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Polymeric structure of disodium *p*-terphenyl-4,4″-disulfonate [$Na_2(O_3S\text{-}C_6H_4\text{-}C_6H_4\text{-}C_6H_4\text{-}SO_3)$]

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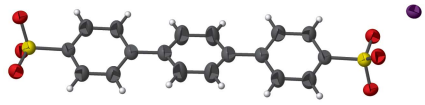
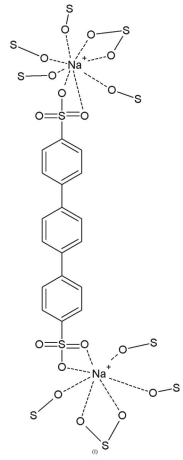
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $2Na^+\cdot C_{18}H_{12}O_6S_2^{2-}$, the sodium ion is sevenfold coordinated by O atoms of five sulfonate groups (two in a chelating and three in a monodentate binding mode). They form (100) layers of edge-, corner- and face-sharing [NaO_7] polyherdra which are interconnected by the terphenyl moieties. The asymmetric unit contains one sodium cation and one *p*-terphenyl-4,4″-disulfonate anion on a centre of inversion.

3D view



Chemical scheme



Structure description

The title compund is shown in Fig. 1. The layers built up by the NaO_7 polyhedra and the connection between these layers through the organic ligand are shown in Fig. 2.

Synthesis and crystallization

Disodium *para*-terphenyl-4,4″disulfonate was synthesized according to the procedure given by Muesmann *et al.* (2011). The compound was heated at 130°C solvothermally for 4 h in dilute nitric acid. After cooling to room temperature for 4 d crystals were obtained.

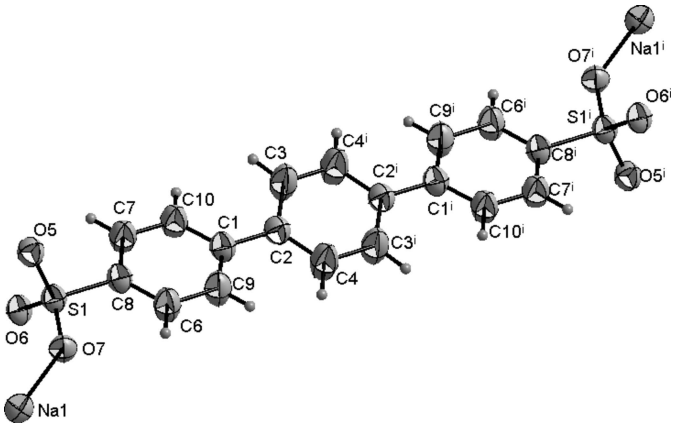


Figure 1
Part of the crystal structure of the title compound with labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $1-x, 2-y, -z$]

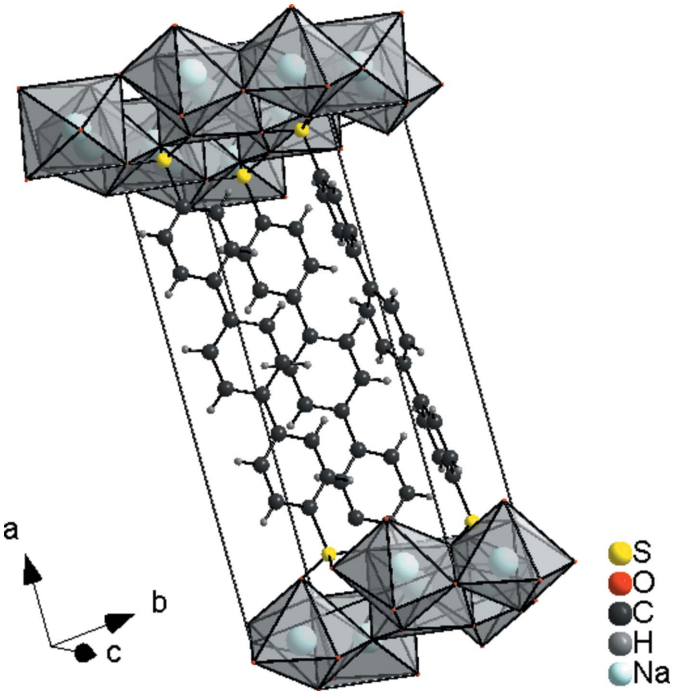


Figure 2
Part of the crystal structure of the title compound. The layers built up by the NaO_7 polyhedra and the connection between these layers through the organic ligand are shown.

