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4′-Chlorobiphenyl-3-yl 2,2,2-trichloroethyl sulfate

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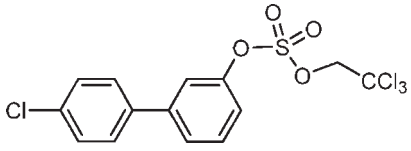
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 18.1.

The title compound, $C_{14}H_{10}Cl_4O_4S$, is a 2,2,2-trichloroethyl-protected precursor of 4′-chlorobiphenyl-3-yl sulfate, a sulfuric acid ester of 4′-chlorobiphenyl-3-ol. The $C_{aromatic}$—O and O—S bond lengths of the $C_{aromatic}$—O—S unit are comparable to those in structurally analogous biphenyl-4-yl 2,2,2-trichloroethyl sulfates with no electronegative chlorine substituent in the benzene ring with the sulfate ester group. The dihedral angle between the aromatic rings is 27.47 (6)°.

Related literature

For similar structures of sulfuric acid biphenyl-4-yl ester 2,2,2-trichloro-ethyl esters, see: Li *et al.* (2008, 2010*a*,*b*,*c*). For a review of structures of sulfuric acid aryl mono esters, see: Brandao *et al.* (2005). For further discussion of dihedral angles in chlorinated biphenyl derivatives, see: Lehmler *et al.* (2002); Shaikh *et al.* (2008); Vyas *et al.* (2006). For additional background to hydroxylated polychlorinated biphenyls, see: Bergman *et al.* (1994); Buckman *et al.* (2006); Dirtu *et al.* (2010); Liu *et al.* (2006, 2009); Nomiyama *et al.* (2010); Wang *et al.* (2006).



Experimental

Crystal data

$C_{14}H_{10}Cl_4O_4S$
M_r = 416.08
Monoclinic, $I2/a$
a = 21.1900 (3) Å
b = 5.8543 (1) Å
c = 26.6803 (5) Å
β = 98.304 (1)°
V = 3275.06 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 90 K
0.41 × 0.22 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.718, T_{max} = 0.950
30021 measured reflections
3759 independent reflections
3242 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.05
3759 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and local procedures.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2350).

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supplementary materials

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4'-Chlorobiphenyl-3-yl 2,2,2-trichloroethyl sulfate

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Comment

Hydroxylated metabolites of polychlorinated biphenyls (OHPCBs) are present in the serum of humans (Bergman *et al.*, 1994; Dirtu *et al.*, 2010) and other animals (Buckman *et al.*, 2006; Nomiyama *et al.*, 2010). Recent studies also indicate that the mammalian cytosolic sulfotransferases catalyze the formation of sulfuric acid esters from OHPCBs (Liu *et al.*, 2006; Liu *et al.*, 2009; Wang *et al.*, 2006). However, our knowledge of the metabolic and toxicologic significance of these sulfation reactions has been hindered by a lack of information on the structural and chemical properties of the sulfuric acid ester products. As one component of our continuing studies on the properties of the sulfuric acid esters of OHPCBs, we report here the structure of 4'-chloro-biphenyl-3-yl 2,2,2-trichloroethyl sulfate.

Several authors have proposed that the $C_{aromatic}$—O and the corresponding O—S bond lengths are correlated with the stability of sulfuric acid conjugates (Brandao *et al.*, 2005; Li *et al.*, 2010*a*-*c*; Li *et al.*, 2008). The $C_{aromatic}$—O (*i.e.*, C3'-O1) and O—S (*i.e.*, O1—S1) bond lengths of the title compound are 1.4338 (17) Å and 1.5685 (11) Å, respectively. These values are comparable to the corresponding bond lengths reported for analogous biphenyl-4-yl 2,2,2-trichloroethyl sulfates with no electronegative chlorine substituent in the sulfated benzene ring (Li *et al.*, 2010*a*-*c*; Li *et al.*, 2008), which suggest that, analogous to biphenyl-4-yl sulfates, the 4'-chloro-biphenyl-3-yl sulfate corresponding to the title compound may be stable under physiological conditions (Brandao *et al.*, 2005; Li *et al.*, 2010*c*).

