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2-(Tritylsulfanyl)ethyl 3-iodobenzoate

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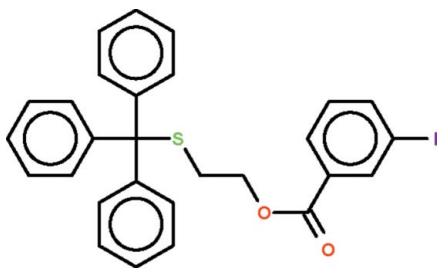
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.045; wR factor = 0.126; data-to-parameter ratio = 14.7.

The triphenylmethyl group in the title compound, $\text{C}_{28}\text{H}_{23}\text{IO}_2\text{S}$, has the methine carbon slightly flattened out [$\Sigma\text{C}_{\text{phenyl}}-\text{C}-\text{C}_{\text{phenyl}} = 332.8$ (6)°]. The $-\text{C}-\text{O}-\text{C}-\text{C}-\text{S}-$ chain connecting the triphenylmethyl group and the aromatic ring adopts an extended zigzag conformation, these five atoms being approximately co-planar (r.m.s. deviation 0.260 Å).

Related literature

For the 2-iodobenzoate analog, see: Zhu *et al.* (2011).

Experimental

Crystal data

$\text{C}_{28}\text{H}_{23}\text{IO}_2\text{S}$	$\gamma = 65.663$ (1)°
$M_r = 550.42$	$V = 1223.9$ (2) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.1634$ (8) Å	Mo $K\alpha$ radiation
$b = 8.8413$ (9) Å	$\mu = 1.42$ mm ⁻¹
$c = 18.9968$ (18) Å	$T = 293$ K
$\alpha = 89.493$ (1)°	$0.40 \times 0.35 \times 0.20$ mm
$\beta = 79.270$ (2)°	

Data collection

Bruker SMART APEX diffractometer	5948 measured reflections
Absorption correction: multi-scan (SADABS, Sheldrick, 1996)	4254 independent reflections
$T_{\min} = 0.601$, $T_{\max} = 0.765$	3375 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	290 parameters
$wR(F^2) = 0.126$	H-atom parameters constrained
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.89$ e Å ⁻³
4254 reflections	$\Delta\rho_{\text{min}} = -1.33$ e Å ⁻³

Data collection: *APEX2* (Bruker, 2007); cell refinement: *S SAINT* (Bruker, 2007); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2142).

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supplementary materials

Acta Cryst. (2011). E67, o2631 [doi:10.1107/S1600536811036427]

2-(Tritylsulfanyl)ethyl 3-iodobenzoate

X. Zhu and S. W. Ng

Comment

Triphenylmethyl is an important *S*-protecting group that prevents a thiol group from reacting with sensitive functional groups. The compound $C_{28}H_{23}IO_2S$ (Scheme I) was synthesized for the purpose of examining copper(I) chloride-catalyzed cleavage reactions, the present study following a previous structural determination of the 2-iodobenzoate analog (Zhu *et al.*, 2011). The methine carbon is slightly flattened out ($\Sigma C_{\text{phenyl}}-C-C_{\text{phenyl}}$ 332.8 (6) °) owing to decreased crowding by the S atom. The $-C-O-C-S-$ chain connecting the triphenylmethyl group and the aromatic ring adopts an extended zigzag conformation, these five atoms lying on an approximate plane (r.m.s. deviation 0.260 Å) (Fig. 1).

Experimental

A solution of 3-iodobenzoic acid (0.74 g, 3 mmol), dicyclohexylcarbodiimide (1.03 g, 5 mmol) and 4-dimethylaminopyridine (0.61 g, 8 mmol) in THF (20 ml) was stirred for an hour. 2-(tritylthio)ethanol (0.96 g, 3 mmol) was added. The reaction was stirred for 36 h. The compound was purified by column chromatography with petroleum ether–acetone (2:1) as the eluent and was isolated upon evaporation of the solvent as yellow crystals (2.30 g, 80% yield).

