₀) the molecular symmetry is C₁. The molecular volume of P2₁₀₀ (435.2 (3) Å³/molecule) is greater than P4₁₀₀ (433.6 (1) Å³/molecule). The thirteen non-H atoms of the three central rings in P2₁₀₀ and P4₁₀₀ are arranged similarly with best molecular fit $\delta_{\text{r.m.s.}} = 0.066$ Å. The most pronounced structural difference between P2₁₀₀ and P4₁₀₀ is in the orientation of the phenyl rings. In P4₁₀₀, two equivalent O—C—C torsions of -14.5 (3)° become +32.4 (2)° and -51.7 (2)° in P2₁₀₀. The global minimum conformation of this molecule has been calculated using *MM2* (Winn & Goodman, 2001) and confirmed by us (Cambridgesoft, 2010). Like the tetragonal form, the minimum conformation has C₂ symmetry, but the two equivalent O—C—C torsions representing the orientation of the phenyl rings are -56°.

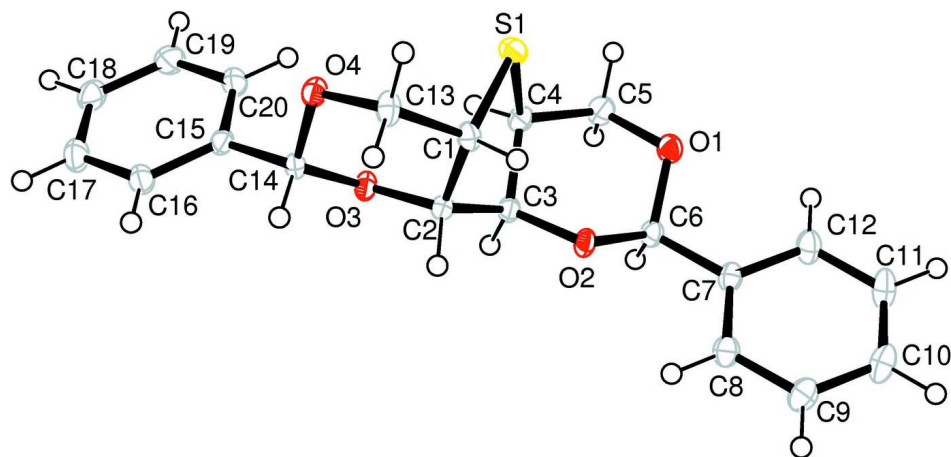
Based on the Flack parameter $x = 0.02$ (5) (Flack, 1983) and Hooft parameters $y = 0.00$ (3) and P2(true) = 1.000 for 2730 Bijvoet pairs (Hooft *et al.*, 2008), the absolute configurations of the tetragonal and monoclinic forms are identical at 100 K, with stereochemical specification (2*R*,4*aS*,5*aS*,8*R*,9*aS*,9*bS*)-2,8-diphenylhexahydrothieno[3,2 - d:4,5 - d'] bis-([1,3]dioxine).

S2. Experimental

The title compound was prepared by Dr. Ronald Voll according to the scheme reported by Rao *et al.* (1988). A suitable single-crystal was obtained by recrystallization from ethanol.

S3. Refinement

All H atoms were placed in calculated positions, guided by difference maps, with C—H bond distances 0.95 (aromatic C), 0.99 (CH₂), 1.00 Å, (R₃CH) and $U_{\text{iso}} = 1.2U_{\text{eq}}$, thereafter refined as riding. The absolute configuration, based on 2730 Bijvoet pairs with Flack parameter $x = 0.02$ (5), Hooft parameter $y = 0.00$ (3) and Hooft P2(true) = 1.000, is consistent with that of the starting materials.

**Figure 1**

View of (I) (50% probability displacement ellipsoids).