The dihedral angle of the biphenyl moiety of OHPCBs and, consequently, their sulfuric acid conjugates is associated with their affinity for cellular target molecules and, therefore, may correlate with their toxicity. The title compound adopts a solid state dihedral angle of 27.47 (6)°. The solid state dihedral angles of structurally related biphenyl-4-yl 2,2,2-trichloroethyl sulfates without *ortho* chlorine substituents ranges from 4.9 (2)° to 41.84 (16)° (Li *et al.*, 2010*a*,*b*; Li *et al.*, 2008). This large range of dihedral angles suggests, similar to the parent PCBs (Lehmler *et al.,* 2002; Shaikh *et al.*, 2008; Vyas *et al.*, 2006), a conformational flexibility of the biphenyl moiety that allows the title compound and analogous biphenyl-4-yl sulfates to adopt an energetically less favorable conformation in the solid state due to crystal packing effects.

Experimental

The title compound was synthesized from 3',4'-dichlorobiphenyl-4-ol by sulfation with 2,2,2-trichloroethyl sulfonyl chloride using 4-dimethylaminopyridine as catalyst (Li *et al.*, 2010*c*). Crystals suitable for crystal structure analysis were obtained by slowly evaporating a methanolic solution of the title compound.

Refinement

H atoms were placed in idealized positions and were constrained with distances of 0.99 Å for CH_2 and 0.95 Å for $C_{ar}H$, and with $U_{iso}(H) = 1.2U_{eq}$ of their attached C atom.

Figures

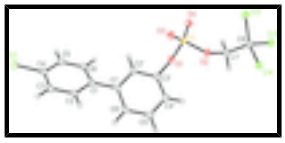


Fig. 1. View of the title compound showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

4'-Chlorobiphenyl-3-yl 2,2,2-trichloroethyl sulfate

Crystal data

$C_{14}H_{10}Cl_4O_4S$	$F(000) = 1680$
$M_r = 416.08$	$D_x = 1.688$ Mg m^{-3}
Monoclinic, *I*2/*a*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -I 2ya	Cell parameters from 4127 reflections
a = 21.1900 (3) Å	θ = 1.0–27.5°
b = 5.8543 (1) Å	μ = 0.87 mm^{-1}
c = 26.6803 (5) Å	*T* = 90 K
β = 98.304 (1)°	Plate, colourless
V = 3275.06 (10) Å^3	0.41 × 0.22 × 0.06 mm
Z = 8	

Data collection

Nonius KappaCCD diffractometer	3759 independent reflections
Radiation source: fine-focus sealed tube	3242 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.041$
Detector resolution: 18 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 1.5°$
ω scans at fixed χ = 55°	*h* = −27→27
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)	*k* = −7→7
$T_{min} = 0.718$, $T_{max} = 0.950$	*l* = −34→34
30021 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.067$	H-atom parameters constrained
S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 3.9224P]$ where $P = (F_o^2 + 2F_c^2)/3$
3759 reflections	$(\Delta/\sigma)_{max} = 0.001$
208 parameters	$\Delta\rho_{max} = 0.39$ e Å^{-3}

