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Sodium 4,*N*-dichlorobenzenesulfonamidate sesquihydrate

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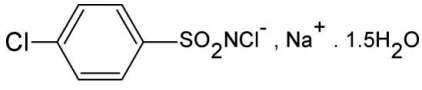
Key indicators: single-crystal X-ray study; T = 303 K; mean σ(C–C) = 0.010 Å; R factor = 0.068; wR factor = 0.140; data-to-parameter ratio = 15.3.

The structure of the title compound, $Na^+\cdot C_6H_4Cl_2NO_2S^-\cdot 1.5H_2O$, resembles the structures of the sodium salts of *N*-chlorobenzenesulfonamide, *N*-chloro-4-methylbenzenesulfonamide and *N*-chloro-2-methyl-4-chlorobenzenesulfonamide. There are two formula units per asymmetric unit. There is no interaction between N and Na, and the Na^+ cation is attached to three O atoms from water molecules and three sulfonyl O atoms of three different 4,*N*-dichlorobenzenesulfonamide anions. There are several hydrogen bonds. The S—N distances of 1.584 (5) and 1.590 (5) Å are consistent with an S=N double bond.

Related literature

For related literature, see: George *et al.* (2000); Gowda & Kumar (2003); Gowda & Shetty (2004); Gowda *et al.* (2002, 2005, 2007); Gowda, D'Souza & Fuess (2003); Gowda, D'Souza & Kumar (2003); Gowda, Jyothi, Kozisek & Fuess (2003); Olmstead & Power (1986).



Experimental

Crystal data

$Na^+\cdot C_6H_4Cl_2NO_2S^-\cdot 1.5H_2O$
M_r = 275.09
Orthorhombic, $P2_12_12_1$
a = 6.7041 (4) Å
b = 10.4763 (8) Å
c = 30.037 (2) Å
V = 2109.6 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 303 (2) K
0.30 × 0.12 × 0.04 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: analytical *CrysAlis RED* (Oxford Diffraction, 2002)
T_{min} = 0.865, T_{max} = 0.962
14393 measured reflections
4281 independent reflections
2959 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.140
S = 1.10
4281 reflections
280 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 1777 Friedel pairs
Flack parameter: 0.22 (12)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H41O···Cl1	0.842 (19)	2.70 (2)	3.523 (5)	167 (5)
O4—H42O···N2^{i}	0.841 (19)	2.06 (2)	2.903 (7)	177 (7)
O4—H42O···S2^{i}	0.841 (19)	2.91 (4)	3.633 (5)	145 (6)
O5—H51O···N2^{ii}	0.848 (19)	2.06 (2)	2.899 (6)	170 (7)
O5—H51O···Cl2^{ii}	0.848 (19)	2.89 (3)	3.631 (5)	147 (4)
O5—H52O···N1^{ii}	0.861 (19)	2.16 (2)	3.006 (6)	169 (7)
O5—H52O···Cl1^{ii}	0.861 (19)	2.82 (3)	3.522 (5)	139 (4)
O6—H61O···Cl2^{iii}	0.87 (2)	2.61 (5)	3.305 (5)	138 (6)
O6—H61O···O2^{iv}	0.87 (2)	2.63 (6)	3.212 (6)	125 (6)
O6—H62O···N1	0.86 (2)	2.00 (2)	2.845 (7)	167 (6)
O6—H62O···S1	0.86 (2)	3.00 (4)	3.687 (5)	138 (5)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $x-1, y, z$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2356).

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supplementary materials

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Sodium 4,*N*-dichlorobenzenesulfonamidate sesquihydrate

B. T. Gowda, K. Jyothi, S. Foro, J. Kozísek and H. Fuess

Comment

The chemistry of arylsulfonamides and their N-halo compounds is of interest as they show distinct physical, chemical and biological properties. Many of these compounds exhibit pharmacological, fungicidal and herbicidal activities due to their oxidizing action in aqueous, partial aqueous and non-aqueous media. Thus N-halo arylsulfonamides are of interest in synthetic, mechanistic, analytical and biological chemistry (Gowda *et al.*, 2002; Gowda, D'Souza & Fuess 2003; Gowda, D'Souza & Kumar, 2003; Gowda, Jyothi *et al.*, 2003; Gowda & Shetty 2004; Gowda & Kumar, 2003; Gowda *et al.*, 2005; Gowda *et al.*, 2007). In the present work, the structure of the sodium salt of *N*-chloro, 4-chlorobenzenesulfonamde has been determined to explore the effect substituent on the solid state structures of sulfonamides and N-halo arylsulfonamides. The structure (Fig. 1) resembles those of the sodium salts of *N*-chlorobenzenesulfonamde (George *et al.*, 2000), *N*-chloro-4-methylbenzenesulfonamde (Olmstead & Power, 1986) and *N*-chloro-2-methyl-4-chlorobenzenesulfonamde (Gowda *et al.*, 2007). There is no interaction between the nitrogen and sodium atoms in the molecule, and Na+ is attached to one of the sulfonyl O atoms. Na+ coordination sphere involves oxygen from waters of crystallization and neighbouring molecules. Na+ ion coordination in the structure is also similar giving rise to several hydrogen bonding between water hydrogen, oxygen and other atoms in the molecule as shown in Figures 2 and 3. The S—N distances of 1.584 (5)Å and 1.590 (5)Å are in agreement with those of similar compounds, consistent with a S—N double bond.