2,5-dideoxy-2,5-epithio-1,3:4,6-bis-O-[(*R*)-phenylmethylene]-L-idoitol*Crystal data*C₂₀H₂₀O₄S $M_r = 356.42$ Monoclinic, *P*2₁

Hall symbol: P 2yb

 $a = 6.158 (1) \text{ \AA}$ $b = 9.223 (2) \text{ \AA}$ $c = 15.407 (4) \text{ \AA}$ $\beta = 95.785 (8)^\circ$ $V = 870.6 (3) \text{ \AA}^3$ $Z = 2$ $F(000) = 376$ $D_x = 1.36 \text{ Mg m}^{-3}$

Melting point: 481.5(5) K

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3254 reflections

 $\theta = 2.5\text{--}33.1^\circ$ $\mu = 0.21 \text{ mm}^{-1}$ $T = 100 \text{ K}$

Lath, colorless

 $0.25 \times 0.22 \times 0.10 \text{ mm}$ *Data collection*

Nonius KappaCCD

diffractometer

Radiation source: sealed tube

Horizontally mounted graphite crystal

monochromator

Detector resolution: 9 pixels mm^{-1} ω and φ scans

Absorption correction: multi-scan

(SCALEPACK; Otwinowski & Minor, 1997)

 $T_{\min} = 0.950, T_{\max} = 0.980$

6225 measured reflections

6225 independent reflections

5648 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0$ $\theta_{\max} = 33.1^\circ, \theta_{\min} = 2.6^\circ$ $h = -9 \rightarrow 9$ $k = -14 \rightarrow 13$ $l = 0 \rightarrow 23$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.037$ $wR(F^2) = 0.088$ $S = 1.05$

6225 reflections

227 parameters

1 restraint

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-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.1562P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.29 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$

Absolute structure: Flack (1983), 2730 Bijvoet pairs

Absolute structure parameter: 0.02 (5)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7808 (2)	0.62050 (15)	0.17832 (8)	0.0169 (2)
H1	0.7275	0.5554	0.1288	0.02*
C2	0.6502 (2)	0.76146 (15)	0.17125 (8)	0.0163 (2)
H2	0.4915	0.7418	0.1554	0.02*
C3	0.7424 (2)	0.85423 (15)	0.10263 (8)	0.0161 (2)
H3	0.681	0.9546	0.1024	0.019*
C4	0.9911 (2)	0.85639 (15)	0.12534 (8)	0.0168 (2)
H4	1.0276	0.9279	0.1734	0.02*
C5	1.1053 (2)	0.90189 (16)	0.04642 (9)	0.0212 (3)
H5A	1.086	1.0075	0.0369	0.025*
H5B	1.2636	0.8822	0.058	0.025*
C6	0.7929 (2)	0.84807 (15)	-0.04585 (8)	0.0167 (2)
H6	0.7622	0.9546	-0.0476	0.02*
C7	0.7107 (2)	0.78161 (14)	-0.13235 (8)	0.0172 (2)
C8	0.4961 (2)	0.73435 (15)	-0.14903 (9)	0.0198 (2)
H8	0.3999	0.7395	-0.1047	0.024*
C9	0.4225 (2)	0.67920 (18)	-0.23124 (8)	0.0229 (2)
H9	0.2771	0.6445	-0.2422	0.027*
C10	0.5608 (2)	0.67481 (19)	-0.29699 (8)	0.0259 (3)
H10	0.509	0.6391	-0.3531	0.031*
C11	0.7744 (3)	0.72253 (17)	-0.28063 (9)	0.0279 (3)
H11	0.8695	0.7192	-0.3255	0.033*
C12	0.8496 (2)	0.77535 (16)	-0.19836 (9)	0.0232 (3)
H12	0.9964	0.8073	-0.1872	0.028*
C13	0.7489 (2)	0.54497 (15)	0.26421 (8)	0.0197 (2)
H13A	0.5992	0.5049	0.2613	0.024*
H13B	0.853	0.4633	0.2733	0.024*
C14	0.6415 (2)	0.76351 (14)	0.32492 (8)	0.0161 (2)
H14	0.4857	0.7313	0.3201	0.019*
C15	0.6900 (2)	0.85965 (15)	0.40299 (8)	0.0168 (2)
C16	0.5382 (2)	0.87628 (16)	0.46339 (9)	0.0204 (3)
H16	0.4012	0.8282	0.4547	0.025*
C17	0.5876 (3)	0.96367 (17)	0.53664 (9)	0.0252 (3)
H17	0.4838	0.9756	0.5777	0.03*
C18	0.7877 (3)	1.03315 (17)	0.54964 (9)	0.0255 (3)
H18	0.8216	1.0916	0.5999	0.031*
C19	0.9390 (2)	1.01740 (18)	0.48917 (9)	0.0263 (3)

