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Poly[(μ_4-chloranilato)bis(saccharin)-disodium(I)]

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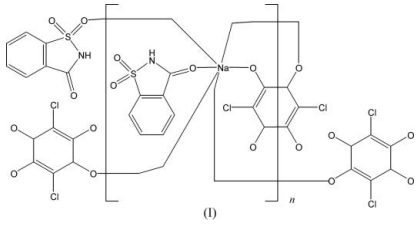
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; some non-H atoms missing; R factor = 0.035; wR factor = 0.089; data-to-parameter ratio = 18.8.

In the title compound {systematic name: poly[(μ_4-2,5-dichloro-3,6-dihydroxy-1,4-benzoquinonato)bis[1,2-benziso-thiazol-3(2*H*)-one 1,1-dioxide]disodium(I)]}, $[Na_2(C_6Cl_2O_4)(C_7H_5NO_3S)_2]_n$, the Na^I atom is coordinated by six O atoms from three chloranilate ions and two saccharin ligands in a distorted octahedral geometry. There is an intramolecular N—H···O hydrogen bond between the saccharin ligand and the chloranilate dianion. Each O atom of the chloranilate ion bonds to two Na^I atoms, while the saccharin ligand bridges the Na^I atoms *via* the carbonyl O atom and one of the sulfonyl O atoms. The Na atoms and bridging ligands form layers parallel to the *ab* plane at z = 0 and $z = \frac{1}{2}$. The shortest Na···Na and Na···Cl distances in the layer are 3.6006 (12) and 3.0680 (7) Å, respectively.

Related literature

There are a large number of metal complexes coordinated by the saccharinate anion obtained by deprotonation of the N—H group of saccharin (Baran, 2005; Baran & Yilmaz, 2006; Gumus *et al.*, 2007). However, no crystal data for metal complexes with neutral saccharin as a ligand are available in the Cambridge Structural Database (Version 5.28; Allen, 2002).



(I)

Experimental

Crystal data

$[Na_2(C_6Cl_2O_4)(C_7H_5NO_3S)_2]$
M_r = 619.30
Monoclinic, $C2/c$
a = 14.6795 (7) Å
b = 6.2247 (3) Å
c = 25.2114 (12) Å
β = 99.9052 (16)°
V = 2269.36 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 170 (2) K
0.55 × 0.23 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.704, T_{max} = 0.961
12067 measured reflections
3306 independent reflections
2886 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.089
S = 1.05
3306 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Na1—O1	2.4024 (11)	Na1—O2^{iii}	2.3664 (12)
Na1—O1^{i}	2.4527 (12)	Na1—O3^{iv}	2.5624 (13)
Na1—O2^{ii}	2.3663 (11)	Na1—O5	2.3198 (13)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.84 (3)	2.01 (2)	2.7938 (16)	156 (2)

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2333).

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supplementary materials

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Poly[(μ_4-chloranilato)bis(saccharin)disodium(I)]

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Comment

The Na^I atom of the title compound is at the centre of a distorted octahedron and deviates by 0.3422 (8) Å from the mean plane of atoms O1, $O2^{ii}$, $O2^{iii}$ and O5, which form the equatorial plane (Figs. 1 and 2) [symmetry codes: (ii) −*x*, −*y* + 2, −*z* + 1; (iii) *x* + 1/2, *y* + 1/2, *z*]. The Na—O bond lengths in this plane range from 2.3663 (11) to 2.4024 (11) Å. Atoms $O1^i$ and $O3^{iv}$ occupy the axial positions [Na—$O1^i$ = 2.4527 (12) and Na—$O3^{iv}$ = 2.5624 (13) Å; symmetry codes: (i) −*x* + 1/2, −*y* + 3/2, −*z* + 1; (iv) *x*, 1 + *y*, *z*].

There is an intermolecular N—H···O hydrogen bond (Table 2). The chloranilate and saccharin ligands bridge the Na^I atoms, forming layers parallel to the *ab* plane at *z* = 0 and *z* = 1/2 (Fig. 3).

