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Sodium benzenesulfonothioate

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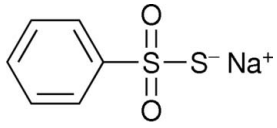
Key indicators: single-crystal X-ray study; T = 100 K, P = 0.0 kPa; mean σ(Na–O) = 0.002 Å; disorder in main residue; R factor = 0.032; wR factor = 0.079; data-to-parameter ratio = 15.3.

The title compound, $Na^+\cdot C_6H_5O_2S_2^-$, at 100 (2) K has orthorhombic (*Cmca*) symmetry. The compound has a network structure. It is of interest with respect to inclusion phenomena and structure–activity relationships. The Na atoms are chelated by two different benzenesulfonothioate anions via α-S and O atoms. Additional coordination by O atoms of two other benzenesulfonothioate anions results in coordination number 6 for each Na atom in the extended two-dimensional polymeric structure. The structure exhibits disorder of the anion in the two-dimensional arrangement. The phenyl group is disordered equally over two positions.

Related literature

For related literature, see: El-khateeb *et al.* (2006).



Experimental

Crystal data

$Na^+\cdot C_6H_5O_2S_2^-$
M_r = 196.21
Orthorhombic, *Cmca*
a = 9.5579 (10) Å
b = 7.0127 (8) Å
c = 24.231 (3) Å
V = 1624.1 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 100 (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: numerical (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.829, T_{max} = 0.881
6658 measured reflections
1053 independent reflections
874 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.079
S = 1.05
1053 reflections
69 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2202).

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supplementary materials

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Sodium benzenesulfonothioate

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Comment

The stucture of the title compound, (I), is shown below (Fig. 1). Dimensions are available in the archived CIF. I forms a two-dimensional polymeric arrangement in the solid state and may serve in future as a polydentate ligand with hard and soft donor centres.

For related literature, see El-khateeb *et al.*, 2006.

Experimental

The compound was prepared by aerobic oxidation of phenylthiol and subsequent treatment with sodium sulfide in THF (yield 10%).

Refinement

All H atoms were positioned in calculated positions and refined using a riding model, with C—H = 0.95 Å, and with U_{iso}(H) = 1.2Ueq(C).

Figures

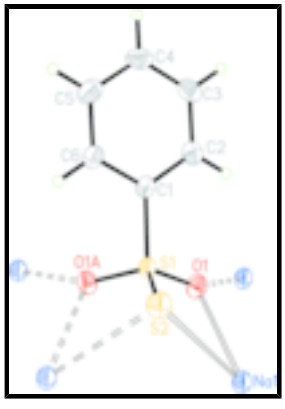

Fig. 1. Structure of the title compound in the solid state (displacement ellipsoids are at the 50% probability level). Connections to neighbouring sodium atoms are indicated by dashed bonds.

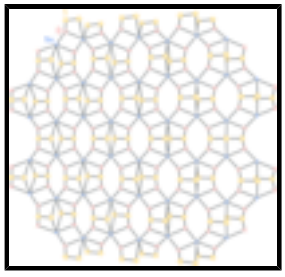

Fig. 2. Packing of the title compound in the solid state (without phenyl groups).

Sodium benzenesulfonothioate

Crystal data

$Na^+ \cdot C_6H_5O_2S_2^-$	$D_x = 1.605$ Mg m^{-3}
$M_r = 196.21$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, *Cmca*	Cell parameters from 6649 reflections
Hall symbol: -c 2ac 2	$\theta = 3.3–56.5°$
$a = 9.5579$ (10) Å	$\mu = 0.65$ mm^{-1}
$b = 7.0127$ (8) Å	$T = 100$ (2) K
$c = 24.231$ (3) Å	Cell measurement pressure: 100 kPa
$V = 1624.1$ (3) Å^3	Block, colourless
$Z = 8$	0.30 × 0.30 × 0.20 mm
$F_{000} = 800$	

Data collection

Stoe IPDS 2 diffractometer	1053 independent reflections
Radiation source: fine-focus sealed tube	874 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.054$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 28.3°$
$T = 100(2)$ K	$\theta_{min} = 1.7°$
rotation scans	$h = -12 \rightarrow 12$
Absorption correction: numerical (X-RED32; Stoe & Cie, 2002)	$k = -9 \rightarrow 9$
$T_{min} = 0.829$, $T_{max} = 0.881$	$l = -32 \rightarrow 32$
6658 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 1.7243P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
1053 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
69 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The phenyl groups are disordered over two positions (50:50). This disorder is static and a consequence of the symmetry operations.