Refinement

Carbon-bound H-atoms were placed in calculated positions ($C-H = 0.93$ to 0.97 Å) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(H)$ set to $1.2U_{\text{eq}}(C)$. The final difference Fourier map had a peak in the vicinity of I1.

Figures

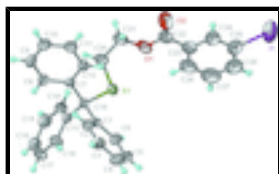


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{28}H_{23}IO_2S$ at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

2-(Tritylsulfanyl)ethyl 3-iodobenzoate

Crystal data

$C_{28}H_{23}IO_2S$

$M_r = 550.42$

Triclinic, *PT*

Hall symbol: -P 1

$Z = 2$

$F(000) = 552$

$D_x = 1.494 \text{ Mg m}^{-3}$

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

supplementary materials

$a = 8.1634$ (8) Å	Cell parameters from 2381 reflections
$b = 8.8413$ (9) Å	$\theta = 2.9\text{--}25.0^\circ$
$c = 18.9968$ (18) Å	$\mu = 1.42$ mm ⁻¹
$\alpha = 89.493$ (1)°	$T = 293$ K
$\beta = 79.270$ (2)°	Prism, yellow
$\gamma = 65.663$ (1)°	$0.40 \times 0.35 \times 0.20$ mm
$V = 1223.9$ (2) Å ³	

Data collection

Bruker SMART APEX diffractometer	4254 independent reflections
Radiation source: fine-focus sealed tube	3375 reflections with $I > 2\sigma(I)$
graphite	$R_{\text{int}} = 0.018$
ω scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (SADABS, Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.601$, $T_{\text{max}} = 0.765$	$k = -10 \rightarrow 10$
5948 measured reflections	$l = -22 \rightarrow 19$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.126$	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 1.4533P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
4254 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
290 parameters	$\Delta\rho_{\text{max}} = 0.89$ e Å ⁻³
0 restraints	$\Delta\rho_{\text{min}} = -1.33$ e Å ⁻³
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0354 (19)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Il	0.70737 (7)	0.61227 (5)	0.60081 (2)	0.1219 (3)
S1	0.73375 (12)	-0.09689 (11)	0.27224 (4)	0.0482 (2)
O1	0.9395 (4)	-0.0436 (4)	0.37588 (14)	0.0733 (8)
O2	1.0491 (6)	0.1484 (5)	0.3642 (2)	0.1083 (13)
C1	0.5442 (4)	-0.0134 (3)	0.16643 (17)	0.0376 (7)
C2	0.5437 (4)	0.0440 (4)	0.09843 (18)	0.0446 (7)
H2	0.6475	-0.0058	0.0623	0.054*
C3	0.3903 (5)	0.1748 (5)	0.0836 (2)	0.0569 (9)
H3	0.3920	0.2127	0.0378	0.068*