Experimental

The title compound was prepared by mixing chloroform–methanol (1:1 *v*/*v*) solutions (20 and 20 ml, respectively) of saccharin sodium (1.0 mmol) and chloranilic acid (1.0 mmol). The combined solution was left at room temperature for 12 h to give red crystals, which were filtered and washed several times with dichloromethane and then dried.

Refinement

All H atoms were located in a difference map. The N-bound H atom was refined freely, while other H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

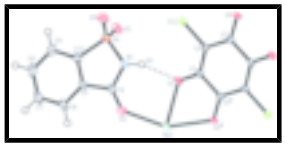

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The intermolecular hydrogen bond is indicated by a dashed line. [Symmetry code: (ii) −*x*, −*y* + 2, −*z* + 1.]

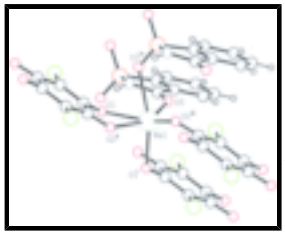

Fig. 2. A view of the polymeric fragment of (I), showing the distorted octahedral coordination geometry. [Symmetry codes: (i) −*x* + 1/2, −*y* + 3/2, −*z* + 1; (ii) −*x*, −*y* + 2, −*z* + 1; (iii) *x* + 1/2, *y* + 1/2, *z*; (iv) *x*, 1 + *y*, *z*.]

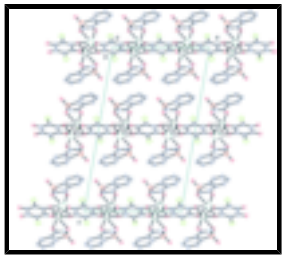

Fig. 3. The molecular packing of (I), viewed along the *b* axis. H atoms have been omitted for clarity.

poly[(μ4 2,5-dichloro-3,6-dihydroxy-1,4-benzoquinonato)bis[1,2- benzisothiazol-3(2*H*)-one 1,1-dioxide]disodium(I)]

Crystal data

$[Na_2(C_6Cl_2O_4)(C_7H_5NO_3S)_2]$	F_{000} = 1248
M_r = 619.30	D_x = 1.818 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: -C 2yc	Cell parameters from 10738 reflections
a = 14.6795 (7) Å	θ = 3.0–30.0º
b = 6.2247 (3) Å	μ = 0.57 mm^{-1}
c = 25.2114 (12) Å	*T* = 170 (2) K
β = 99.9052 (16)º	Platelet, red
V = 2269.36 (19) Å^3	0.55 × 0.23 × 0.07 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	2886 reflections with $I > 2\sigma(I)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.041
ω scans	θ_{max} = 30.0º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −20→20
T_{min} = 0.704, T_{max} = 0.961	*k* = −8→8
12067 measured reflections	*l* = −35→35
3306 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 1.5311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.089	$(\Delta/\sigma)_{max} < 0.001$
S = 1.05	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
3306 reflections	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
176 parameters	Extinction correction: none