Table 1
Experimental details.

Crystal data	
Chemical formula	$2Na^+ \cdot C_{18}H_{12}O_6S_2^{2-}$
M_r	434.38
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	17.662 (4), 8.2854 (17), 5.9719 (12)
β (°)	91.38 (3)
V (Å^3)	873.7 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	0.16 × 0.11 × 0.05
Data collection	
Diffractometer	Stoe *IPDS2* diffractometer
Absorption correction	Numerical (*X-SHAPE* and *X-RED*; Stoe, 2008)
T_{min}, T_{max}	0.902, 0.975
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1958, 1958, 1076
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.648
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.103, 1.05
No. of reflections	1958
No. of parameters	127
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.40

Computer programs: *X-AREA* (Stoe, 2008), *SHELXS2014/7* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999), *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

The authors like to thank Inke Jess for collecting the single-crystal data.

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full crystallographic data

IUCrData (2016). **1**, x160039 [doi:10.1107/S2414314616000390]

Polymeric structure of disodium *p*-terphenyl-4,4′′-disulfonate [$Na_2(O_3S$-C_6H_4-C_6H_4-C_6H_4-SO_3]

Martin Albat and Norbert Stock

Disodium *p*-terphenyl-4,4′′-disulfonate

Crystal data

$2Na^+ \cdot C_{18}H_{12}O_6S_2^{2-}$
M_r = 434.38
Monoclinic, $P2_1/c$
a = 17.662 (4) Å
b = 8.2854 (17) Å
c = 5.9719 (12) Å
β = 91.38 (3)°
V = 873.7 (3) Å^3
Z = 2
$F(000)$ = 444
D_x = 1.651 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8528 reflections
θ = 2.3–27.5°
μ = 0.39 mm^{-1}
T = 293 K
Needle, light brown
0.16 × 0.11 × 0.05 mm

