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2-(Tritylsulfanyl)ethyl 2-iodobenzoate

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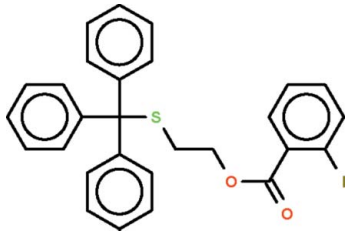
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.096; data-to-parameter ratio = 19.3.

The methine C atom of the triphenylmethyl group in the title compound, $C_{28}H_{23}IO_2S$, is slightly flattened out [$\Sigma C_{phenyl}—C—C_{phenyl}$ = 335.6 (5)°]. 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 = 0.120 Å).

Related literature

For the copper(I)-catalysed cleavage of *S*-tritylmethyl thioethers, see: Ma *et al.* (2007); Zhang *et al.* (2009).



Experimental

Crystal data

$C_{28}H_{23}IO_2S$
M_r = 550.42
Monoclinic, $C2/c$
a = 28.4378 (4) Å
b = 9.6154 (1) Å
c = 18.3808 (2) Å
β = 106.618 (1)°
V = 4816.13 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.672, T_{max} = 0.870
15633 measured reflections
5564 independent reflections
4506 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.096
S = 1.01
5564 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 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: XU5302).

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2-(Tritylsulfanyl)ethyl 2-iodobenzoate

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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 cupper(I) chloride-catalyzed cleavage investigation (Ma *et al.*, 2007; Zhang *et al.*, 2009). The methine carbon slightly flattened out (ΣC_{phenyl}–*C*–C_{phenyl} 335.6 (5) °) 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 0.120 Å) (Fig. 1).

S2. Experimental

A solution of 2-iodobenzoic acid (1.24 g, 5 mmol), dicyclohexylcarbodiimide (1.65 g, 8 mmol) and 4-dimethylamino-pyridine (0.98 g, 8 mmol) in THF (20 ml) was stirred for an hour. 2-(Tritylthio)ethanol (1.60 g, 5 mmol) was added. The reaction was stirred for 48 h. The compound was purified by column chromatography with petroleumether–chloroform (3:1) as the eluent. The compound was isolated upon evaporation of the solvent as yellow crystals (2.02 g, 70% 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*(H) set to 1.2*U*(C).

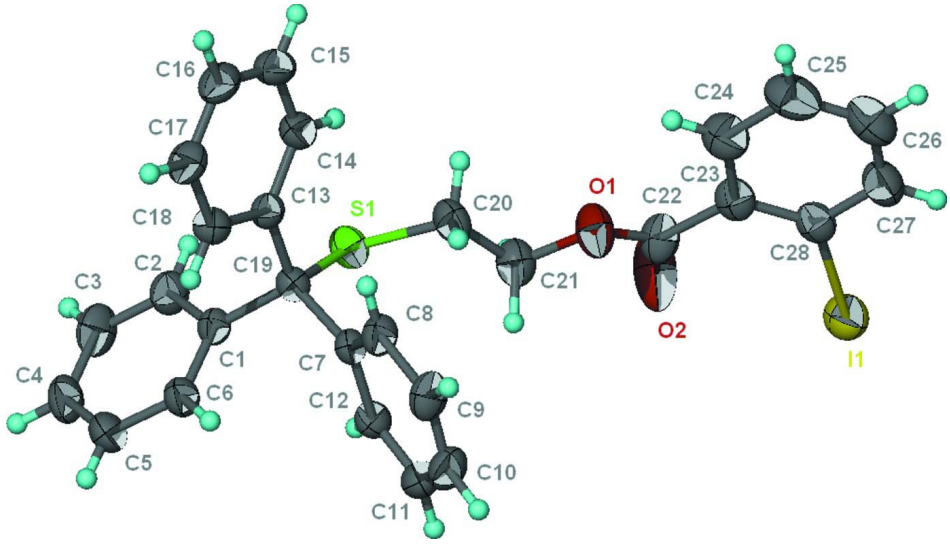

Figure 1

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-[(triphenylmethyl)sulfanyl]ethyl 2-iodobenzoate