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 $F^2 > \sigma(F^2)$ 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}
Cl1	−0.04269 (2)	0.57417 (5)	0.431471 (13)	0.01939 (9)
S1	0.14374 (2)	0.30306 (6)	0.354874 (14)	0.01869 (9)
Na1	0.27054 (4)	0.99825 (9)	0.46736 (2)	0.01851 (13)
O1	0.14132 (7)	0.76727 (16)	0.47271 (4)	0.01704 (19)
O2	−0.17515 (7)	0.85677 (17)	0.47486 (4)	0.0179 (2)
O3	0.13973 (8)	0.14915 (19)	0.39671 (5)	0.0262 (2)
O4	0.06485 (8)	0.3162 (2)	0.31285 (5)	0.0282 (3)
O5	0.29399 (8)	0.77774 (18)	0.39676 (5)	0.0255 (2)
N1	0.17091 (9)	0.5440 (2)	0.38105 (5)	0.0205 (2)
C1	0.07295 (9)	0.8707 (2)	0.48321 (5)	0.0141 (2)
C2	−0.01884 (9)	0.8108 (2)	0.46768 (5)	0.0152 (2)
C3	−0.09322 (9)	0.9193 (2)	0.48437 (5)	0.0143 (2)
C4	0.25872 (10)	0.6137 (2)	0.37689 (6)	0.0185 (3)
C5	0.30221 (10)	0.4592 (2)	0.34423 (6)	0.0190 (3)
C6	0.38975 (11)	0.4763 (3)	0.33085 (6)	0.0263 (3)
H6	0.4266	0.5962	0.3406	0.032*
C7	0.42019 (12)	0.3072 (3)	0.30234 (7)	0.0329 (4)
H7	0.4792	0.3125	0.2936	0.039*
C8	0.36383 (13)	0.1295 (3)	0.28656 (7)	0.0324 (4)
H8	0.3856	0.0196	0.2671	0.039*
C9	0.27599 (12)	0.1142 (3)	0.29944 (6)	0.0256 (3)
H9	0.2379	−0.0028	0.2887	0.031*
C10	0.24751 (10)	0.2814 (2)	0.32910 (6)	0.0194 (3)
H1	0.1459 (17)	0.599 (4)	0.4051 (10)	0.041 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01556 (15)	0.01872 (16)	0.02493 (17)	−0.00330 (12)	0.00638 (12)	−0.00676 (12)
S1	0.01455 (16)	0.02209 (17)	0.02003 (17)	−0.00378 (12)	0.00463 (12)	0.00048 (12)
Na1	0.0136 (3)	0.0178 (3)	0.0256 (3)	−0.0015 (2)	0.0077 (2)	−0.0026 (2)
O1	0.0108 (4)	0.0185 (5)	0.0231 (5)	0.0011 (4)	0.0067 (3)	−0.0014 (4)

O2	0.0092 (4)	0.0205 (5)	0.0246 (5)	−0.0033 (4)	0.0051 (3)	−0.0039 (4)
O3	0.0252 (6)	0.0282 (6)	0.0266 (5)	−0.0036 (5)	0.0081 (4)	0.0057 (4)
O4	0.0175 (5)	0.0391 (7)	0.0265 (6)	−0.0066 (5)	−0.0003 (4)	0.0015 (5)
O5	0.0258 (6)	0.0227 (5)	0.0303 (6)	−0.0070 (4)	0.0111 (4)	−0.0061 (4)
N1	0.0148 (5)	0.0229 (6)	0.0257 (6)	−0.0014 (5)	0.0089 (5)	−0.0050 (5)
C1	0.0111 (5)	0.0152 (6)	0.0172 (5)	−0.0003 (5)	0.0057 (4)	0.0008 (5)
C2	0.0114 (5)	0.0148 (6)	0.0201 (6)	−0.0020 (5)	0.0044 (5)	−0.0046 (5)
C3	0.0109 (5)	0.0158 (6)	0.0171 (5)	−0.0009 (5)	0.0047 (4)	−0.0005 (5)
C4	0.0158 (6)	0.0205 (6)	0.0204 (6)	−0.0010 (5)	0.0065 (5)	−0.0002 (5)
C5	0.0168 (6)	0.0225 (6)	0.0191 (6)	−0.0012 (5)	0.0069 (5)	−0.0012 (5)
C6	0.0183 (7)	0.0362 (8)	0.0269 (7)	−0.0025 (6)	0.0104 (6)	−0.0020 (6)
C7	0.0232 (8)	0.0520 (11)	0.0268 (8)	0.0063 (7)	0.0138 (6)	−0.0025 (7)
C8	0.0338 (9)	0.0409 (10)	0.0245 (7)	0.0117 (8)	0.0107 (6)	−0.0067 (7)
C9	0.0299 (8)	0.0254 (7)	0.0218 (7)	0.0015 (6)	0.0057 (6)	−0.0041 (6)
C10	0.0181 (6)	0.0230 (7)	0.0180 (6)	0.0004 (5)	0.0060 (5)	−0.0005 (5)