Experimental

The title compound was prepared according to the literature method (Gowda, D'Souza & Fuess 2003; Gowda, D'Souza & Kumar, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, NMR and NQR spectra. Single crystals of the title compound were obtained from a slow evaporation of its chloroform solution and used for X-ray diffraction studies at room temperature.

Figures

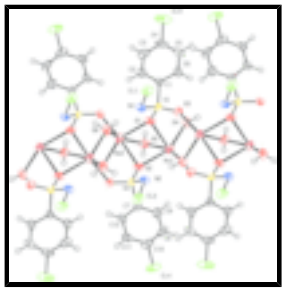

Fig. 1. *ORTEP* view of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

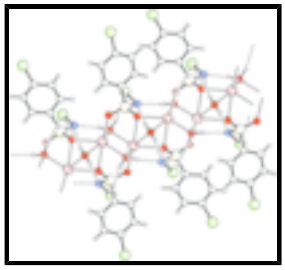

Fig. 2. Packing diagram of the title compound viewed down the axis b.

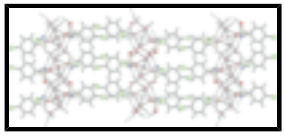

Fig. 3. Typical Hydrogen bond bridges observed in the title compound.

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Crystal data

$Na^{+}\cdot C_6H_4Cl_2NO_2S^{-}\cdot 1.5H_2O$	F_{000} = 1112
M_r = 275.09	D_x = 1.732 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 3193 reflections
a = 6.7041 (4) Å	θ = 3.4–25.5º
b = 10.4763 (8) Å	μ = 0.84 mm^{-1}
c = 30.037 (2) Å	T = 303 (2) K
V = 2109.6 (2) Å^3	Laminar, colourless
Z = 8	0.30 × 0.12 × 0.04 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector	4281 independent reflections
Radiation source: fine-focus sealed tube	2959 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.079
T = 303(2) K	θ_{max} = 26.4º
Rotation method data acquisition using ω scans	θ_{min} = 4.1º
Absorption correction: analytical CrysAlis RED (Oxford Diffraction, 2002)	h = −8→5
T_{min} = 0.865, T_{max} = 0.962	k = −12→13
14393 measured reflections	l = −37→37

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.068	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.140$	$(\Delta/\sigma)_{max} = 0.039$
$S = 1.10$	$\Delta\rho_{max} = 0.41$ e Å^{-3}
4281 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
280 parameters	Extinction correction: none
9 restraints	Absolute structure: Flack (1983), 1777 Friedel pairs'
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.22 (12)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.2166 (9)	0.6230 (6)	0.1339 (2)	0.0233 (15)
C2	0.1376 (9)	0.5182 (7)	0.1569 (2)	0.0363 (17)
H2	0.1420	0.4366	0.1448	0.044*
C3	0.0543 (10)	0.5394 (8)	0.1977 (2)	0.045 (2)
H3	−0.0031	0.4715	0.2130	0.054*
C4	0.0533 (10)	0.6565 (8)	0.2162 (2)	0.0388 (18)
C5	0.1311 (11)	0.7599 (8)	0.1944 (3)	0.048 (2)
H5	0.1280	0.8402	0.2076	0.058*
C6	0.2147 (10)	0.7438 (6)	0.1525 (2)	0.0376 (18)
H6	0.2684	0.8129	0.1372	0.045*
C7	0.2101 (9)	0.4255 (6)	−0.1317 (2)	0.0219 (14)
C8	0.2049 (11)	0.5461 (7)	−0.1490 (2)	0.0412 (18)
H8	0.2560	0.6134	−0.1323	0.049*
C9	0.1272 (10)	0.5704 (7)	−0.1899 (3)	0.042 (2)
H9	0.1270	0.6528	−0.2015	0.050*
C10	0.0489 (10)	0.4707 (8)	−0.2138 (2)	0.0407 (19)
C11	0.0500 (11)	0.3466 (7)	−0.1974 (2)	0.0390 (18)
H11	−0.0017	0.2797	−0.2141	0.047*
C12	0.1303 (9)	0.3247 (6)	−0.1551 (2)	0.0326 (17)
H12	0.1298	0.2431	−0.1430	0.039*
N1	0.4918 (6)	0.4958 (5)	0.08230 (17)	0.0320 (13)
N2	0.5112 (7)	0.4835 (5)	−0.07515 (16)	0.0275 (12)
O1	0.1710 (6)	0.5457 (4)	0.05205 (13)	0.0322 (11)