0 restraints $\Delta\rho_{min} = -0.38$ e Å^{-3}

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.205499 (17)	0.54226 (7)	0.300571 (14)	0.01597 (9)
O1	0.18726 (5)	0.4208 (2)	0.24808 (4)	0.0172 (2)
O2	0.19895 (5)	0.3440 (2)	0.33919 (4)	0.0183 (2)
O3	0.15849 (5)	0.7045 (2)	0.30865 (4)	0.0221 (2)
O4	0.27060 (5)	0.6040 (2)	0.30274 (4)	0.0248 (3)
Cl1	−0.064775 (19)	1.32997 (7)	0.026719 (15)	0.02388 (10)
Cl2	0.279773 (19)	0.45519 (7)	0.437358 (15)	0.02180 (10)
Cl3	0.333188 (17)	0.00690 (7)	0.427046 (15)	0.02125 (10)
Cl4	0.199083 (17)	0.05436 (7)	0.434813 (14)	0.01980 (10)
C1	0.01131 (7)	0.7573 (3)	0.13260 (5)	0.0141 (3)
C2	−0.05371 (7)	0.8102 (3)	0.12421 (6)	0.0169 (3)
H2	−0.0823	0.7255	0.1414	0.020*
C3	−0.07744 (7)	0.9834 (3)	0.09145 (6)	0.0182 (3)
H3	−0.1217	1.0176	0.0863	0.022*
C4	−0.03566 (7)	1.1058 (3)	0.06635 (6)	0.0173 (3)
C5	0.02901 (7)	1.0572 (3)	0.07324 (6)	0.0179 (3)
H5	0.0571	1.1412	0.0555	0.021*
C6	0.05201 (7)	0.8843 (3)	0.10634 (6)	0.0169 (3)
H6	0.0964	0.8512	0.1114	0.020*
C1'	0.03627 (7)	0.5740 (3)	0.16854 (5)	0.0139 (3)
C2'	0.09909 (7)	0.5839 (3)	0.19354 (5)	0.0147 (3)
H2'	0.1259	0.7090	0.1881	0.018*
C3'	0.12148 (7)	0.4097 (3)	0.22605 (5)	0.0150 (3)
C4'	0.08533 (7)	0.2238 (3)	0.23630 (6)	0.0169 (3)
H4'	0.1025	0.1062	0.2588	0.020*
C5'	0.02240 (7)	0.2170 (3)	0.21209 (6)	0.0175 (3)
H5'	−0.0044	0.0935	0.2186	0.021*
C6'	−0.00152 (7)	0.3877 (3)	0.17880 (5)	0.0155 (3)
H6'	−0.0444	0.3785	0.1625	0.019*
C7	0.25272 (7)	0.1927 (3)	0.35354 (6)	0.0166 (3)
H7A	0.2910	0.2522	0.3406	0.020*

H7B	0.2431	0.0387	0.3391	0.020*
C8	0.26470 (7)	0.1800 (3)	0.41106 (6)	0.0153 (3)

Atomic displacement parameters (Å^2)