H19	1.0756	1.0658	0.4979	0.032*
C20	0.8902 (2)	0.93077 (17)	0.41595 (9)	0.0225 (3)
H20	0.9937	0.92	0.3746	0.027*
O1	1.02017 (15)	0.82585 (11)	-0.03065 (6)	0.01980 (19)
O2	0.68339 (15)	0.78354 (10)	0.02114 (5)	0.01686 (18)
O3	0.68371 (15)	0.84402 (11)	0.24980 (6)	0.01752 (18)
O4	0.78222 (15)	0.64292 (10)	0.33617 (6)	0.01824 (19)
S1	1.06220 (5)	0.67372 (4)	0.16652 (2)	0.01900 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0184 (6)	0.0173 (6)	0.0159 (5)	-0.0023 (4)	0.0049 (4)	-0.0009 (4)
C2	0.0156 (6)	0.0206 (6)	0.0127 (5)	0.0006 (4)	0.0016 (4)	-0.0001 (4)
C3	0.0186 (5)	0.0169 (6)	0.0130 (5)	0.0019 (5)	0.0022 (4)	0.0002 (4)
C4	0.0191 (5)	0.0158 (6)	0.0153 (5)	-0.0015 (5)	0.0009 (4)	0.0016 (4)
C5	0.0204 (6)	0.0236 (7)	0.0196 (6)	-0.0057 (5)	0.0024 (5)	0.0012 (5)
C6	0.0190 (5)	0.0181 (6)	0.0135 (5)	-0.0011 (5)	0.0035 (4)	0.0022 (4)
C7	0.0232 (6)	0.0146 (6)	0.0139 (5)	-0.0006 (5)	0.0029 (4)	0.0016 (4)
C8	0.0241 (6)	0.0181 (6)	0.0176 (5)	-0.0016 (5)	0.0036 (5)	0.0002 (5)
C9	0.0290 (6)	0.0186 (6)	0.0203 (5)	-0.0035 (6)	-0.0009 (5)	-0.0014 (5)
C10	0.0401 (7)	0.0211 (6)	0.0165 (5)	-0.0059 (7)	0.0020 (5)	-0.0034 (6)
C11	0.0402 (8)	0.0282 (8)	0.0168 (6)	-0.0065 (6)	0.0107 (5)	-0.0039 (5)
C12	0.0278 (7)	0.0255 (7)	0.0175 (6)	-0.0051 (5)	0.0073 (5)	-0.0010 (5)
C13	0.0287 (7)	0.0148 (6)	0.0164 (5)	-0.0010 (5)	0.0070 (5)	-0.0002 (4)
C14	0.0169 (5)	0.0195 (6)	0.0123 (5)	0.0018 (4)	0.0037 (4)	-0.0004 (4)
C15	0.0203 (6)	0.0174 (6)	0.0127 (5)	0.0036 (5)	0.0009 (4)	0.0010 (4)
C16	0.0218 (6)	0.0214 (7)	0.0187 (6)	0.0012 (5)	0.0048 (5)	-0.0010 (5)
C17	0.0307 (7)	0.0272 (8)	0.0184 (6)	0.0033 (6)	0.0067 (5)	-0.0028 (5)
C18	0.0309 (7)	0.0258 (7)	0.0190 (6)	0.0045 (6)	-0.0013 (5)	-0.0060 (5)
C19	0.0222 (7)	0.0315 (8)	0.0244 (7)	-0.0006 (6)	-0.0018 (5)	-0.0061 (6)
C20	0.0200 (6)	0.0290 (7)	0.0189 (6)	0.0003 (5)	0.0032 (5)	-0.0045 (5)
O1	0.0184 (4)	0.0243 (5)	0.0173 (4)	-0.0027 (4)	0.0045 (3)	-0.0002 (3)
O2	0.0193 (4)	0.0209 (5)	0.0107 (4)	-0.0027 (3)	0.0031 (3)	0.0004 (3)
O3	0.0244 (5)	0.0167 (4)	0.0119 (4)	0.0027 (4)	0.0038 (3)	0.0003 (3)
O4	0.0243 (4)	0.0164 (5)	0.0139 (4)	0.0029 (3)	0.0017 (3)	-0.0001 (3)
S1	0.01709 (13)	0.01938 (15)	0.02103 (13)	0.00212 (12)	0.00436 (10)	0.00274 (12)