O2	0.1801 (6)	0.4532 (4)	−0.04620 (14)	0.0345 (11)
O3	0.3891 (7)	0.7264 (4)	0.06666 (15)	0.0413 (13)
O4	0.8701 (7)	0.7723 (4)	0.04198 (15)	0.0366 (12)
H41O	0.839 (10)	0.724 (4)	0.0632 (14)	0.044*
H42O	0.915 (9)	0.842 (3)	0.0521 (18)	0.044*
O5	−0.2356 (6)	0.5018 (6)	0.00285 (14)	0.0383 (11)
H51O	−0.306 (7)	0.487 (7)	−0.0200 (10)	0.046*
H52O	−0.319 (6)	0.510 (7)	0.0245 (11)	0.046*
O6	0.3547 (7)	0.2708 (4)	0.03900 (16)	0.0398 (12)
H61O	0.376 (10)	0.204 (3)	0.0553 (18)	0.048*
H62O	0.411 (9)	0.332 (4)	0.0535 (18)	0.048*
O7	0.3489 (6)	0.2636 (4)	−0.07503 (14)	0.0346 (11)
S1	0.3222 (2)	0.60178 (14)	0.08011 (5)	0.0255 (4)
S2	0.3159 (2)	0.39894 (14)	−0.07852 (5)	0.0241 (4)
Cl1	0.6828 (3)	0.54516 (18)	0.11769 (6)	0.0432 (5)
Cl2	0.6858 (3)	0.43230 (17)	−0.11428 (6)	0.0436 (5)
Cl3	−0.0432 (3)	0.6788 (3)	0.26962 (6)	0.0706 (7)
Cl4	−0.0464 (3)	0.4965 (2)	−0.26702 (6)	0.0584 (6)
Na1	0.5463 (4)	0.8486 (2)	0.01367 (8)	0.0327 (6)
Na2	0.0289 (4)	0.3492 (2)	0.01858 (8)	0.0336 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.021 (3)	0.023 (4)	0.026 (3)	−0.007 (3)	−0.003 (3)	−0.003 (3)
C2	0.041 (4)	0.033 (4)	0.035 (4)	0.004 (3)	0.008 (3)	−0.002 (3)
C3	0.038 (4)	0.061 (6)	0.036 (4)	−0.001 (4)	0.011 (4)	0.012 (4)
C4	0.025 (4)	0.071 (6)	0.021 (4)	−0.004 (4)	0.006 (3)	−0.013 (4)
C5	0.056 (5)	0.049 (5)	0.039 (5)	−0.003 (4)	0.001 (4)	−0.020 (4)
C6	0.044 (4)	0.028 (4)	0.041 (4)	0.003 (4)	0.014 (4)	−0.002 (3)
C7	0.015 (3)	0.027 (4)	0.023 (3)	0.012 (3)	−0.001 (3)	0.002 (3)
C8	0.047 (4)	0.037 (4)	0.039 (4)	−0.004 (4)	−0.010 (4)	0.003 (3)
C9	0.040 (4)	0.042 (4)	0.043 (5)	−0.008 (4)	−0.015 (4)	0.021 (4)
C10	0.023 (3)	0.066 (6)	0.033 (4)	0.009 (4)	−0.002 (3)	0.020 (4)
C11	0.049 (4)	0.039 (4)	0.030 (4)	−0.003 (4)	−0.016 (4)	−0.009 (3)
C12	0.038 (4)	0.026 (4)	0.034 (4)	−0.003 (3)	−0.001 (3)	−0.007 (3)
N1	0.027 (3)	0.038 (3)	0.031 (3)	−0.001 (3)	−0.007 (2)	−0.005 (3)
N2	0.025 (3)	0.035 (3)	0.022 (3)	0.001 (2)	0.004 (2)	−0.005 (3)
O1	0.029 (2)	0.041 (3)	0.027 (2)	0.006 (2)	−0.008 (2)	−0.004 (2)
O2	0.035 (2)	0.045 (3)	0.023 (2)	0.004 (2)	0.011 (2)	0.001 (2)
O3	0.059 (3)	0.031 (3)	0.034 (3)	−0.010 (2)	0.006 (2)	0.004 (2)
O4	0.039 (3)	0.027 (3)	0.044 (3)	−0.002 (2)	0.003 (2)	−0.005 (2)
O5	0.029 (2)	0.054 (3)	0.031 (3)	0.004 (3)	−0.002 (2)	−0.002 (2)
O6	0.040 (3)	0.031 (3)	0.049 (3)	0.006 (3)	−0.002 (2)	0.000 (2)
O7	0.049 (3)	0.028 (2)	0.027 (2)	0.003 (2)	−0.005 (2)	−0.003 (2)
S1	0.0274 (9)	0.0283 (9)	0.0206 (8)	0.0012 (8)	−0.0010 (8)	0.0019 (7)
S2	0.0274 (9)	0.0252 (9)	0.0198 (8)	−0.0001 (8)	−0.0027 (8)	0.0005 (7)
Cl1	0.0306 (9)	0.0603 (12)	0.0386 (10)	−0.0009 (9)	−0.0082 (9)	0.0034 (10)

Cl2	0.0330 (10)	0.0552 (11)	0.0426 (11)	0.0059 (9)	0.0097 (9)	0.0101 (9)
Cl3	0.0490 (11)	0.128 (2)	0.0349 (11)	−0.0072 (13)	0.0123 (11)	−0.0199 (13)
Cl4	0.0469 (10)	0.0969 (17)	0.0313 (10)	0.0015 (12)	−0.0133 (10)	0.0145 (11)
Na1	0.0331 (14)	0.0343 (15)	0.0307 (14)	−0.0085 (13)	0.0027 (13)	0.0041 (12)
Na2	0.0316 (14)	0.0309 (15)	0.0384 (15)	−0.0046 (13)	0.0013 (13)	0.0051 (12)

Geometric parameters (Å, °)