Crystal data

$C_{28}H_{23}IO_2S$
$M_r = 550.42$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 28.4378$ (4) Å
$b = 9.6154$ (1) Å
$c = 18.3808$ (2) Å
$\beta = 106.618$ (1)°
$V = 4816.13$ (10) Å^3
$Z = 8$
$F(000) = 2208$
$D_x = 1.518$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6921 reflections
$\theta = 2.4$–$27.4°$
$\mu = 1.44$ mm^{-1}
$T = 293$ K
Prism, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.672$, $T_{max} = 0.870$
15633 measured reflections
5564 independent reflections
4506 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.7°$, $\theta_{min} = 2.3°$
$h = -37 \rightarrow 33$
$k = -11 \rightarrow 12$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.096$
$S = 1.01$
5564 reflections
289 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
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 3.6231P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.613888 (7)	0.54548 (2)	0.524788 (11)	0.06653 (9)
S1	0.42074 (2)	1.00910 (7)	0.68754 (4)	0.04999 (15)
O1	0.48562 (7)	0.6866 (2)	0.62115 (13)	0.0667 (5)
O2	0.56063 (9)	0.7361 (3)	0.6179 (2)	0.1131 (11)
C1	0.34622 (8)	1.1936 (2)	0.64315 (12)	0.0395 (4)
C2	0.36875 (10)	1.2693 (3)	0.70807 (14)	0.0538 (6)
H2	0.3901	1.2249	0.7494	0.065*
C3	0.35972 (11)	1.4105 (3)	0.71197 (17)	0.0653 (7)
H3	0.3759	1.4599	0.7554	0.078*
C4	0.32767 (12)	1.4781 (3)	0.65340 (18)	0.0632 (7)
H4	0.3219	1.5727	0.6566	0.076*
C5	0.30396 (11)	1.4042 (3)	0.58932 (16)	0.0581 (6)
H5	0.2814	1.4488	0.5494	0.070*

C6	0.31346 (9)	1.2644 (3)	0.58382 (13)	0.0477 (5)
H6	0.2977	1.2165	0.5396	0.057*
C7	0.34474 (8)	0.9869 (2)	0.55660 (12)	0.0378 (4)
C8	0.31287 (9)	0.8805 (3)	0.52546 (13)	0.0477 (5)
H8	0.2971	0.8321	0.5556	0.057*
C9	0.30400 (10)	0.8445 (3)	0.44904 (14)	0.0583 (6)
H9	0.2826	0.7721	0.4288	0.070*
C10	0.32654 (11)	0.9150 (3)	0.40389 (14)	0.0607 (7)
H10	0.3197	0.8927	0.3527	0.073*
C11	0.35946 (11)	1.0193 (3)	0.43456 (15)	0.0557 (6)
H11	0.3754	1.0662	0.4042	0.067*
C12	0.36889 (9)	1.0546 (2)	0.51009 (13)	0.0466 (5)
H12	0.3916	1.1242	0.5304	0.056*
C13	0.32141 (8)	0.9602 (2)	0.68042 (12)	0.0394 (4)
C14	0.33881 (9)	0.8611 (3)	0.73632 (13)	0.0485 (5)
H14	0.3721	0.8396	0.7514	0.058*
C15	0.30749 (11)	0.7933 (3)	0.77023 (14)	0.0563 (6)
H15	0.3199	0.7259	0.8070	0.068*
C16	0.25806 (10)	0.8250 (3)	0.74968 (14)	0.0562 (6)
H16	0.2371	0.7797	0.7724	0.067*
C17	0.24038 (10)	0.9249 (3)	0.69503 (15)	0.0532 (6)
H17	0.2072	0.9480	0.6812	0.064*
C18	0.27160 (9)	0.9912 (3)	0.66036 (13)	0.0467 (5)
H18	0.2590	1.0576	0.6231	0.056*
C19	0.35420 (8)	1.0362 (2)	0.63906 (12)	0.0385 (4)
C20	0.43229 (9)	0.8328 (3)	0.66178 (16)	0.0551 (6)
H20A	0.4385	0.7730	0.7060	0.066*
H20B	0.4037	0.7976	0.6236	0.066*
C21	0.47580 (10)	0.8317 (3)	0.63140 (17)	0.0601 (6)
H21A	0.4686	0.8811	0.5835	0.072*
H21B	0.5038	0.8752	0.6670	0.072*
C22	0.52920 (9)	0.6522 (3)	0.61484 (16)	0.0581 (6)
C23	0.53339 (9)	0.4982 (3)	0.60730 (14)	0.0515 (6)
C24	0.50377 (11)	0.4115 (4)	0.63571 (18)	0.0675 (7)
H24	0.4814	0.4507	0.6580	0.081*
C25	0.50676 (12)	0.2688 (4)	0.6317 (2)	0.0801 (9)
H25	0.4869	0.2125	0.6516	0.096*
C26	0.53938 (13)	0.2107 (4)	0.5980 (2)	0.0790 (9)
H26	0.5415	0.1145	0.5950	0.095*
C27	0.56871 (11)	0.2933 (3)	0.56890 (16)	0.0652 (7)
H27	0.5904	0.2527	0.5457	0.078*
C28	0.56646 (9)	0.4366 (3)	0.57364 (14)	0.0506 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.05710 (13)	0.06887 (15)	0.07605 (15)	0.00487 (8)	0.02295 (9)	0.00746 (9)
S1	0.0392 (3)	0.0480 (3)	0.0585 (3)	0.0024 (2)	0.0071 (2)	0.0001 (3)