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
S1	0.5000	0.24418 (9)	0.43057 (3)	0.01877 (16)	
S2	0.5000	−0.02166 (10)	0.40674 (3)	0.02647 (18)	
Na1	0.28026 (10)	0.0000	0.5000	0.0222 (2)	
O1	0.37188 (13)	0.2896 (2)	0.46085 (5)	0.0245 (3)	
C1	0.5122 (3)	0.3934 (3)	0.37218 (8)	0.0208 (6)	0.50
C2	0.4003 (2)	0.5052 (4)	0.35502 (10)	0.0236 (7)	0.50
H2	0.3147	0.5024	0.3749	0.028*	0.50
C3	0.4137 (2)	0.6210 (3)	0.30877 (11)	0.0276 (8)	0.50
H3	0.3372	0.6975	0.2970	0.033*	0.50
C4	0.5390 (3)	0.6251 (3)	0.27968 (9)	0.0297 (10)	0.50
H4	0.5482	0.7043	0.2481	0.036*	0.50
C5	0.6509 (2)	0.5133 (4)	0.29684 (10)	0.0306 (9)	0.50
H5	0.7366	0.5160	0.2770	0.037*	0.50
C6	0.6375 (2)	0.3974 (3)	0.34309 (10)	0.0251 (8)	0.50
H6	0.7140	0.3210	0.3548	0.030*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0143 (3)	0.0198 (3)	0.0222 (3)	0.000	0.000	−0.0004 (2)
S2	0.0264 (3)	0.0217 (3)	0.0313 (4)	0.000	0.000	−0.0030 (3)
Na1	0.0168 (5)	0.0210 (5)	0.0288 (5)	0.000	0.000	0.0000 (4)
O1	0.0189 (6)	0.0270 (7)	0.0277 (7)	0.0020 (5)	0.0052 (5)	−0.0020 (5)
C1	0.0183 (16)	0.0218 (12)	0.0224 (12)	0.000 (2)	0.001 (2)	−0.0009 (10)
C2	0.0222 (16)	0.0253 (18)	0.0232 (17)	0.0019 (15)	−0.0015 (14)	−0.0040 (15)
C3	0.031 (2)	0.0244 (18)	0.027 (2)	−0.0005 (17)	−0.0087 (17)	0.0003 (16)
C4	0.039 (3)	0.0242 (17)	0.0262 (18)	−0.0063 (14)	−0.0034 (15)	0.0057 (15)
C5	0.029 (2)	0.033 (2)	0.030 (2)	−0.0069 (18)	0.0044 (16)	0.0017 (18)
C6	0.0201 (17)	0.029 (2)	0.0257 (19)	−0.0029 (16)	0.0008 (15)	0.0015 (16)

Geometric parameters (Å, °)