C1—C6	1.382 (9)	O2—S2	1.447 (4)
C1—C2	1.401 (9)	O2—Na2	2.450 (5)
C1—S1	1.779 (6)	O2—Na1^{i}	2.464 (5)
C2—C3	1.363 (9)	O3—S1	1.438 (5)
C2—H2	0.9300	O3—Na1	2.298 (5)
C3—C4	1.348 (10)	O4—Na1^{ii}	2.407 (5)
C3—H3	0.9300	O4—Na1	2.465 (5)
C4—C5	1.369 (10)	O4—H41O	0.842 (19)
C4—Cl3	1.745 (7)	O4—H42O	0.841 (19)
C5—C6	1.389 (10)	O5—Na2	2.433 (5)
C5—H5	0.9300	O5—Na1^{i}	2.505 (5)
C6—H6	0.9300	O5—H51O	0.848 (19)
C7—C8	1.366 (9)	O5—H52O	0.861 (19)
C7—C12	1.377 (8)	O6—Na2	2.413 (5)
C7—S2	1.770 (6)	O6—Na2^{iii}	2.437 (6)
C8—C9	1.360 (9)	O6—H61O	0.87 (2)
C8—H8	0.9300	O6—H62O	0.86 (2)
C9—C10	1.372 (10)	O7—S2	1.439 (4)
C9—H9	0.9300	O7—Na2^{iii}	2.393 (5)
C10—C11	1.391 (9)	Na1—O4^{i}	2.407 (5)
C10—Cl4	1.742 (7)	Na1—O1^{ii}	2.413 (5)
C11—C12	1.397 (9)	Na1—O2^{ii}	2.464 (5)
C11—H11	0.9300	Na1—O5^{ii}	2.505 (5)
C12—H12	0.9300	Na1—Na2^{ii}	3.313 (3)
N1—S1	1.590 (5)	Na1—Na1^{i}	4.022 (3)
N1—Cl1	1.743 (5)	Na1—Na1^{ii}	4.022 (3)
N2—S2	1.584 (5)	Na2—O7^{iv}	2.393 (5)
N2—Cl2	1.743 (5)	Na2—O6^{iv}	2.437 (6)
O1—S1	1.443 (4)	Na2—Na1^{i}	3.313 (3)
O1—Na1^{i}	2.413 (5)	Na2—Na2^{iv}	4.100 (3)
O1—Na2	2.481 (5)	Na2—Na2^{iii}	4.100 (3)
C6—C1—C2	121.0 (6)	O2—S2—C7	107.0 (3)
C6—C1—S1	119.0 (5)	N2—S2—C7	107.5 (3)
C2—C1—S1	120.0 (5)	O3—Na1—O4^{i}	87.87 (18)
C3—C2—C1	118.1 (7)	O3—Na1—O1^{ii}	168.82 (19)
C3—C2—H2	121.0	O4^{i}—Na1—O1^{ii}	80.99 (17)
C1—C2—H2	121.0	O3—Na1—O2^{ii}	111.21 (17)

C4—C3—C2	121.4 (7)	O4^{i}—Na1—O2^{ii}	153.84 (19)
C4—C3—H3	119.3	O1^{ii}—Na1—O2^{ii}	79.13 (16)
C2—C3—H3	119.3	O3—Na1—O4	89.11 (18)
C3—C4—C5	121.4 (6)	O4^{i}—Na1—O4	120.08 (15)
C3—C4—Cl3	120.2 (6)	O1^{ii}—Na1—O4	97.22 (17)
C5—C4—Cl3	118.4 (6)	O2^{ii}—Na1—O4	79.37 (16)
C4—C5—C6	119.5 (7)	O3—Na1—O5^{ii}	98.04 (18)
C4—C5—H5	120.3	O4^{i}—Na1—O5^{ii}	79.73 (17)
C6—C5—H5	120.3	O1^{ii}—Na1—O5^{ii}	79.17 (16)
C1—C6—C5	118.7 (7)	O2^{ii}—Na1—O5^{ii}	79.97 (17)
C1—C6—H6	120.6	O4—Na1—O5^{ii}	159.34 (19)
C5—C6—H6	120.6	O3—Na1—Na2^{ii}	135.94 (16)
C8—C7—C12	120.3 (6)	O4^{i}—Na1—Na2^{ii}	106.41 (15)
C8—C7—S2	119.9 (5)	O1^{ii}—Na1—Na2^{ii}	48.27 (12)
C12—C7—S2	119.7 (5)	O2^{ii}—Na1—Na2^{ii}	47.43 (11)
C9—C8—C7	121.8 (7)	O4—Na1—Na2^{ii}	116.21 (14)
C9—C8—H8	119.1	O5^{ii}—Na1—Na2^{ii}	46.95 (13)
C7—C8—H8	119.1	O3—Na1—Na1^{i}	58.21 (13)
C8—C9—C10	118.5 (7)	O4^{i}—Na1—Na1^{i}	34.82 (13)
C8—C9—H9	120.8	O1^{ii}—Na1—Na1^{i}	110.94 (14)
C10—C9—H9	120.8	O2^{ii}—Na1—Na1^{i}	144.81 (14)
C9—C10—C11	121.6 (6)	O4—Na1—Na1^{i}	129.66 (16)
C9—C10—Cl4	120.1 (6)	O5^{ii}—Na1—Na1^{i}	69.65 (13)
C11—C10—Cl4	118.2 (6)	Na2^{ii}—Na1—Na1^{i}	113.68 (9)
C10—C11—C12	118.6 (7)	O3—Na1—Na1^{ii}	103.73 (16)
C10—C11—H11	120.7	O4^{i}—Na1—Na1^{ii}	89.82 (15)
C12—C11—H11	120.7	O1^{ii}—Na1—Na1^{ii}	77.28 (12)
C7—C12—C11	119.2 (6)	O2^{ii}—Na1—Na1^{ii}	102.14 (12)
C7—C12—H12	120.4	O4—Na1—Na1^{ii}	33.89 (11)
C11—C12—H12	120.4	O5^{ii}—Na1—Na1^{ii}	155.46 (15)
S1—N1—Cl1	110.1 (3)	Na2^{ii}—Na1—Na1^{ii}	117.42 (9)
S2—N2—Cl2	109.9 (3)	Na1^{i}—Na1—Na1^{ii}	112.90 (12)
S1—O1—Na1^{i}	122.3 (3)	O7^{iv}—Na2—O6	96.20 (18)
S1—O1—Na2	147.6 (3)	O7^{iv}—Na2—O5	95.44 (17)
Na1^{i}—O1—Na2	85.19 (15)	O6—Na2—O5	158.84 (19)
S2—O2—Na2	128.2 (3)	O7^{iv}—Na2—O6^{iv}	90.36 (17)
S2—O2—Na1^{i}	145.7 (3)	O6—Na2—O6^{iv}	116.01 (15)
Na2—O2—Na1^{i}	84.77 (15)	O5—Na2—O6^{iv}	81.49 (18)
S1—O3—Na1	147.5 (3)	O7^{iv}—Na2—O2	172.32 (18)
Na1^{ii}—O4—Na1	111.29 (19)	O6—Na2—O2	88.76 (17)
Na1^{ii}—O4—H41O	109 (4)	O5—Na2—O2	81.69 (16)