Geometric parameters (Å, °)

C1—C13	1.5256 (18)	C9—H9	0.95
C1—C2	1.5266 (19)	C10—C11	1.386 (2)
C1—S1	1.8279 (13)	C10—H10	0.95
C1—H1	1	C11—C12	1.3928 (19)
C2—O3	1.4271 (15)	C11—H11	0.95
C2—C3	1.5144 (18)	C12—H12	0.95
C2—H2	1	C13—O4	1.4287 (16)
C3—O2	1.4288 (15)	C13—H13A	0.99

C3—C4	1.5360 (18)	C13—H13B	0.99
C3—H3	1	C14—O4	1.4100 (15)
C4—C5	1.5236 (19)	C14—O3	1.4211 (15)
C4—S1	1.8376 (14)	C14—C15	1.5000 (17)
C4—H4	1	C14—H14	1
C5—O1	1.4322 (16)	C15—C16	1.3925 (18)
C5—H5A	0.99	C15—C20	1.3928 (19)
C5—H5B	0.99	C16—C17	1.3952 (19)
C6—O1	1.4103 (16)	C16—H16	0.95
C6—O2	1.4195 (15)	C17—C18	1.386 (2)
C6—C7	1.5073 (18)	C17—H17	0.95
C6—H6	1	C18—C19	1.390 (2)
C7—C8	1.3907 (19)	C18—H18	0.95
C7—C12	1.3945 (19)	C19—C20	1.390 (2)
C8—C9	1.3974 (18)	C19—H19	0.95
C8—H8	0.95	C20—H20	0.95
C9—C10	1.3879 (19)		
C13—C1—C2	109.75 (11)	C11—C10—C9	119.92 (12)
C13—C1—S1	114.52 (9)	C11—C10—H10	120
C2—C1—S1	105.18 (9)	C9—C10—H10	120
C13—C1—H1	109.1	C10—C11—C12	119.93 (13)
C2—C1—H1	109.1	C10—C11—H11	120
S1—C1—H1	109.1	C12—C11—H11	120
O3—C2—C3	104.97 (10)	C11—C12—C7	120.40 (14)
O3—C2—C1	111.34 (10)	C11—C12—H12	119.8
C3—C2—C1	107.41 (11)	C7—C12—H12	119.8
O3—C2—H2	111	O4—C13—C1	111.31 (11)
C3—C2—H2	111	O4—C13—H13A	109.4
C1—C2—H2	111	C1—C13—H13A	109.4
O2—C3—C2	105.99 (10)	O4—C13—H13B	109.4
O2—C3—C4	111.45 (10)	C1—C13—H13B	109.4
C2—C3—C4	106.47 (10)	H13A—C13—H13B	108
O2—C3—H3	110.9	O4—C14—O3	110.58 (10)
C2—C3—H3	110.9	O4—C14—C15	107.30 (10)
C4—C3—H3	110.9	O3—C14—C15	107.83 (11)
C5—C4—C3	110.57 (10)	O4—C14—H14	110.4
C5—C4—S1	114.52 (10)	O3—C14—H14	110.4
C3—C4—S1	105.32 (9)	C15—C14—H14	110.4
C5—C4—H4	108.8	C16—C15—C20	119.77 (12)
C3—C4—H4	108.8	C16—C15—C14	120.53 (12)
S1—C4—H4	108.8	C20—C15—C14	119.69 (12)
O1—C5—C4	111.54 (11)	C15—C16—C17	119.85 (14)
O1—C5—H5A	109.3	C15—C16—H16	120.1
C4—C5—H5A	109.3	C17—C16—H16	120.1
O1—C5—H5B	109.3	C18—C17—C16	120.16 (14)
C4—C5—H5B	109.3	C18—C17—H17	119.9
H5A—C5—H5B	108	C16—C17—H17	119.9