O1	0.0485 (10)	0.0558 (11)	0.0997 (14)	0.0031 (9)	0.0275 (9)	−0.0087 (11)
O2	0.0711 (14)	0.0704 (16)	0.215 (3)	−0.0192 (13)	0.0685 (18)	−0.0479 (19)
C1	0.0402 (10)	0.0371 (11)	0.0428 (10)	−0.0014 (9)	0.0145 (8)	−0.0039 (9)
C2	0.0558 (14)	0.0530 (15)	0.0490 (12)	0.0005 (11)	0.0094 (10)	−0.0101 (11)
C3	0.0713 (17)	0.0556 (16)	0.0688 (16)	−0.0108 (14)	0.0200 (14)	−0.0277 (14)
C4	0.0789 (19)	0.0374 (14)	0.0806 (19)	0.0029 (13)	0.0346 (16)	−0.0084 (13)
C5	0.0715 (17)	0.0439 (14)	0.0613 (14)	0.0122 (13)	0.0226 (13)	0.0062 (12)
C6	0.0531 (13)	0.0414 (13)	0.0472 (11)	0.0047 (10)	0.0122 (10)	−0.0028 (10)
C7	0.0406 (10)	0.0333 (10)	0.0404 (10)	0.0039 (8)	0.0128 (8)	−0.0014 (8)
C8	0.0500 (12)	0.0442 (13)	0.0520 (12)	−0.0025 (10)	0.0197 (10)	−0.0074 (10)
C9	0.0576 (14)	0.0584 (16)	0.0587 (14)	−0.0045 (12)	0.0161 (11)	−0.0207 (13)
C10	0.0691 (16)	0.0694 (18)	0.0443 (12)	0.0090 (14)	0.0175 (11)	−0.0094 (12)
C11	0.0704 (16)	0.0532 (15)	0.0497 (13)	0.0091 (13)	0.0269 (12)	0.0060 (11)
C12	0.0542 (13)	0.0389 (12)	0.0489 (12)	0.0010 (10)	0.0184 (10)	0.0017 (10)
C13	0.0457 (11)	0.0358 (11)	0.0376 (10)	−0.0016 (9)	0.0133 (8)	−0.0049 (8)
C14	0.0562 (13)	0.0424 (13)	0.0471 (11)	0.0038 (11)	0.0152 (10)	0.0015 (10)
C15	0.0778 (17)	0.0461 (14)	0.0486 (12)	−0.0006 (13)	0.0238 (12)	0.0049 (11)
C16	0.0701 (16)	0.0510 (15)	0.0561 (13)	−0.0126 (13)	0.0315 (12)	−0.0054 (12)
C17	0.0498 (13)	0.0575 (15)	0.0570 (13)	−0.0053 (11)	0.0228 (11)	−0.0069 (12)
C18	0.0483 (12)	0.0465 (13)	0.0456 (11)	0.0010 (10)	0.0141 (10)	0.0020 (10)
C19	0.0377 (10)	0.0362 (11)	0.0406 (10)	0.0010 (8)	0.0098 (8)	0.0012 (8)
C20	0.0473 (13)	0.0479 (14)	0.0692 (15)	0.0100 (11)	0.0154 (11)	0.0047 (12)
C21	0.0527 (14)	0.0559 (16)	0.0718 (16)	0.0020 (12)	0.0181 (12)	−0.0063 (13)
C22	0.0429 (12)	0.0636 (17)	0.0682 (15)	−0.0021 (12)	0.0164 (11)	−0.0129 (13)
C23	0.0399 (12)	0.0550 (14)	0.0537 (13)	0.0027 (11)	0.0038 (10)	−0.0012 (12)
C24	0.0514 (14)	0.0707 (19)	0.0801 (19)	0.0011 (14)	0.0182 (13)	0.0079 (16)
C25	0.0674 (19)	0.072 (2)	0.098 (2)	−0.0073 (17)	0.0195 (17)	0.0247 (19)
C26	0.083 (2)	0.0524 (18)	0.095 (2)	0.0014 (16)	0.0163 (18)	0.0085 (17)
C27	0.0673 (17)	0.0558 (17)	0.0693 (16)	0.0127 (14)	0.0146 (13)	0.0021 (14)
C28	0.0438 (12)	0.0512 (14)	0.0512 (12)	0.0043 (10)	0.0048 (10)	0.0019 (11)