S1—O1	1.4627 (13)	Na1—Na1^{iv}	3.5537 (5)
S1—O1^{i}	1.4627 (13)	Na1—Na1^{vi}	3.5537 (5)
S1—C1^{i}	1.7636 (18)	Na1—Na1^{ii}	4.201 (2)
S1—C1	1.7636 (18)	O1—Na1^{iv}	2.2784 (14)
S1—S2	1.9517 (10)	C1—C2	1.3900
S1—Na1	3.1896 (8)	C1—C6	1.3900
S1—Na1^{ii}	3.1897 (8)	C2—C3	1.3900
S2—Na1	3.0889 (9)	C2—H2	0.9500
S2—Na1^{ii}	3.0889 (9)	C3—C4	1.3900
Na1—O1^{iii}	2.2784 (14)	C3—H3	0.9500
Na1—O1^{iv}	2.2784 (14)	C4—C5	1.3900
Na1—O1	2.4065 (14)	C4—H4	0.9500
Na1—O1^{v}	2.4066 (14)	C5—C6	1.3900
Na1—S2^{ii}	3.0889 (9)	C5—H5	0.9500
Na1—S1^{ii}	3.1896 (8)	C6—H6	0.9500
O1—S1—O1^{i}	113.68 (11)	S2—Na1—S1	36.176 (19)
O1—S1—C1^{i}	102.58 (11)	S1^{ii}—Na1—S1	97.63 (3)
O1^{i}—S1—C1^{i}	109.19 (11)	O1^{iii}—Na1—Na1^{iv}	122.35 (5)
O1—S1—C1	109.19 (10)	O1^{iv}—Na1—Na1^{iv}	42.03 (4)
O1^{i}—S1—C1	102.58 (11)	O1—Na1—Na1^{iv}	39.34 (3)
C1^{i}—S1—C1	7.60 (18)	O1^{v}—Na1—Na1^{iv}	153.11 (4)
O1—S1—S2	110.89 (6)	S2^{ii}—Na1—Na1^{iv}	93.56 (2)
O1^{i}—S1—S2	110.89 (6)	S2—Na1—Na1^{iv}	99.16 (2)
C1^{i}—S1—S2	109.23 (9)	S1^{ii}—Na1—Na1^{iv}	129.56 (3)
C1—S1—S2	109.23 (9)	S1—Na1—Na1^{iv}	65.01 (2)
O1—S1—Na1	45.66 (6)	O1^{iii}—Na1—Na1^{vi}	42.03 (4)
O1^{i}—S1—Na1	113.80 (6)	O1^{iv}—Na1—Na1^{vi}	122.35 (5)
C1^{i}—S1—Na1	134.27 (9)	O1—Na1—Na1^{vi}	153.11 (4)
C1—S1—Na1	141.75 (9)	O1^{v}—Na1—Na1^{vi}	39.34 (3)
S2—S1—Na1	69.10 (2)	S2^{ii}—Na1—Na1^{vi}	99.16 (2)
O1—S1—Na1^{ii}	113.80 (6)	S2—Na1—Na1^{vi}	93.56 (2)
O1^{i}—S1—Na1^{ii}	45.66 (6)	S1^{ii}—Na1—Na1^{vi}	65.01 (2)
C1^{i}—S1—Na1^{ii}	141.75 (9)	S1—Na1—Na1^{vi}	129.56 (3)
C1—S1—Na1^{ii}	134.27 (9)	Na1^{iv}—Na1—Na1^{vi}	161.27 (6)
S2—S1—Na1^{ii}	69.10 (2)	O1^{iii}—Na1—Na1^{ii}	129.66 (4)
Na1—S1—Na1^{ii}	82.37 (3)	O1^{iv}—Na1—Na1^{ii}	129.66 (4)
S1—S2—Na1	74.72 (2)	O1—Na1—Na1^{ii}	68.66 (4)
S1—S2—Na1^{ii}	74.72 (2)	O1^{v}—Na1—Na1^{ii}	68.66 (4)
Na1—S2—Na1^{ii}	85.68 (3)	S2^{ii}—Na1—Na1^{ii}	47.160 (17)