Na1—O4—H41O	104 (5)	O6^{iv}—Na2—O2	82.19 (17)
Na1^{ii}—O4—H42O	122 (4)	O7^{iv}—Na2—O1	108.44 (17)
Na1—O4—H42O	99 (5)	O6—Na2—O1	80.31 (16)
H41O—O4—H42O	110 (3)	O5—Na2—O1	79.27 (17)
Na2—O5—Na1^{i}	84.24 (14)	O6^{iv}—Na2—O1	154.16 (19)
Na2—O5—H51O	116 (5)	O2—Na2—O1	78.11 (16)
Na1^{i}—O5—H51O	112 (4)	O7^{iv}—Na2—Na1^{i}	134.19 (15)
Na2—O5—H52O	113 (4)	O6—Na2—Na1^{i}	111.57 (14)
Na1^{i}—O5—H52O	125 (4)	O5—Na2—Na1^{i}	48.80 (13)
H51O—O5—H52O	106 (3)	O6^{iv}—Na2—Na1^{i}	107.62 (15)
Na2—O6—Na2^{iii}	115.42 (19)	O2—Na2—Na1^{i}	47.80 (12)
Na2—O6—H61O	125 (4)	O1—Na2—Na1^{i}	46.54 (11)
Na2^{iii}—O6—H61O	84 (5)	O7^{iv}—Na2—Na2^{iv}	61.98 (12)
Na2—O6—H62O	106 (4)	O6—Na2—Na2^{iv}	129.55 (16)
Na2^{iii}—O6—H62O	122 (5)	O5—Na2—Na2^{iv}	71.60 (13)
H61O—O6—H62O	104 (3)	O6^{iv}—Na2—Na2^{iv}	32.11 (12)
S2—O7—Na2^{iii}	128.0 (3)	O2—Na2—Na2^{iv}	110.35 (15)
O3—S1—O1	115.1 (3)	O1—Na2—Na2^{iv}	147.69 (13)
O3—S1—N1	115.0 (3)	Na1^{i}—Na2—Na2^{iv}	115.72 (10)
O1—S1—N1	104.0 (3)	O7^{iv}—Na2—Na2^{iii}	110.76 (15)
O3—S1—C1	105.4 (3)	O6—Na2—Na2^{iii}	32.47 (11)
O1—S1—C1	107.6 (3)	O5—Na2—Na2^{iii}	151.17 (16)
N1—S1—C1	109.5 (3)	O6^{iv}—Na2—Na2^{iii}	86.37 (15)
O7—S2—O2	115.8 (3)	O2—Na2—Na2^{iii}	70.77 (12)
O7—S2—N2	114.8 (3)	O1—Na2—Na2^{iii}	102.54 (11)
O2—S2—N2	104.9 (3)	Na1^{i}—Na2—Na2^{iii}	112.10 (9)
O7—S2—C7	106.4 (3)	Na2^{iv}—Na2—Na2^{iii}	109.70 (12)
C6—C1—C2—C3	1.7 (10)	S1—O3—Na1—O2^{ii}	−157.2 (5)
S1—C1—C2—C3	−178.6 (5)	S1—O3—Na1—O4	−78.9 (6)
C1—C2—C3—C4	−2.3 (10)	S1—O3—Na1—O5^{ii}	120.5 (5)
C2—C3—C4—C5	1.8 (11)	S1—O3—Na1—Na2^{ii}	152.8 (5)
C2—C3—C4—Cl3	−176.7 (5)	S1—O3—Na1—Na1^{i}	60.6 (5)
C3—C4—C5—C6	−0.7 (11)	S1—O3—Na1—Na1^{ii}	−48.1 (6)
Cl3—C4—C5—C6	177.9 (5)	Na1^{ii}—O4—Na1—O3	116.7 (2)
C2—C1—C6—C5	−0.6 (10)	Na1^{ii}—O4—Na1—O4^{i}	29.7 (2)
S1—C1—C6—C5	179.7 (5)	Na1^{ii}—O4—Na1—O1^{ii}	−54.1 (2)
C4—C5—C6—C1	0.1 (11)	Na1^{ii}—O4—Na1—O2^{ii}	−131.5 (2)
C12—C7—C8—C9	−1.9 (11)	Na1^{ii}—O4—Na1—O5^{ii}	−132.5 (5)
S2—C7—C8—C9	179.2 (6)	Na1^{ii}—O4—Na1—Na2^{ii}	−100.81 (19)
C7—C8—C9—C10	1.2 (11)	Na1^{ii}—O4—Na1—Na1^{i}	70.9 (3)
C8—C9—C10—C11	−0.8 (11)	Na2^{iii}—O6—Na2—O7^{iv}	119.6 (2)