Data collection

Stoe IPDS-2 diffractometer
Radiation source: fine-focus sealed tube
Phi scan
Absorption correction: numerical (*X-SHAPE* and *X-RED*; Stoe, 2008)
T_{min} = 0.902, T_{max} = 0.975
1958 measured reflections
1958 independent reflections
1076 reflections with $I > 2\sigma(I)$
θ_{max} = 27.4°, θ_{min} = 2.3°
h = −5→7
k = −10→10
l = −22→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.103
S = 1.05
1958 reflections
127 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.10160 (5)	1.00677 (12)	0.39209 (13)	0.0449 (2)
O5	0.08018 (12)	1.1730 (3)	0.4403 (4)	0.0498 (6)
O6	0.05617 (12)	0.9457 (3)	0.2019 (4)	0.0474 (6)
C1	0.34588 (18)	1.0039 (5)	0.1584 (5)	0.0493 (7)
C2	0.42455 (18)	1.0013 (5)	0.0773 (5)	0.0505 (8)
C9	0.3260 (2)	0.9301 (6)	0.3564 (6)	0.0654 (11)
H9A	0.3633	0.8790	0.4428	0.079*
C3	0.4476 (2)	1.1005 (7)	−0.0914 (8)	0.0807 (14)
H3A	0.4127	1.1710	−0.1574	0.097*
C4	0.4789 (2)	0.9009 (6)	0.1670 (8)	0.0817 (14)
H4A	0.4660	0.8314	0.2822	0.098*
C10	0.2884 (2)	1.0803 (6)	0.0367 (7)	0.0645 (11)
H10A	0.3000	1.1319	−0.0965	0.077*
C6	0.2524 (2)	0.9299 (6)	0.4299 (6)	0.0634 (11)
H6A	0.2407	0.8782	0.5628	0.076*
C7	0.2145 (2)	1.0822 (5)	0.1072 (7)	0.0649 (11)
H7A	0.1770	1.1339	0.0220	0.078*
C8	0.19665 (17)	1.0068 (5)	0.3051 (5)	0.0463 (7)
O7	0.09890 (13)	0.8979 (3)	0.5831 (4)	0.0505 (6)
Na1	0.02020 (7)	0.81590 (17)	0.8734 (2)	0.0487 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0426 (4)	0.0493 (5)	0.0430 (4)	−0.0006 (5)	0.0020 (3)	−0.0003 (5)
O5	0.0458 (13)	0.0521 (15)	0.0517 (13)	0.0020 (11)	0.0052 (10)	−0.0035 (12)
O6	0.0448 (12)	0.0556 (16)	0.0413 (11)	−0.0021 (10)	−0.0059 (9)	−0.0040 (10)
C1	0.0439 (16)	0.056 (2)	0.0484 (16)	0.000 (2)	0.0054 (13)	−0.001 (2)
C2	0.0453 (16)	0.053 (2)	0.0529 (18)	0.002 (2)	0.0064 (14)	0.002 (2)
C9	0.0453 (19)	0.093 (3)	0.058 (2)	0.007 (2)	0.0037 (17)	0.018 (2)
C3	0.049 (2)	0.109 (4)	0.085 (3)	0.016 (2)	0.013 (2)	0.040 (3)
C4	0.053 (2)	0.114 (4)	0.079 (3)	0.019 (3)	0.021 (2)	0.042 (3)
C10	0.0454 (19)	0.085 (3)	0.064 (2)	0.006 (2)	0.0119 (17)	0.024 (2)
C6	0.0454 (19)	0.089 (3)	0.056 (2)	0.004 (2)	0.0047 (17)	0.016 (2)
C7	0.047 (2)	0.083 (3)	0.065 (2)	0.006 (2)	0.0078 (17)	0.026 (2)
C8	0.0422 (16)	0.054 (2)	0.0432 (15)	0.0004 (18)	0.0050 (13)	−0.0035 (18)
O7	0.0488 (13)	0.0572 (15)	0.0455 (12)	0.0003 (12)	0.0026 (10)	0.0134 (12)
Na1	0.0523 (8)	0.0521 (8)	0.0416 (6)	0.0023 (7)	0.0004 (6)	−0.0007 (6)

Geometric parameters (Å, º)

S1—O7	1.456 (2)	C4—H4A	0.9300
S1—O5	1.459 (3)	C10—C7	1.381 (5)
S1—O6	1.465 (2)	C10—H10A	0.9300
S1—C8	1.769 (3)	C6—C8	1.377 (5)

S1—Na1^{i}	3.0225 (17)	C6—H6A	0.9300
S1—Na1^{ii}	3.0363 (18)	C7—C8	1.380 (5)
O5—Na1^{iii}	2.424 (3)	C7—H7A	0.9300
O5—Na1^{i}	2.550 (3)	O7—Na1	2.348 (3)
O6—Na1^{iv}	2.313 (3)	O7—Na1^{ii}	2.560 (3)
O6—Na1^{i}	2.428 (3)	Na1—O6^{vi}	2.313 (3)
O6—Na1^{ii}	2.487 (3)	Na1—O5^{vii}	2.424 (3)
C1—C9	1.384 (5)	Na1—O6^{i}	2.428 (3)
C1—C10	1.388 (5)	Na1—O6^{viii}	2.487 (3)
C1—C2	1.483 (5)	Na1—O5^{i}	2.550 (3)
C2—C3	1.369 (5)	Na1—O7^{viii}	2.560 (3)
C2—C4	1.369 (5)	Na1—S1^{i}	3.0225 (17)
C9—C6	1.381 (5)	Na1—S1^{viii}	3.0363 (18)
C9—H9A	0.9300	Na1—Na1^{ii}	3.1794 (11)
C3—C4^{v}	1.385 (5)	Na1—Na1^{viii}	3.1794 (11)
C3—H3A	0.9300	Na1—Na1^{ix}	3.486 (3)
C4—C3^{v}	1.385 (5)		