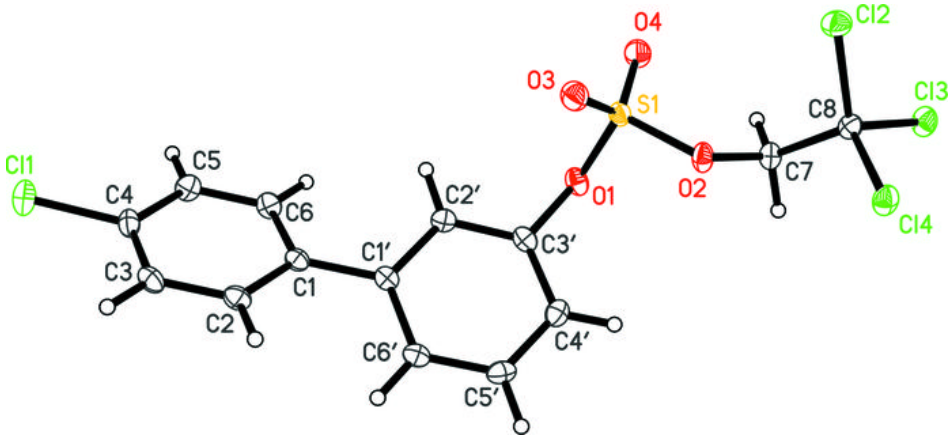
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01324 (17)	0.0176 (2)	0.01656 (19)	−0.00114 (14)	0.00035 (13)	0.00386 (14)
O1	0.0119 (5)	0.0242 (6)	0.0157 (5)	0.0030 (4)	0.0023 (4)	0.0016 (5)
O2	0.0130 (5)	0.0241 (6)	0.0179 (5)	0.0007 (4)	0.0025 (4)	0.0087 (5)
O3	0.0221 (6)	0.0204 (6)	0.0228 (6)	0.0036 (5)	0.0000 (4)	−0.0015 (5)
O4	0.0158 (5)	0.0291 (7)	0.0282 (6)	−0.0073 (5)	−0.0011 (4)	0.0095 (5)
Cl1	0.0251 (2)	0.0248 (2)	0.0220 (2)	0.00861 (17)	0.00412 (15)	0.00689 (16)
Cl2	0.0263 (2)	0.0171 (2)	0.0219 (2)	−0.00104 (15)	0.00333 (15)	−0.00356 (15)
Cl3	0.01544 (17)	0.0210 (2)	0.0267 (2)	0.00532 (15)	0.00114 (14)	0.00543 (16)
Cl4	0.01582 (17)	0.0237 (2)	0.02059 (19)	−0.00115 (15)	0.00512 (14)	0.00656 (15)
C1	0.0139 (7)	0.0161 (7)	0.0124 (7)	−0.0002 (6)	0.0017 (5)	−0.0024 (6)
C2	0.0122 (7)	0.0210 (8)	0.0178 (7)	−0.0024 (6)	0.0032 (5)	−0.0008 (6)
C3	0.0115 (7)	0.0231 (8)	0.0196 (8)	0.0011 (6)	0.0003 (6)	−0.0021 (6)
C4	0.0196 (7)	0.0177 (8)	0.0137 (7)	0.0047 (6)	0.0000 (6)	0.0007 (6)
C5	0.0179 (7)	0.0195 (8)	0.0175 (8)	−0.0004 (6)	0.0066 (6)	0.0017 (6)
C6	0.0120 (7)	0.0203 (8)	0.0190 (7)	0.0020 (6)	0.0048 (5)	−0.0003 (6)
C1'	0.0127 (6)	0.0173 (8)	0.0123 (7)	0.0005 (6)	0.0034 (5)	−0.0017 (6)
C2'	0.0132 (7)	0.0170 (8)	0.0149 (7)	−0.0011 (6)	0.0050 (5)	−0.0005 (6)
C3'	0.0109 (6)	0.0199 (8)	0.0144 (7)	0.0023 (6)	0.0027 (5)	−0.0021 (6)
C4'	0.0213 (7)	0.0158 (8)	0.0143 (7)	0.0018 (6)	0.0051 (6)	0.0006 (6)
C5'	0.0215 (8)	0.0166 (8)	0.0155 (7)	−0.0053 (6)	0.0067 (6)	−0.0028 (6)
C6'	0.0145 (7)	0.0186 (8)	0.0138 (7)	−0.0019 (6)	0.0034 (5)	−0.0033 (6)
C7	0.0168 (7)	0.0180 (8)	0.0152 (7)	0.0029 (6)	0.0030 (5)	0.0024 (6)
C8	0.0136 (7)	0.0145 (7)	0.0180 (7)	0.0016 (6)	0.0031 (5)	0.0009 (6)

Geometric parameters (Å, °)

S1—O3	1.4153 (12)	C4—C5	1.386 (2)
S1—O4	1.4191 (11)	C5—C6	1.385 (2)
S1—O1	1.5685 (11)	C5—H5	0.9500
S1—O2	1.5714 (11)	C6—H6	0.9500
O1—C3'	1.4338 (17)	C1'—C2'	1.401 (2)
O2—C7	1.4503 (18)	C1'—C6'	1.403 (2)
Cl1—C4	1.7412 (16)	C2'—C3'	1.378 (2)
Cl2—C8	1.7677 (16)	C2'—H2'	0.9500
Cl3—C8	1.7710 (15)	C3'—C4'	1.381 (2)
Cl4—C8	1.7693 (15)	C4'—C5'	1.396 (2)
C1—C2	1.398 (2)	C4'—H4'	0.9500
C1—C6	1.401 (2)	C5'—C6'	1.384 (2)
C1—C1'	1.485 (2)	C5'—H5'	0.9500
C2—C3	1.385 (2)	C6'—H6'	0.9500
C2—H2	0.9500	C7—C8	1.521 (2)
C3—C4	1.385 (2)	C7—H7A	0.9900
C3—H3	0.9500	C7—H7B	0.9900