C8—C9—C10—Cl4	−178.3 (6)	Na2^{iii}—O6—Na2—O5	−117.4 (5)
C9—C10—C11—C12	1.0 (11)	Na2^{iii}—O6—Na2—O6^{iv}	26.1 (2)
Cl4—C10—C11—C12	178.6 (5)	Na2^{iii}—O6—Na2—O2	−54.6 (2)
C8—C7—C12—C11	2.1 (10)	Na2^{iii}—O6—Na2—O1	−132.7 (2)
S2—C7—C12—C11	−179.0 (5)	Na2^{iii}—O6—Na2—Na1^{i}	−97.6 (2)
C10—C11—C12—C7	−1.7 (10)	Na2^{iii}—O6—Na2—Na2^{iv}	61.1 (3)
Na1—O3—S1—O1	−64.0 (6)	Na1^{i}—O5—Na2—O7^{iv}	147.92 (16)
Na1—O3—S1—N1	56.9 (6)	Na1^{i}—O5—Na2—O6	24.8 (6)
Na1—O3—S1—C1	177.6 (5)	Na1^{i}—O5—Na2—O6^{iv}	−122.54 (16)
Na1^{i}—O1—S1—O3	1.5 (4)	Na1^{i}—O5—Na2—O2	−39.25 (15)
Na2—O1—S1—O3	145.6 (5)	Na1^{i}—O5—Na2—O1	40.13 (15)
Na1^{i}—O1—S1—N1	−125.2 (3)	Na1^{i}—O5—Na2—Na2^{iv}	−154.02 (14)
Na2—O1—S1—N1	18.9 (5)	Na1^{i}—O5—Na2—Na2^{iii}	−56.4 (3)
Na1^{i}—O1—S1—C1	118.7 (3)	S2—O2—Na2—O7^{iv}	−81.8 (15)
Na2—O1—S1—C1	−97.2 (5)	Na1^{i}—O2—Na2—O7^{iv}	108.5 (14)
Cl1—N1—S1—O3	56.3 (4)	S2—O2—Na2—O6	48.6 (3)
Cl1—N1—S1—O1	−176.9 (3)	Na1^{i}—O2—Na2—O6	−121.07 (17)
Cl1—N1—S1—C1	−62.1 (4)	S2—O2—Na2—O5	−150.3 (3)
C6—C1—S1—O3	0.2 (6)	Na1^{i}—O2—Na2—O5	39.99 (16)
C2—C1—S1—O3	−179.5 (5)	S2—O2—Na2—O6^{iv}	−67.8 (3)
C6—C1—S1—O1	−123.1 (5)	Na1^{i}—O2—Na2—O6^{iv}	122.47 (17)
C2—C1—S1—O1	57.2 (6)	S2—O2—Na2—O1	129.0 (3)
C6—C1—S1—N1	124.5 (5)	Na1^{i}—O2—Na2—O1	−40.71 (14)
C2—C1—S1—N1	−55.3 (6)	S2—O2—Na2—Na1^{i}	169.7 (4)
Na2^{iii}—O7—S2—O2	−70.9 (4)	S2—O2—Na2—Na2^{iv}	−83.5 (3)
Na2^{iii}—O7—S2—N2	51.7 (4)	Na1^{i}—O2—Na2—Na2^{iv}	106.77 (14)
Na2^{iii}—O7—S2—C7	170.4 (3)	S2—O2—Na2—Na2^{iii}	21.0 (3)
Na2—O2—S2—O7	7.5 (4)	Na1^{i}—O2—Na2—Na2^{iii}	−148.67 (15)
Na1^{i}—O2—S2—O7	169.1 (4)	S1—O1—Na2—O7^{iv}	75.7 (5)
Na2—O2—S2—N2	−120.1 (3)	Na1^{i}—O1—Na2—O7^{iv}	−134.14 (17)
Na1^{i}—O2—S2—N2	41.4 (5)	S1—O1—Na2—O6	−17.7 (5)
Na2—O2—S2—C7	125.9 (3)	Na1^{i}—O1—Na2—O6	132.51 (17)
Na1^{i}—O2—S2—C7	−72.5 (5)	S1—O1—Na2—O5	167.9 (5)
Cl2—N2—S2—O7	54.2 (4)	Na1^{i}—O1—Na2—O5	−41.93 (15)
Cl2—N2—S2—O2	−177.6 (3)	S1—O1—Na2—O6^{iv}	−149.6 (4)
Cl2—N2—S2—C7	−64.0 (4)	Na1^{i}—O1—Na2—O6^{iv}	0.6 (5)
C8—C7—S2—O7	−164.6 (6)	S1—O1—Na2—O2	−108.4 (5)
C12—C7—S2—O7	16.5 (6)	Na1^{i}—O1—Na2—O2	41.73 (15)
C8—C7—S2—O2	71.0 (6)	S1—O1—Na2—Na1^{i}	−150.2 (6)
C12—C7—S2—O2	−107.9 (5)	S1—O1—Na2—Na2^{iv}	142.2 (4)
C8—C7—S2—N2	−41.2 (6)	Na1^{i}—O1—Na2—Na2^{iv}	−67.7 (3)