O7—S1—O5	114.63 (15)	O6^{vi}—Na1—O6^{viii}	133.41 (10)
O7—S1—O6	111.47 (15)	O7—Na1—O6^{viii}	77.66 (9)
O5—S1—O6	109.83 (14)	O5^{vii}—Na1—O6^{viii}	87.72 (9)
O7—S1—C8	106.21 (15)	O6^{i}—Na1—O6^{viii}	141.19 (6)
O5—S1—C8	108.07 (17)	O6^{vi}—Na1—O5^{i}	141.12 (10)
O6—S1—C8	106.16 (14)	O7—Na1—O5^{i}	81.99 (9)
O7—S1—Na1^{i}	132.52 (10)	O5^{vii}—Na1—O5^{i}	81.46 (8)
O5—S1—Na1^{i}	57.32 (10)	O6^{i}—Na1—O5^{i}	57.40 (8)
O6—S1—Na1^{i}	52.52 (10)	O6^{viii}—Na1—O5^{i}	84.76 (8)
C8—S1—Na1^{i}	120.96 (12)	O6^{vi}—Na1—O7^{viii}	76.82 (9)
O7—S1—Na1^{ii}	57.24 (11)	O7—Na1—O7^{viii}	103.72 (10)
O5—S1—Na1^{ii}	135.55 (10)	O5^{vii}—Na1—O7^{viii}	80.34 (9)
O6—S1—Na1^{ii}	54.37 (10)	O6^{i}—Na1—O7^{viii}	161.12 (9)
C8—S1—Na1^{ii}	116.17 (14)	O6^{viii}—Na1—O7^{viii}	57.13 (8)
Na1^{i}—S1—Na1^{ii}	94.50 (3)	O5^{i}—Na1—O7^{viii}	138.08 (10)
S1—O5—Na1^{iii}	138.38 (14)	O6^{vi}—Na1—S1^{i}	113.35 (8)
S1—O5—Na1^{i}	93.89 (12)	O7—Na1—S1^{i}	84.18 (7)
Na1^{iii}—O5—Na1^{i}	79.42 (8)	O5^{vii}—Na1—S1^{i}	87.65 (7)
S1—O6—Na1^{iv}	162.26 (15)	O6^{i}—Na1—S1^{i}	28.61 (5)
S1—O6—Na1^{i}	98.87 (12)	O6^{viii}—Na1—S1^{i}	113.16 (7)
Na1^{iv}—O6—Na1^{i}	94.66 (9)	O5^{i}—Na1—S1^{i}	28.79 (6)
S1—O6—Na1^{ii}	97.02 (12)	O7^{viii}—Na1—S1^{i}	164.60 (8)
Na1^{iv}—O6—Na1^{ii}	82.89 (8)	O6^{vi}—Na1—S1^{viii}	104.97 (7)
Na1^{i}—O6—Na1^{ii}	129.73 (10)	O7—Na1—S1^{viii}	89.64 (8)
C9—C1—C10	116.8 (3)	O5^{vii}—Na1—S1^{viii}	84.49 (7)
C9—C1—C2	122.2 (3)	O6^{i}—Na1—S1^{viii}	169.62 (7)
C10—C1—C2	121.0 (3)	O6^{viii}—Na1—S1^{viii}	28.61 (5)
C3—C2—C4	115.8 (3)	O5^{i}—Na1—S1^{viii}	112.26 (7)
C3—C2—C1	122.0 (3)	O7^{viii}—Na1—S1^{viii}	28.58 (5)
C4—C2—C1	122.3 (3)	S1^{i}—Na1—S1^{viii}	141.04 (5)