C4	0.2358 (5)	0.2489 (5)	0.1365 (2)	0.0626 (10)
H4	0.1326	0.3365	0.1265	0.075*
C5	0.2343 (5)	0.1929 (4)	0.2040 (2)	0.0591 (10)
H5	0.1303	0.2440	0.2400	0.071*
C6	0.3854 (4)	0.0617 (4)	0.21896 (19)	0.0482 (8)
H6	0.3815	0.0227	0.2646	0.058*
C7	0.8838 (4)	-0.1952 (4)	0.12723 (16)	0.0362 (6)
C8	0.9698 (4)	-0.3353 (4)	0.08007 (18)	0.0455 (7)
H8	0.9232	-0.4155	0.0825	0.055*
C9	1.1256 (5)	-0.3583 (5)	0.0288 (2)	0.0576 (9)
H9	1.1830	-0.4543	-0.0022	0.069*
C10	1.1947 (5)	-0.2414 (5)	0.0235 (2)	0.0565 (9)
H10	1.2975	-0.2564	-0.0115	0.068*
C11	1.1113 (5)	-0.1011 (5)	0.0702 (2)	0.0549 (9)
H11	1.1589	-0.0216	0.0673	0.066*
C12	0.9576 (4)	-0.0776 (4)	0.12155 (18)	0.0462 (8)
H12	0.9024	0.0180	0.1528	0.055*
C13	0.6642 (4)	-0.3178 (4)	0.18842 (17)	0.0385 (7)
C14	0.7540 (5)	-0.4510 (4)	0.2265 (2)	0.0510 (8)
H14	0.8427	-0.4480	0.2502	0.061*
C15	0.7132 (5)	-0.5887 (4)	0.2296 (2)	0.0601 (10)
H15	0.7749	-0.6769	0.2555	0.072*
C16	0.5843 (5)	-0.5972 (4)	0.1953 (2)	0.0625 (10)
H16	0.5566	-0.6895	0.1982	0.075*
C17	0.4959 (6)	-0.4673 (5)	0.1566 (3)	0.0659 (11)
H17	0.4090	-0.4722	0.1323	0.079*
C18	0.5353 (5)	-0.3291 (4)	0.1533 (2)	0.0557 (9)
H18	0.4738	-0.2420	0.1269	0.067*
C19	0.7098 (4)	-0.1647 (4)	0.18310 (16)	0.0364 (6)
C20	0.9669 (5)	-0.2308 (5)	0.2817 (2)	0.0594 (9)
H20A	0.9645	-0.3123	0.3160	0.071*
H20B	1.0386	-0.2898	0.2359	0.071*
C21	1.0527 (6)	-0.1264 (6)	0.3073 (2)	0.0700 (11)
H21A	1.1769	-0.1958	0.3127	0.084*
H21B	1.0567	-0.0452	0.2731	0.084*
C22	0.9472 (6)	0.0942 (6)	0.3973 (2)	0.0688 (11)
C23	0.8168 (6)	0.1760 (6)	0.4656 (2)	0.0694 (11)
C24	0.8162 (6)	0.3195 (6)	0.4935 (2)	0.0754 (12)
H24	0.8964	0.3620	0.4696	0.090*
C25	0.6974 (7)	0.4010 (7)	0.5568 (2)	0.0841 (14)
C26	0.5784 (8)	0.3367 (10)	0.5919 (3)	0.1035 (19)
H26	0.4970	0.3913	0.6342	0.124*
C27	0.5801 (8)	0.1935 (11)	0.5645 (3)	0.114 (2)
H27	0.5005	0.1506	0.5886	0.137*
C28	0.6994 (7)	0.1116 (8)	0.5013 (2)	0.0902 (16)
H28	0.7003	0.0140	0.4829	0.108*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
II	0.1472 (5)	0.1016 (4)	0.0882 (3)	-0.0278 (3)	-0.0128 (3)	-0.0138 (2)
S1	0.0494 (5)	0.0535 (5)	0.0438 (5)	-0.0241 (4)	-0.0075 (4)	-0.0034 (4)