C12—C7—S2—N2	139.9 (5)	S1—O1—Na2—Na2^{iii}	−41.5 (5)
S1—O3—Na1—O4^{i}	41.2 (6)	Na1^{i}—O1—Na2—Na2^{iii}	108.68 (13)
S1—O3—Na1—O1^{ii}	45.8 (14)		

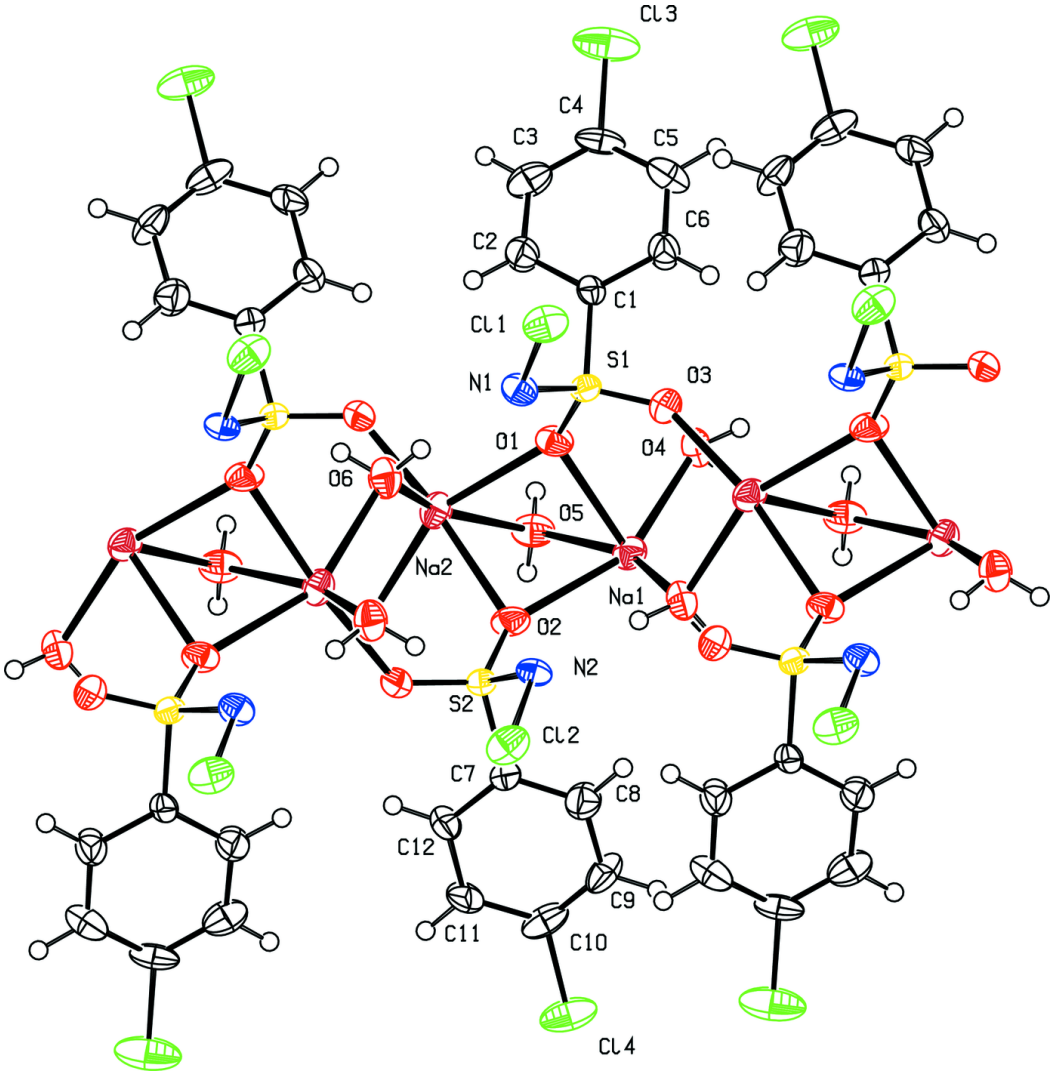
Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*; (ii) *x*+1/2, −*y*+3/2, −*z*; (iii) *x*+1/2, −*y*+1/2, −*z*; (iv) *x*−1/2, −*y*+1/2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H41O···Cl1	0.842 (19)	2.70 (2)	3.523 (5)	167 (5)
O4—H42O···N2^{ii}	0.841 (19)	2.06 (2)	2.903 (7)	177 (7)
O4—H42O···S2^{ii}	0.841 (19)	2.91 (4)	3.633 (5)	145 (6)
O5—H51O···N2^{v}	0.848 (19)	2.06 (2)	2.899 (6)	170 (7)
O5—H51O···Cl2^{v}	0.848 (19)	2.89 (3)	3.631 (5)	147 (4)
O5—H52O···N1^{v}	0.861 (19)	2.16 (2)	3.006 (6)	169 (7)
O5—H52O···Cl1^{v}	0.861 (19)	2.82 (3)	3.522 (5)	139 (4)
O6—H61O···Cl2^{iv}	0.87 (2)	2.61 (5)	3.305 (5)	138 (6)
O6—H61O···O2^{iii}	0.87 (2)	2.63 (6)	3.212 (6)	125 (6)
O6—H62O···N1	0.86 (2)	2.00 (2)	2.845 (7)	167 (6)
O6—H62O···S1	0.86 (2)	3.00 (4)	3.687 (5)	138 (5)