O1^{iii}—Na1—O1^{iv}	100.68 (8)	S2—Na1—Na1^{ii}	47.161 (17)
O1^{iii}—Na1—O1	127.93 (6)	S1^{ii}—Na1—Na1^{ii}	48.816 (15)
O1^{iv}—Na1—O1	81.37 (5)	S1—Na1—Na1^{ii}	48.817 (15)
O1^{iii}—Na1—O1^{v}	81.37 (5)	Na1^{iv}—Na1—Na1^{ii}	99.37 (3)
O1^{iv}—Na1—O1^{v}	127.92 (6)	Na1^{vi}—Na1—Na1^{ii}	99.37 (3)
O1—Na1—O1^{v}	137.32 (8)	S1—O1—Na1^{iv}	152.16 (9)
O1^{iii}—Na1—S2^{ii}	140.39 (4)	S1—O1—Na1	108.58 (8)
O1^{iv}—Na1—S2^{ii}	95.60 (4)	Na1^{iv}—O1—Na1	98.63 (5)
O1—Na1—S2^{ii}	89.97 (4)	C2—C1—C6	120.0
O1^{v}—Na1—S2^{ii}	60.38 (4)	C2—C1—S1	121.58 (15)
O1^{iii}—Na1—S2	95.60 (4)	C6—C1—S1	118.42 (15)
O1^{iv}—Na1—S2	140.39 (4)	C1—C2—C3	120.0
O1—Na1—S2	60.38 (4)	C1—C2—H2	120.0
O1^{v}—Na1—S2	89.97 (4)	C3—C2—H2	120.0
S2^{ii}—Na1—S2	94.32 (3)	C4—C3—C2	120.0
O1^{iii}—Na1—S1^{ii}	106.99 (4)	C4—C3—H3	120.0
O1^{iv}—Na1—S1^{ii}	123.25 (4)	C2—C3—H3	120.0
O1—Na1—S1^{ii}	114.92 (5)	C3—C4—C5	120.0
O1^{v}—Na1—S1^{ii}	25.76 (3)	C3—C4—H4	120.0
S2^{ii}—Na1—S1^{ii}	36.175 (19)	C5—C4—H4	120.0
S2—Na1—S1^{ii}	84.94 (3)	C4—C5—C6	120.0
O1^{iii}—Na1—S1	123.25 (4)	C4—C5—H5	120.0
O1^{iv}—Na1—S1	106.99 (4)	C6—C5—H5	120.0
O1—Na1—S1	25.76 (3)	C5—C6—C1	120.0
O1^{v}—Na1—S1	114.92 (5)	C5—C6—H6	120.0
S2^{ii}—Na1—S1	84.94 (3)	C1—C6—H6	120.0
O1—S1—S2—Na1	−18.83 (6)	C1^{i}—S1—Na1—S1^{ii}	167.38 (13)
O1^{i}—S1—S2—Na1	108.46 (7)	C1—S1—Na1—S1^{ii}	165.36 (14)
C1^{i}—S1—S2—Na1	−131.16 (10)	S2—S1—Na1—S1^{ii}	70.48 (2)
C1—S1—S2—Na1	−139.21 (9)	O1—S1—Na1—Na1^{iv}	−4.18 (7)
Na1^{ii}—S1—S2—Na1	89.63 (3)	O1^{i}—S1—Na1—Na1^{iv}	96.36 (7)
O1—S1—S2—Na1^{ii}	−108.46 (7)	C1^{i}—S1—Na1—Na1^{iv}	−62.35 (13)
O1^{i}—S1—S2—Na1^{ii}	18.82 (6)	C1—S1—Na1—Na1^{iv}	−64.36 (14)
C1^{i}—S1—S2—Na1^{ii}	139.21 (9)	S2—S1—Na1—Na1^{iv}	−159.24 (3)
C1—S1—S2—Na1^{ii}	131.16 (10)	Na1^{ii}—S1—Na1—Na1^{iv}	130.28 (2)
Na1—S1—S2—Na1^{ii}	−89.63 (3)	O1—S1—Na1—Na1^{vi}	161.79 (9)
S1—S2—Na1—O1^{iii}	143.07 (4)	O1^{i}—S1—Na1—Na1^{vi}	−97.67 (7)
Na1^{ii}—S2—Na1—O1^{iii}	−141.60 (4)	C1^{i}—S1—Na1—Na1^{vi}	103.62 (13)
S1—S2—Na1—O1^{iv}	28.83 (7)	C1—S1—Na1—Na1^{vi}	101.61 (14)
Na1^{ii}—S2—Na1—O1^{iv}	104.16 (7)	S2—S1—Na1—Na1^{vi}	6.73 (4)
S1—S2—Na1—O1	12.17 (4)	Na1^{ii}—S1—Na1—Na1^{vi}	−63.75 (4)