Geometric parameters (Å, º)

I1—C28	2.101 (3)	C12—H12	0.9300
S1—C20	1.815 (3)	C13—C14	1.385 (3)
S1—C19	1.865 (2)	C13—C18	1.390 (3)
O1—C22	1.319 (3)	C13—C19	1.544 (3)
O1—C21	1.445 (4)	C14—C15	1.387 (4)
O2—C22	1.193 (4)	C14—H14	0.9300
C1—C2	1.388 (3)	C15—C16	1.381 (4)
C1—C6	1.392 (3)	C15—H15	0.9300
C1—C19	1.536 (3)	C16—C17	1.376 (4)
C2—C3	1.387 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.388 (4)
C3—C4	1.360 (5)	C17—H17	0.9300
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.375 (4)	C20—C21	1.496 (4)
C4—H4	0.9300	C20—H20A	0.9700

C5—C6	1.381 (4)	C20—H20B	0.9700
C5—H5	0.9300	C21—H21A	0.9700
C6—H6	0.9300	C21—H21B	0.9700
C7—C8	1.378 (3)	C22—C23	1.495 (4)
C7—C12	1.401 (3)	C23—C24	1.389 (4)
C7—C19	1.537 (3)	C23—C28	1.397 (4)
C8—C9	1.398 (3)	C24—C25	1.378 (5)
C8—H8	0.9300	C24—H24	0.9300
C9—C10	1.365 (4)	C25—C26	1.373 (5)
C9—H9	0.9300	C25—H25	0.9300
C10—C11	1.378 (4)	C26—C27	1.366 (5)
C10—H10	0.9300	C26—H26	0.9300
C11—C12	1.379 (3)	C27—C28	1.383 (4)
C11—H11	0.9300	C27—H27	0.9300

C20—S1—C19	103.90 (11)	C17—C16—H16	120.5
C22—O1—C21	118.3 (2)	C15—C16—H16	120.5
C2—C1—C6	117.3 (2)	C16—C17—C18	120.5 (2)
C2—C1—C19	121.4 (2)	C16—C17—H17	119.7
C6—C1—C19	121.23 (19)	C18—C17—H17	119.7
C3—C2—C1	120.7 (2)	C17—C18—C13	121.1 (2)
C3—C2—H2	119.6	C17—C18—H18	119.4
C1—C2—H2	119.6	C13—C18—H18	119.4
C4—C3—C2	121.2 (3)	C1—C19—C7	111.43 (17)
C4—C3—H3	119.4	C1—C19—C13	108.88 (17)
C2—C3—H3	119.4	C7—C19—C13	112.31 (17)
C3—C4—C5	119.0 (3)	C1—C19—S1	104.96 (14)
C3—C4—H4	120.5	C7—C19—S1	107.20 (14)
C5—C4—H4	120.5	C13—C19—S1	111.83 (14)
C4—C5—C6	120.5 (3)	C21—C20—S1	109.6 (2)
C4—C5—H5	119.8	C21—C20—H20A	109.8
C6—C5—H5	119.8	S1—C20—H20A	109.8
C5—C6—C1	121.3 (2)	C21—C20—H20B	109.8
C5—C6—H6	119.3	S1—C20—H20B	109.8
C1—C6—H6	119.3	H20A—C20—H20B	108.2
C8—C7—C12	118.1 (2)	O1—C21—C20	105.5 (2)
C8—C7—C19	123.2 (2)	O1—C21—H21A	110.6
C12—C7—C19	118.7 (2)	C20—C21—H21A	110.6
C7—C8—C9	120.6 (2)	O1—C21—H21B	110.6
C7—C8—H8	119.7	C20—C21—H21B	110.6
C9—C8—H8	119.7	H21A—C21—H21B	108.8
C10—C9—C8	120.5 (3)	O2—C22—O1	122.4 (3)
C10—C9—H9	119.8	O2—C22—C23	126.5 (3)
C8—C9—H9	119.8	O1—C22—C23	111.0 (2)
C9—C10—C11	119.7 (2)	C24—C23—C28	118.0 (3)
C9—C10—H10	120.2	C24—C23—C22	119.1 (3)
C11—C10—H10	120.2	C28—C23—C22	122.9 (2)
C10—C11—C12	120.3 (2)	C25—C24—C23	121.7 (3)