Symmetry codes: (ii) *x*+1/2, −*y*+3/2, −*z*; (v) *x*−1, *y*, *z*; (iv) *x*−1/2, −*y*+1/2, −*z*; (iii) *x*+1/2, −*y*+1/2, −*z*.

Fig. 1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C5
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C1
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O1
O4
O6
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N2
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Cl2
C7
C8
C12
C9
C11
C10
Cl4

Fig. 2

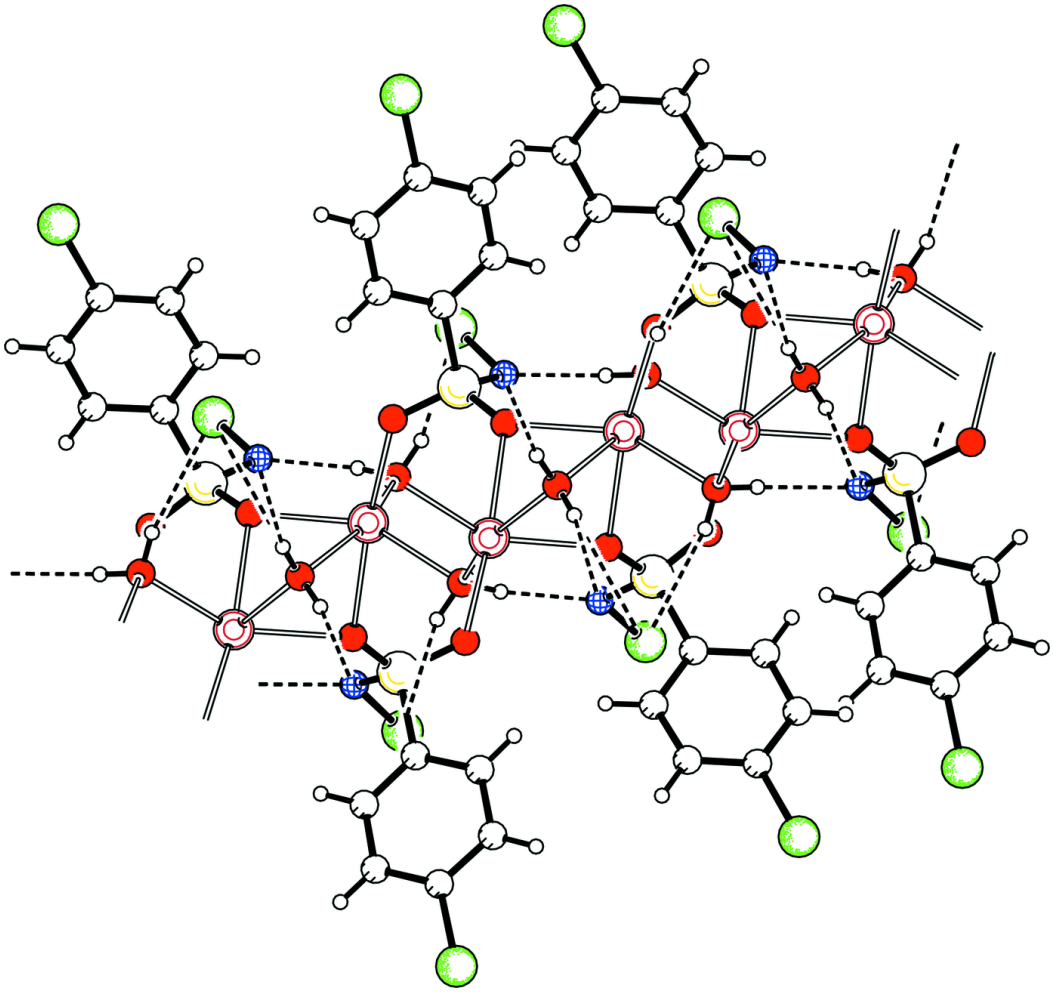

Fig. 3