O1	0.085 (2)	0.115 (2)	0.0464 (15)	-0.0680 (19)	-0.0136 (14)	0.0030 (15)
O2	0.131 (3)	0.129 (3)	0.082 (2)	-0.093 (3)	0.032 (2)	-0.024 (2)
C1	0.0354 (15)	0.0313 (15)	0.0498 (18)	-0.0184 (13)	-0.0062 (13)	0.0012 (13)
C2	0.0424 (17)	0.0432 (17)	0.0494 (19)	-0.0198 (15)	-0.0074 (14)	0.0049 (14)
C3	0.054 (2)	0.056 (2)	0.065 (2)	-0.0259 (18)	-0.0183 (18)	0.0207 (18)
C4	0.045 (2)	0.045 (2)	0.092 (3)	-0.0110 (16)	-0.018 (2)	0.0169 (19)
C5	0.0410 (19)	0.047 (2)	0.077 (3)	-0.0113 (16)	0.0002 (17)	0.0031 (18)
C6	0.0423 (18)	0.0459 (18)	0.053 (2)	-0.0179 (15)	-0.0026 (15)	0.0062 (15)
C7	0.0326 (15)	0.0367 (15)	0.0403 (16)	-0.0152 (12)	-0.0078 (12)	0.0046 (12)
C8	0.0420 (17)	0.0408 (17)	0.0540 (19)	-0.0196 (14)	-0.0045 (15)	0.0006 (14)
C9	0.050 (2)	0.053 (2)	0.059 (2)	-0.0162 (17)	0.0039 (17)	-0.0092 (17)
C10	0.0441 (19)	0.065 (2)	0.058 (2)	-0.0262 (17)	0.0034 (16)	0.0054 (18)
C11	0.051 (2)	0.055 (2)	0.070 (2)	-0.0343 (17)	-0.0078 (17)	0.0108 (18)
C12	0.0462 (18)	0.0416 (17)	0.055 (2)	-0.0243 (15)	-0.0048 (15)	-0.0004 (14)
C13	0.0369 (15)	0.0309 (15)	0.0475 (17)	-0.0172 (13)	-0.0005 (13)	0.0001 (12)
C14	0.0467 (19)	0.0408 (18)	0.067 (2)	-0.0198 (15)	-0.0118 (16)	0.0074 (16)
C15	0.061 (2)	0.0365 (18)	0.079 (3)	-0.0205 (17)	-0.006 (2)	0.0131 (17)
C16	0.061 (2)	0.0404 (19)	0.089 (3)	-0.0312 (18)	0.003 (2)	-0.0027 (18)
C17	0.064 (2)	0.055 (2)	0.095 (3)	-0.038 (2)	-0.023 (2)	0.002 (2)
C18	0.058 (2)	0.0453 (19)	0.076 (3)	-0.0291 (17)	-0.0241 (19)	0.0108 (17)
C19	0.0361 (15)	0.0337 (15)	0.0412 (16)	-0.0173 (13)	-0.0058 (12)	0.0012 (12)
C20	0.055 (2)	0.071 (2)	0.058 (2)	-0.0274 (19)	-0.0214 (18)	0.0077 (18)
C21	0.064 (2)	0.106 (3)	0.054 (2)	-0.048 (2)	-0.0177 (19)	0.004 (2)
C22	0.069 (3)	0.097 (3)	0.052 (2)	-0.048 (2)	-0.010 (2)	0.004 (2)
C23	0.064 (2)	0.105 (3)	0.047 (2)	-0.041 (2)	-0.0158 (19)	0.011 (2)
C24	0.074 (3)	0.097 (3)	0.054 (2)	-0.037 (3)	-0.007 (2)	0.007 (2)
C25	0.078 (3)	0.107 (4)	0.055 (3)	-0.025 (3)	-0.016 (2)	0.003 (2)
C26	0.078 (3)	0.166 (6)	0.058 (3)	-0.049 (4)	-0.002 (2)	-0.006 (3)
C27	0.097 (4)	0.203 (7)	0.066 (3)	-0.092 (5)	0.000 (3)	0.006 (4)
C28	0.088 (3)	0.147 (5)	0.059 (3)	-0.075 (3)	-0.008 (2)	0.008 (3)