O3—S1—O4	121.62 (8)	C6'—C1'—C1	121.85 (13)
O3—S1—O1	110.62 (6)	C3'—C2'—C1'	119.08 (14)
O4—S1—O1	105.34 (7)	C3'—C2'—H2'	120.5
O3—S1—O2	105.39 (7)	C1'—C2'—H2'	120.5
O4—S1—O2	109.79 (6)	C2'—C3'—C4'	123.88 (14)
O1—S1—O2	102.53 (6)	C2'—C3'—O1	116.77 (13)
C3'—O1—S1	119.08 (9)	C4'—C3'—O1	119.27 (14)
C7—O2—S1	118.95 (9)	C3'—C4'—C5'	116.82 (14)
C2—C1—C6	117.78 (14)	C3'—C4'—H4'	121.6
C2—C1—C1'	120.96 (13)	C5'—C4'—H4'	121.6
C6—C1—C1'	121.26 (13)	C6'—C5'—C4'	120.90 (14)
C3—C2—C1	121.53 (14)	C6'—C5'—H5'	119.6
C3—C2—H2	119.2	C4'—C5'—H5'	119.6
C1—C2—H2	119.2	C5'—C6'—C1'	121.33 (14)
C2—C3—C4	119.01 (14)	C5'—C6'—H6'	119.3
C2—C3—H3	120.5	C1'—C6'—H6'	119.3
C4—C3—H3	120.5	O2—C7—C8	107.85 (12)
C3—C4—C5	121.24 (15)	O2—C7—H7A	110.1
C3—C4—Cl1	119.25 (12)	C8—C7—H7A	110.1
C5—C4—Cl1	119.48 (12)	O2—C7—H7B	110.1
C6—C5—C4	119.01 (14)	C8—C7—H7B	110.1
C6—C5—H5	120.5	H7A—C7—H7B	108.5
C4—C5—H5	120.5	C7—C8—Cl2	110.51 (11)
C5—C6—C1	121.43 (14)	C7—C8—Cl4	110.88 (11)
C5—C6—H6	119.3	Cl2—C8—Cl4	110.07 (8)
C1—C6—H6	119.3	C7—C8—Cl3	106.40 (10)
C2'—C1'—C6'	117.97 (14)	Cl2—C8—Cl3	109.34 (8)
C2'—C1'—C1	120.18 (13)	Cl4—C8—Cl3	109.56 (8)
O3—S1—O1—C3'	−24.84 (13)	C2—C1—C1'—C6'	27.7 (2)
O4—S1—O1—C3'	−158.01 (11)	C6—C1—C1'—C6'	−152.88 (15)
O2—S1—O1—C3'	87.12 (11)	C6'—C1'—C2'—C3'	1.4 (2)
O3—S1—O2—C7	−158.44 (11)	C1—C1'—C2'—C3'	−178.90 (13)
O4—S1—O2—C7	−25.84 (13)	C1'—C2'—C3'—C4'	−0.8 (2)
O1—S1—O2—C7	85.75 (11)	C1'—C2'—C3'—O1	176.06 (13)
C6—C1—C2—C3	−0.5 (2)	S1—O1—C3'—C2'	91.88 (14)
C1'—C1—C2—C3	178.90 (14)	S1—O1—C3'—C4'	−91.13 (15)
C1—C2—C3—C4	0.2 (2)	C2'—C3'—C4'—C5'	−0.5 (2)
C2—C3—C4—C5	0.4 (2)	O1—C3'—C4'—C5'	−177.25 (13)
C2—C3—C4—Cl1	−177.88 (12)	C3'—C4'—C5'—C6'	1.2 (2)
C3—C4—C5—C6	−0.7 (2)	C4'—C5'—C6'—C1'	−0.6 (2)
Cl1—C4—C5—C6	177.54 (12)	C2'—C1'—C6'—C5'	−0.7 (2)
C4—C5—C6—C1	0.4 (2)	C1—C1'—C6'—C5'	179.55 (14)
C2—C1—C6—C5	0.2 (2)	S1—O2—C7—C8	129.66 (11)
C1'—C1—C6—C5	−179.25 (14)	O2—C7—C8—Cl2	−58.24 (14)
C2—C1—C1'—C2'	−152.01 (15)	O2—C7—C8—Cl4	64.09 (14)
C6—C1—C1'—C2'	27.4 (2)	O2—C7—C8—Cl3	−176.84 (10)

Fig. 1


O4
Cl2
O3
S1
Cl3
C8
Cl1
C5
C4
C6
C2′
O1
O2
C7
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C1′
C3′
C3
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C2
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C4′
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