C6—C9—C1	122.2 (3)	O6^{vi}—Na1—Na1^{ii}	161.83 (7)
C6—C9—H9A	118.9	O7—Na1—Na1^{ii}	52.60 (7)
C1—C9—H9A	118.9	O5^{vii}—Na1—Na1^{ii}	106.25 (8)
C2—C3—C4^{v}	122.2 (4)	O6^{i}—Na1—Na1^{ii}	96.78 (7)
C2—C3—H3A	118.9	O6^{viii}—Na1—Na1^{ii}	46.20 (7)
C4^{v}—C3—H3A	118.9	O5^{i}—Na1—Na1^{ii}	48.55 (6)
C2—C4—C3^{v}	122.1 (4)	O7^{viii}—Na1—Na1^{ii}	102.09 (8)
C2—C4—H4A	119.0	S1^{i}—Na1—Na1^{ii}	71.96 (4)
C3^{v}—C4—H4A	119.0	S1^{viii}—Na1—Na1^{ii}	73.82 (5)
C7—C10—C1	122.0 (3)	O6^{vi}—Na1—Na1^{viii}	50.90 (6)
C7—C10—H10A	119.0	O7—Na1—Na1^{viii}	143.71 (6)
C1—C10—H10A	119.0	O5^{vii}—Na1—Na1^{viii}	52.03 (7)
C8—C6—C9	119.6 (3)	O6^{i}—Na1—Na1^{viii}	116.16 (7)
C8—C6—H6A	120.2	O6^{viii}—Na1—Na1^{viii}	95.35 (8)
C9—C6—H6A	120.2	O5^{i}—Na1—Na1^{viii}	133.37 (7)
C8—C7—C10	119.6 (3)	O7^{viii}—Na1—Na1^{viii}	46.78 (6)
C8—C7—H7A	120.2	S1^{i}—Na1—Na1^{viii}	130.06 (4)
C10—C7—H7A	120.2	S1^{viii}—Na1—Na1^{viii}	70.96 (5)
C7—C8—C6	119.9 (3)	Na1^{ii}—Na1—Na1^{viii}	139.82 (9)
C7—C8—S1	119.3 (3)	O6^{vi}—Na1—Na1^{ix}	43.95 (6)
C6—C8—S1	120.8 (3)	O7—Na1—Na1^{ix}	101.42 (9)
S1—O7—Na1	142.06 (15)	O5^{vii}—Na1—Na1^{ix}	93.94 (8)
S1—O7—Na1^{ii}	94.19 (12)	O6^{i}—Na1—Na1^{ix}	41.39 (6)
Na1—O7—Na1^{ii}	80.62 (8)	O6^{viii}—Na1—Na1^{ix}	176.86 (9)
O6^{vi}—Na1—O7	109.65 (10)	O5^{i}—Na1—Na1^{ix}	98.12 (8)
O6^{vi}—Na1—O5^{vii}	91.54 (9)	O7^{viii}—Na1—Na1^{ix}	120.51 (8)
O7—Na1—O5^{vii}	158.81 (10)	S1^{i}—Na1—Na1^{ix}	69.61 (5)
O6^{vi}—Na1—O6^{i}	85.34 (9)	S1^{viii}—Na1—Na1^{ix}	148.90 (6)
O7—Na1—O6^{i}	87.94 (9)	Na1^{ii}—Na1—Na1^{ix}	135.44 (7)
O5^{vii}—Na1—O6^{i}	94.19 (9)	Na1^{viii}—Na1—Na1^{ix}	83.61 (5)

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, -y+3/2, z-1/2$; (iii) $-x, y+1/2, -z+3/2$; (iv) $x, y, z-1$; (v) $-x+1, -y+2, -z$; (vi) $x, y, z+1$; (vii) $-x, y-1/2, -z+3/2$; (viii) $x, -y+3/2, z+1/2$; (ix) $-x, -y+2, -z+2$.