Na1^{ii}—S2—Na1—O1	87.50 (4)	O1—S1—Na1—Na1^{ii}	−134.45 (8)
S1—S2—Na1—O1^{v}	−135.61 (4)	O1^{i}—S1—Na1—Na1^{ii}	−33.92 (6)
Na1^{ii}—S2—Na1—O1^{v}	−60.28 (4)	C1^{i}—S1—Na1—Na1^{ii}	167.38 (13)
S1—S2—Na1—S2^{ii}	−75.331 (19)	C1—S1—Na1—Na1^{ii}	165.36 (14)
S1—S2—Na1—S1^{ii}	−110.31 (2)	S2—S1—Na1—Na1^{ii}	70.48 (2)
Na1^{ii}—S2—Na1—S1^{ii}	−34.977 (17)	O1^{i}—S1—O1—Na1^{iv}	66.5 (2)
Na1^{ii}—S2—Na1—S1	75.331 (19)	C1^{i}—S1—O1—Na1^{iv}	−51.3 (2)
S1—S2—Na1—Na1^{iv}	18.99 (3)	C1—S1—O1—Na1^{iv}	−47.4 (2)
Na1^{ii}—S2—Na1—Na1^{iv}	94.32 (3)	S2—S1—O1—Na1^{iv}	−167.80 (15)
S1—S2—Na1—Na1^{vi}	−174.81 (3)	Na1—S1—O1—Na1^{iv}	167.3 (2)
Na1^{ii}—S2—Na1—Na1^{vi}	−99.48 (3)	Na1^{ii}—S1—O1—Na1^{iv}	116.62 (17)
S1—S2—Na1—Na1^{ii}	−75.331 (19)	O1^{i}—S1—O1—Na1	−100.80 (10)
O1—S1—Na1—O1^{iii}	109.42 (8)	C1^{i}—S1—O1—Na1	141.44 (10)
O1^{i}—S1—Na1—O1^{iii}	−150.05 (10)	C1—S1—O1—Na1	145.33 (11)
C1^{i}—S1—Na1—O1^{iii}	51.25 (14)	S2—S1—O1—Na1	24.93 (8)
C1—S1—Na1—O1^{iii}	49.23 (15)	Na1^{ii}—S1—O1—Na1	−50.65 (8)
S2—S1—Na1—O1^{iii}	−45.65 (5)	O1^{iii}—Na1—O1—S1	−89.13 (7)
Na1^{ii}—S1—Na1—O1^{iii}	−116.13 (5)	O1^{iv}—Na1—O1—S1	174.02 (11)
O1—S1—Na1—O1^{iv}	−6.18 (11)	O1^{v}—Na1—O1—S1	35.23 (6)
O1^{i}—S1—Na1—O1^{iv}	94.36 (6)	S2^{ii}—Na1—O1—S1	78.36 (7)
C1^{i}—S1—Na1—O1^{iv}	−64.35 (13)	S2—Na1—O1—S1	−16.63 (5)
C1—S1—Na1—O1^{iv}	−66.37 (15)	S1^{ii}—Na1—O1—S1	51.27 (8)
S2—S1—Na1—O1^{iv}	−161.25 (4)	Na1^{iv}—Na1—O1—S1	174.02 (11)
Na1^{ii}—S1—Na1—O1^{iv}	128.27 (4)	Na1^{vi}—Na1—O1—S1	−32.18 (16)
O1^{i}—S1—Na1—O1	100.54 (13)	Na1^{ii}—Na1—O1—S1	35.23 (6)
C1^{i}—S1—Na1—O1	−58.17 (14)	O1^{iii}—Na1—O1—Na1^{iv}	96.85 (9)
C1—S1—Na1—O1	−60.19 (16)	O1^{v}—Na1—O1—Na1^{iv}	−138.80 (5)
S2—S1—Na1—O1	−155.07 (8)	S2^{ii}—Na1—O1—Na1^{iv}	−95.67 (4)
Na1^{ii}—S1—Na1—O1	134.45 (8)	S2—Na1—O1—Na1^{iv}	169.34 (6)
O1—S1—Na1—O1^{v}	−154.46 (6)	S1^{ii}—Na1—O1—Na1^{iv}	−122.75 (4)
O1^{i}—S1—Na1—O1^{v}	−53.92 (9)	S1—Na1—O1—Na1^{iv}	−174.02 (11)
C1^{i}—S1—Na1—O1^{v}	147.37 (13)	Na1^{vi}—Na1—O1—Na1^{iv}	153.79 (12)
C1—S1—Na1—O1^{v}	145.35 (14)	Na1^{ii}—Na1—O1—Na1^{iv}	−138.80 (5)
S2—S1—Na1—O1^{v}	50.48 (4)	O1—S1—C1—C2	−11.20 (17)
Na1^{ii}—S1—Na1—O1^{v}	−20.01 (4)	O1^{i}—S1—C1—C2	−132.10 (14)
O1—S1—Na1—S2^{ii}	−100.50 (8)	C1^{i}—S1—C1—C2	18.88 (14)
O1^{i}—S1—Na1—S2^{ii}	0.04 (7)	S2—S1—C1—C2	110.21 (13)
C1^{i}—S1—Na1—S2^{ii}	−158.67 (13)	Na1—S1—C1—C2	29.9 (2)
C1—S1—Na1—S2^{ii}	−160.69 (14)	Na1^{ii}—S1—C1—C2	−170.60 (10)
S2—S1—Na1—S2^{ii}	104.44 (3)	O1—S1—C1—C6	168.83 (12)
Na1^{ii}—S1—Na1—S2^{ii}	33.953 (17)	O1^{i}—S1—C1—C6	47.94 (15)

O1—S1—Na1—S2	155.07 (8)	C1^{i}—S1—C1—C6	−161.08 (13)
O1^{i}—S1—Na1—S2	−104.40 (7)	S2—S1—C1—C6	−69.76 (14)
C1^{i}—S1—Na1—S2	96.90 (13)	Na1—S1—C1—C6	−150.09 (11)
C1—S1—Na1—S2	94.88 (14)	Na1^{ii}—S1—C1—C6	9.4 (2)
Na1^{ii}—S1—Na1—S2	−70.48 (2)	S1—C1—C2—C3	−180.0 (2)
O1—S1—Na1—S1^{ii}	−134.45 (8)	S1—C1—C6—C5	179.97 (19)
O1^{i}—S1—Na1—S1^{ii}	−33.92 (6)		

Symmetry codes: (i) −*x*+1, *y*, *z*; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*+1/2, *y*−1/2, *z*; (iv) −*x*+1/2, −*y*+1/2, −*z*+1; (v) *x*, −*y*, −*z*+1; (vi) −*x*+1/2, −*y*−1/2, −*z*+1.