C10—C11—H11	119.8	C25—C24—H24	119.2
C12—C11—H11	119.8	C23—C24—H24	119.2
C11—C12—C7	120.8 (2)	C26—C25—C24	119.3 (3)
C11—C12—H12	119.6	C26—C25—H25	120.4
C7—C12—H12	119.6	C24—C25—H25	120.4
C14—C13—C18	117.7 (2)	C27—C26—C25	120.5 (3)
C14—C13—C19	123.5 (2)	C27—C26—H26	119.8
C18—C13—C19	118.74 (19)	C25—C26—H26	119.8
C13—C14—C15	121.2 (2)	C26—C27—C28	120.6 (3)
C13—C14—H14	119.4	C26—C27—H27	119.7
C15—C14—H14	119.4	C28—C27—H27	119.7
C16—C15—C14	120.5 (2)	C27—C28—C23	120.0 (3)
C16—C15—H15	119.8	C27—C28—I1	115.0 (2)
C14—C15—H15	119.8	C23—C28—I1	125.0 (2)
C17—C16—C15	119.0 (2)		

C6—C1—C2—C3	−1.9 (4)	C12—C7—C19—C13	174.8 (2)
C19—C1—C2—C3	−177.5 (2)	C8—C7—C19—S1	119.2 (2)
C1—C2—C3—C4	1.8 (5)	C12—C7—C19—S1	−62.0 (2)
C2—C3—C4—C5	0.0 (5)	C14—C13—C19—C1	−128.4 (2)
C3—C4—C5—C6	−1.6 (4)	C18—C13—C19—C1	52.3 (3)
C4—C5—C6—C1	1.5 (4)	C14—C13—C19—C7	107.7 (2)
C2—C1—C6—C5	0.3 (4)	C18—C13—C19—C7	−71.6 (3)
C19—C1—C6—C5	175.9 (2)	C14—C13—C19—S1	−12.9 (3)
C12—C7—C8—C9	−1.9 (4)	C18—C13—C19—S1	167.80 (17)
C19—C7—C8—C9	177.0 (2)	C20—S1—C19—C1	−166.42 (15)
C7—C8—C9—C10	−0.4 (4)	C20—S1—C19—C7	−47.83 (17)
C8—C9—C10—C11	2.1 (4)	C20—S1—C19—C13	75.69 (17)
C9—C10—C11—C12	−1.3 (4)	C19—S1—C20—C21	129.09 (19)
C10—C11—C12—C7	−1.0 (4)	C22—O1—C21—C20	−161.8 (2)
C8—C7—C12—C11	2.6 (3)	S1—C20—C21—O1	173.37 (18)
C19—C7—C12—C11	−176.3 (2)	C21—O1—C22—O2	0.6 (5)
C18—C13—C14—C15	1.1 (3)	C21—O1—C22—C23	178.1 (2)
C19—C13—C14—C15	−178.2 (2)	O2—C22—C23—C24	153.0 (4)
C13—C14—C15—C16	−1.1 (4)	O1—C22—C23—C24	−24.4 (4)
C14—C15—C16—C17	0.1 (4)	O2—C22—C23—C28	−26.1 (5)
C15—C16—C17—C18	0.9 (4)	O1—C22—C23—C28	156.5 (2)
C16—C17—C18—C13	−0.8 (4)	C28—C23—C24—C25	0.5 (4)
C14—C13—C18—C17	−0.2 (3)	C22—C23—C24—C25	−178.7 (3)
C19—C13—C18—C17	179.2 (2)	C23—C24—C25—C26	−0.8 (5)
C2—C1—C19—C7	−156.2 (2)	C24—C25—C26—C27	0.2 (5)
C6—C1—C19—C7	28.3 (3)	C25—C26—C27—C28	0.8 (5)
C2—C1—C19—C13	79.4 (3)	C26—C27—C28—C23	−1.1 (4)
C6—C1—C19—C13	−96.1 (2)	C26—C27—C28—I1	−179.5 (2)
C2—C1—C19—S1	−40.5 (3)	C24—C23—C28—C27	0.5 (4)
C6—C1—C19—S1	144.05 (18)	C22—C23—C28—C27	179.6 (2)
C8—C7—C19—C1	−126.5 (2)	C24—C23—C28—I1	178.69 (19)
C12—C7—C19—C1	52.3 (3)	C22—C23—C28—I1	−2.2 (3)

C8—C7—C19—C13	−4.0 (3)