Geometric parameters (\AA , $^\circ$)

II—C25	2.091 (6)	C12—H12	0.9300
S1—C20	1.823 (4)	C13—C18	1.383 (5)
S1—C19	1.872 (3)	C13—C14	1.385 (5)
O1—C22	1.317 (5)	C13—C19	1.542 (4)
O1—C21	1.449 (5)	C14—C15	1.387 (5)
O2—C22	1.202 (5)	C14—H14	0.9300
C1—C2	1.384 (4)	C15—C16	1.363 (6)
C1—C6	1.392 (4)	C15—H15	0.9300
C1—C19	1.542 (4)	C16—C17	1.372 (6)
C2—C3	1.384 (5)	C16—H16	0.9300

C2—H2	0.9300	C17—C18	1.384 (5)
C3—C4	1.374 (6)	C17—H17	0.9300
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.371 (6)	C20—C21	1.498 (5)
C4—H4	0.9300	C20—H20A	0.9700
C5—C6	1.377 (5)	C20—H20B	0.9700
C5—H5	0.9300	C21—H21A	0.9700
C6—H6	0.9300	C21—H21B	0.9700
C7—C8	1.378 (4)	C22—C23	1.486 (6)
C7—C12	1.395 (4)	C23—C24	1.378 (7)
C7—C19	1.532 (4)	C23—C28	1.379 (6)
C8—C9	1.392 (5)	C24—C25	1.382 (6)
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.361 (5)	C25—C26	1.385 (8)
C9—H9	0.9300	C26—C27	1.367 (9)
C10—C11	1.375 (5)	C26—H26	0.9300
C10—H10	0.9300	C27—C28	1.384 (8)
C11—C12	1.379 (5)	C27—H27	0.9300
C11—H11	0.9300	C28—H28	0.9300
C20—S1—C19	105.86 (16)	C15—C16—H16	120.6
C22—O1—C21	117.5 (3)	C17—C16—H16	120.6
C2—C1—C6	118.2 (3)	C16—C17—C18	120.5 (4)
C2—C1—C19	121.6 (3)	C16—C17—H17	119.8
C6—C1—C19	120.0 (3)	C18—C17—H17	119.8
C3—C2—C1	120.7 (3)	C17—C18—C13	121.4 (3)
C3—C2—H2	119.6	C17—C18—H18	119.3
C1—C2—H2	119.6	C13—C18—H18	119.3
C4—C3—C2	120.2 (4)	C7—C19—C1	110.8 (2)
C4—C3—H3	119.9	C7—C19—C13	112.6 (2)
C2—C3—H3	119.9	C1—C19—C13	109.4 (2)
C5—C4—C3	119.7 (3)	C7—C19—S1	109.38 (19)
C5—C4—H4	120.2	C1—C19—S1	102.89 (19)
C3—C4—H4	120.2	C13—C19—S1	111.3 (2)
C4—C5—C6	120.5 (3)	C21—C20—S1	109.3 (3)
C4—C5—H5	119.8	C21—C20—H20A	109.8
C6—C5—H5	119.8	S1—C20—H20A	109.8
C5—C6—C1	120.7 (3)	C21—C20—H20B	109.8
C5—C6—H6	119.7	S1—C20—H20B	109.8
C1—C6—H6	119.7	H20A—C20—H20B	108.3
C8—C7—C12	117.8 (3)	O1—C21—C20	106.6 (3)
C8—C7—C19	122.0 (3)	O1—C21—H21A	110.4
C12—C7—C19	120.2 (3)	C20—C21—H21A	110.4
C7—C8—C9	120.8 (3)	O1—C21—H21B	110.4
C7—C8—H8	119.6	C20—C21—H21B	110.4
C9—C8—H8	119.6	H21A—C21—H21B	108.6
C10—C9—C8	120.6 (3)	O2—C22—O1	123.0 (4)
C10—C9—H9	119.7	O2—C22—C23	123.6 (4)
C8—C9—H9	119.7	O1—C22—C23	113.4 (4)
C9—C10—C11	119.5 (3)	C24—C23—C28	120.0 (4)

