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2-(Tritylsulfanyl)ethyl 3-iodobenzoate

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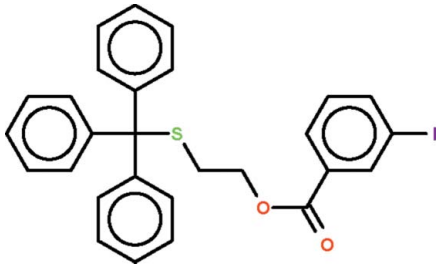
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.045; wR factor = 0.126; data-to-parameter ratio = 14.7.

The triphenylmethyl group in the title compound, $C_{28}H_{23}IO_2S$, has the methine carbon slightly flattened out [$\Sigma C_{phenyl}—C—C_{phenyl}$ = 332.8 (6) °]. The –C–O–C–C–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

$C_{28}H_{23}IO_2S$
M_r = 550.42
Triclinic, $P\overline{1}$
a = 8.1634 (8) Å
b = 8.8413 (9) Å
c = 18.9968 (18) Å
α = 89.493 (1)°
β = 79.270 (2)°
γ = 65.663 (1)°
V = 1223.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 293 K
0.40 × 0.35 × 0.20 mm

Data collection

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

Refinement

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *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: *publCIF* (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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Zhu, X., Lu, P. & Ng, S. W. (2011). *Acta Cryst.* E**67**, o2475.

supporting information

Acta Cryst. (2011). E**67**, o2631 [https://doi.org/10.1107/S1600536811036427]

2-(Tritylsulfanyl)ethyl 3-iodobenzoate

Xin Zhu and Seik Weng Ng

S1. 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 (ΣC_{phenyl}–*C*–C_{phenyl} 332.8 (6) °) owing to decreased crowding by the S atom. The –C–O–C–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).

S2. Experimental

A solution of 3-iodobenzoic acid (0.74 g, 3 mmol), dicyclohexylcarbodiimide (1.03 g, 5 mmol) and 4-dimethylamino-pyridine (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).

S3. 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_{iso}(H) set to 1.2U_{eq}(C). The final difference Fourier map had a peak in the vicinity of I1.

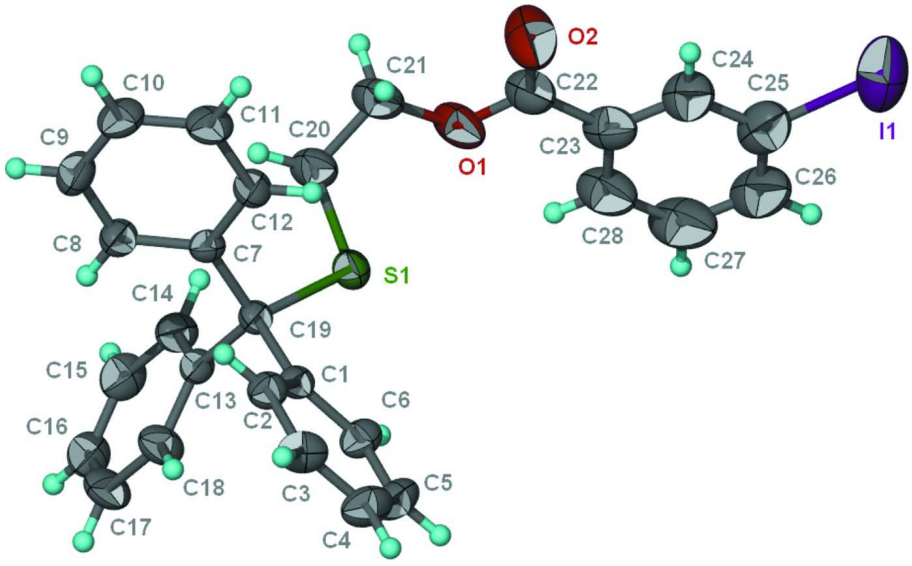

Figure 1

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, $P\overline{1}$
Hall symbol: -P 1
$a = 8.1634$ (8) Å
$b = 8.8413$ (9) Å
$c = 18.9968$ (18) Å
$\alpha = 89.493$ (1)°
$\beta = 79.270$ (2)°
$\gamma = 65.663$ (1)°
$V = 1223.9$ (2) Å^3
$Z = 2$
$F(000) = 552$
$D_x = 1.494$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2381 reflections
$\theta = 2.9$–$25.0°$
$\mu = 1.42$ mm^{-1}
$T = 293$ K
Prism, yellow
0.40 × 0.35 × 0.20 mm

Data collection

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

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.126$
$S = 1.02$
4254 reflections
290 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
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 1.4533P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -1.33$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0354 (19)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	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*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	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 (Å, º)

I1—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)
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—I1	119.9 (4)
C7—C12—H12	119.6	C26—C25—I1	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—I1	177.1 (3)
C8—C7—C19—C13	9.6 (4)	C24—C25—C26—C27	0.7 (8)
C12—C7—C19—C13	−172.1 (3)	I1—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)