O1—C6—O2	110.77 (10)	C17—C18—C19	120.07 (13)
O1—C6—C7	109.08 (11)	C17—C18—H18	120
O2—C6—C7	109.30 (11)	C19—C18—H18	120
O1—C6—H6	109.2	C18—C19—C20	119.97 (14)
O2—C6—H6	109.2	C18—C19—H19	120
C7—C6—H6	109.2	C20—C19—H19	120
C8—C7—C12	119.57 (12)	C19—C20—C15	120.17 (13)
C8—C7—C6	121.27 (12)	C19—C20—H20	119.9
C12—C7—C6	119.06 (12)	C15—C20—H20	119.9
C7—C8—C9	119.79 (12)	C6—O1—C5	109.91 (10)
C7—C8—H8	120.1	C6—O2—C3	110.49 (10)
C9—C8—H8	120.1	C14—O3—C2	112.91 (10)
C10—C9—C8	120.36 (13)	C14—O4—C13	111.41 (9)
C10—C9—H9	119.8	C1—S1—C4	94.89 (6)
C8—C9—H9	119.8		
C13—C1—C2—O3	47.28 (14)	O3—C14—C15—C16	129.50 (12)
S1—C1—C2—O3	-76.39 (11)	O4—C14—C15—C20	67.48 (15)
C13—C1—C2—C3	161.68 (10)	O3—C14—C15—C20	-51.66 (15)
S1—C1—C2—C3	38.02 (11)	C20—C15—C16—C17	-0.2 (2)
O3—C2—C3—O2	-172.01 (9)	C14—C15—C16—C17	178.65 (12)
C1—C2—C3—O2	69.39 (12)	C15—C16—C17—C18	-0.4 (2)
O3—C2—C3—C4	69.21 (12)	C16—C17—C18—C19	0.8 (2)
C1—C2—C3—C4	-49.39 (13)	C17—C18—C19—C20	-0.6 (2)
O2—C3—C4—C5	45.85 (15)	C18—C19—C20—C15	0.0 (2)
C2—C3—C4—C5	160.99 (11)	C16—C15—C20—C19	0.4 (2)
O2—C3—C4—S1	-78.37 (11)	C14—C15—C20—C19	-178.47 (13)
C2—C3—C4—S1	36.77 (11)	O2—C6—O1—C5	-66.02 (13)
C3—C4—C5—O1	-46.70 (16)	C7—C6—O1—C5	173.64 (10)
S1—C4—C5—O1	72.07 (13)	C4—C5—O1—C6	56.52 (14)
O1—C6—C7—C8	153.67 (12)	O1—C6—O2—C3	65.43 (13)
O2—C6—C7—C8	32.42 (17)	C7—C6—O2—C3	-174.35 (10)
O1—C6—C7—C12	-30.07 (16)	C2—C3—O2—C6	-170.15 (10)
O2—C6—C7—C12	-151.31 (12)	C4—C3—O2—C6	-54.71 (13)
C12—C7—C8—C9	0.9 (2)	O4—C14—O3—C2	60.93 (13)
C6—C7—C8—C9	177.15 (13)	C15—C14—O3—C2	177.96 (10)
C7—C8—C9—C10	-1.7 (2)	C3—C2—O3—C14	-169.74 (10)
C8—C9—C10—C11	1.4 (3)	C1—C2—O3—C14	-53.83 (13)
C9—C10—C11—C12	-0.3 (2)	O3—C14—O4—C13	-62.23 (13)
C10—C11—C12—C7	-0.5 (2)	C15—C14—O4—C13	-179.58 (10)
C8—C7—C12—C11	0.2 (2)	C1—C13—O4—C14	57.33 (14)
C6—C7—C12—C11	-176.16 (13)	C13—C1—S1—C4	-134.53 (10)
C2—C1—C13—O4	-49.24 (15)	C2—C1—S1—C4	-13.96 (9)
S1—C1—C13—O4	68.77 (13)	C5—C4—S1—C1	-134.60 (10)
O4—C14—C15—C16	-111.36 (13)	C3—C4—S1—C1	-12.90 (9)