supplementary materials

C9—C10—H10	120.3	C24—C23—C22	118.1 (4)
C11—C10—H10	120.3	C28—C23—C22	121.9 (5)
C12—C11—C10	120.4 (3)	C23—C24—C25	120.5 (5)
C12—C11—H11	119.8	C23—C24—H24	119.7
C10—C11—H11	119.8	C25—C24—H24	119.7
C11—C12—C7	120.9 (3)	C24—C25—C26	119.2 (5)
C11—C12—H12	119.6	C24—C25—H1	119.9 (4)
C7—C12—H12	119.6	C26—C25—H1	120.8 (4)
C18—C13—C14	117.4 (3)	C27—C26—C25	120.3 (5)
C18—C13—C19	120.9 (3)	C27—C26—H26	119.9
C14—C13—C19	121.6 (3)	C25—C26—H26	119.9
C13—C14—C15	120.7 (3)	C26—C27—C28	120.6 (5)
C13—C14—H14	119.7	C26—C27—H27	119.7
C15—C14—H14	119.7	C28—C27—H27	119.7
C16—C15—C14	121.2 (4)	C23—C28—C27	119.5 (6)
C16—C15—H15	119.4	C23—C28—H28	120.3
C14—C15—H15	119.4	C27—C28—H28	120.3
C15—C16—C17	118.8 (3)		
C6—C1—C2—C3	1.3 (5)	C2—C1—C19—C13	-104.0 (3)
C19—C1—C2—C3	176.8 (3)	C6—C1—C19—C13	71.4 (3)
C1—C2—C3—C4	-0.4 (5)	C2—C1—C19—S1	137.6 (2)
C2—C3—C4—C5	0.2 (6)	C6—C1—C19—S1	-46.9 (3)
C3—C4—C5—C6	-0.9 (6)	C18—C13—C19—C7	-98.5 (3)
C4—C5—C6—C1	1.9 (6)	C14—C13—C19—C7	79.5 (4)
C2—C1—C6—C5	-2.0 (5)	C18—C13—C19—C1	25.2 (4)
C19—C1—C6—C5	-177.6 (3)	C14—C13—C19—C1	-156.8 (3)
C12—C7—C8—C9	0.3 (5)	C18—C13—C19—S1	138.2 (3)
C19—C7—C8—C9	178.6 (3)	C14—C13—C19—S1	-43.8 (4)
C7—C8—C9—C10	-0.9 (6)	C20—S1—C19—C7	-42.7 (2)
C8—C9—C10—C11	1.2 (6)	C20—S1—C19—C1	-160.5 (2)
C9—C10—C11—C12	-0.8 (6)	C20—S1—C19—C13	82.4 (2)
C10—C11—C12—C7	0.1 (6)	C19—S1—C20—C21	133.8 (3)
C8—C7—C12—C11	0.1 (5)	C22—O1—C21—C20	-157.3 (4)
C19—C7—C12—C11	-178.2 (3)	S1—C20—C21—O1	59.9 (4)
C18—C13—C14—C15	-0.8 (5)	C21—O1—C22—O2	-3.5 (7)
C19—C13—C14—C15	-178.9 (3)	C21—O1—C22—C23	175.9 (3)
C13—C14—C15—C16	0.1 (6)	O2—C22—C23—C24	-1.8 (7)
C14—C15—C16—C17	0.8 (6)	O1—C22—C23—C24	178.8 (4)
C15—C16—C17—C18	-1.0 (6)	O2—C22—C23—C28	178.7 (5)
C16—C17—C18—C13	0.2 (6)	O1—C22—C23—C28	-0.8 (6)
C14—C13—C18—C17	0.7 (5)	C28—C23—C24—C25	-0.6 (7)
C19—C13—C18—C17	178.7 (3)	C22—C23—C24—C25	179.8 (4)
C8—C7—C19—C1	-113.4 (3)	C23—C24—C25—C26	-0.1 (7)
C12—C7—C19—C1	64.9 (3)	C23—C24—C25—H1	177.1 (3)
C8—C7—C19—C13	9.6 (4)	C24—C25—C26—C27	0.7 (8)
C12—C7—C19—C13	-172.1 (3)	H1—C25—C26—C27	-176.5 (5)
C8—C7—C19—S1	133.9 (3)	C25—C26—C27—C28	-0.5 (10)
C12—C7—C19—S1	-47.8 (3)	C24—C23—C28—C27	0.8 (8)
C2—C1—C19—C7	20.8 (4)	C22—C23—C28—C27	-179.7 (5)

C6—C1—C19—C7

-163.8 (3)

C26—C27—C28—C23

-0.2 (9)

Fig. 1