Fig. 1

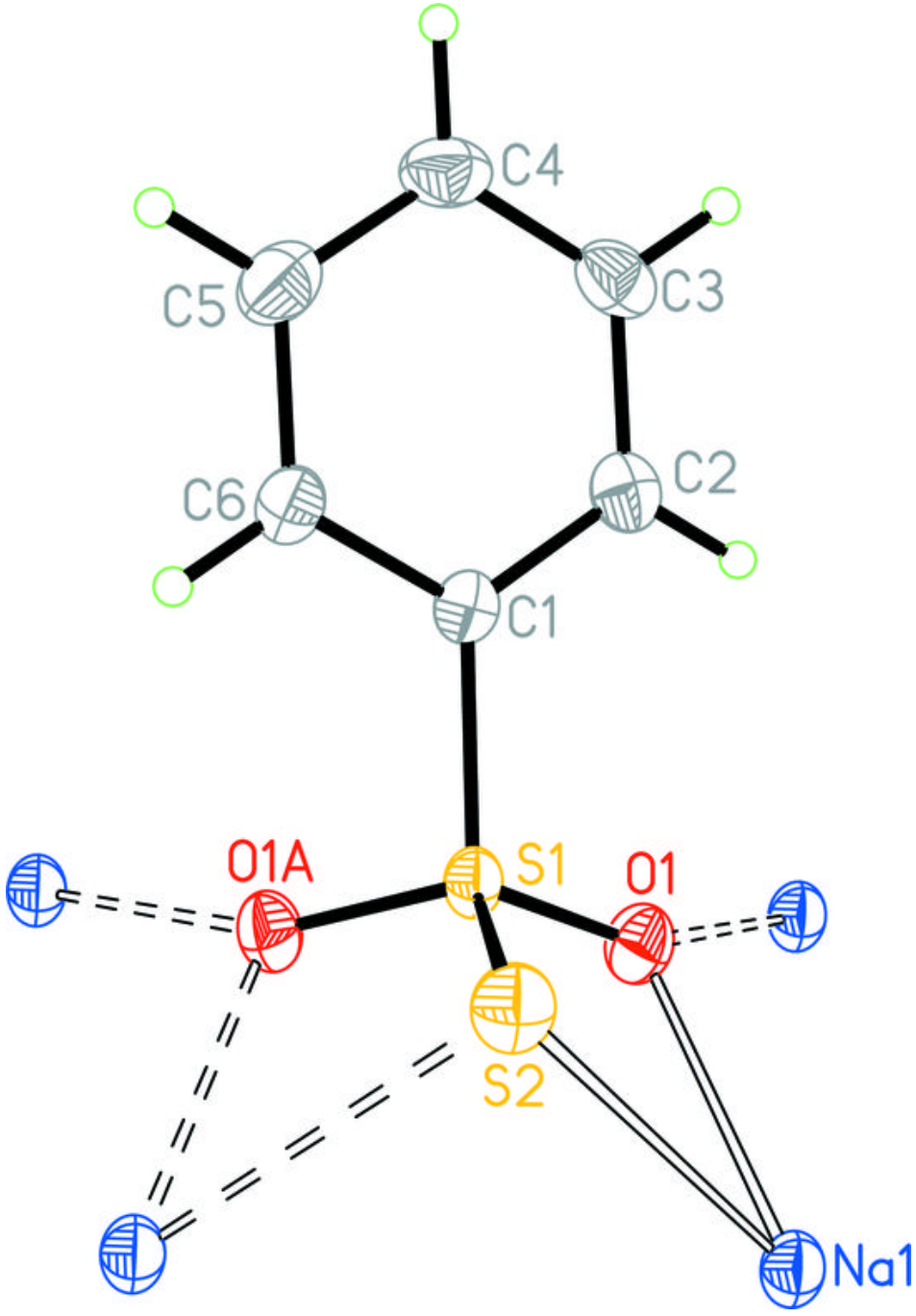

Fig. 2