Geometric parameters (Å, °)

Cl1—C2	1.7365 (13)	N1—H1	0.84 (3)
S1—O3	1.4336 (12)	C1—C2	1.3879 (18)
S1—O4	1.4312 (11)	C1—C3^{ii}	1.5431 (18)
S1—N1	1.6595 (13)	C2—C3	1.4085 (18)
S1—C10	1.7610 (15)	C4—C5	1.480 (2)
Na1—O1	2.4024 (11)	C5—C6	1.388 (2)
Na1—O1^{i}	2.4527 (12)	C5—C10	1.382 (2)
Na1—O2^{ii}	2.3663 (11)	C6—C7	1.391 (2)
Na1—O2^{iii}	2.3664 (12)	C6—H6	0.93
Na1—O3^{iv}	2.5624 (13)	C7—C8	1.398 (3)
Na1—O5	2.3198 (13)	C7—H7	0.93
O1—C1	1.2582 (16)	C8—C9	1.386 (3)
O2—C3	1.2475 (15)	C8—H8	0.93
O5—C4	1.2134 (19)	C9—C10	1.387 (2)
N1—C4	1.3810 (18)	C9—H9	0.93
Na1···Cl1^{iii}	3.0680 (7)	Na1···Na1^{i}	3.6006 (12)
Na1···C1	3.0986 (14)	Na1···Na1^{v}	3.6381 (11)
Na1···C3^{ii}	3.0998 (14)		
O4—S1—O3	116.90 (7)	S1—N1—H1	123.7 (18)
O4—S1—N1	110.57 (7)	O1—C1—C2	125.03 (12)
O3—S1—N1	110.42 (7)	O1—C1—C3^{ii}	117.17 (11)
O4—S1—C10	111.86 (7)	C2—C1—C3^{ii}	117.80 (11)
O3—S1—C10	111.58 (7)	C1—C2—C3	123.49 (12)
N1—S1—C10	92.98 (7)	C1—C2—Cl1	118.31 (10)
O1—Na1—O1^{i}	84.27 (4)	C3—C2—Cl1	117.86 (10)
O2^{ii}—Na1—O1	68.72 (4)	O2—C3—C2	124.33 (12)
O2^{iii}—Na1—O1	144.92 (4)	O2—C3—C1^{ii}	117.26 (11)
O2^{ii}—Na1—O1^{i}	100.55 (4)	C2—C3—C1^{ii}	118.41 (11)

O2^{iii}—Na1—O1^{i}	116.84 (4)	O5—C4—N1	124.78 (14)
O5—Na1—O1	84.94 (4)	O5—C4—C5	125.61 (14)
O5—Na1—O1^{i}	86.66 (4)	N1—C4—C5	109.61 (12)
O2^{ii}—Na1—O2^{iii}	79.52 (4)	C10—C5—C6	120.85 (14)
O5—Na1—O2^{ii}	151.60 (5)	C10—C5—C4	112.84 (13)
O5—Na1—O2^{iii}	121.79 (5)	C6—C5—C4	126.25 (14)
O1—Na1—O3^{iv}	75.75 (4)	C5—C6—C7	117.44 (16)
O1^{i}—Na1—O3^{iv}	158.14 (4)	C5—C6—H6	121.3
O2^{ii}—Na1—O3^{iv}	80.56 (4)	C7—C6—H6	121.3
O2^{iii}—Na1—O3^{iv}	84.93 (4)	C6—C7—C8	121.27 (16)
O5—Na1—O3^{iv}	82.87 (5)	C6—C7—H7	119.4
Na1—O1—Na1^{i}	95.73 (4)	C8—C7—H7	119.4
C1—O1—Na1	111.82 (9)	C9—C8—C7	121.09 (15)
C1—O1—Na1^{i}	124.80 (9)	C9—C8—H8	119.5
C3—O2—Na1^{ii}	114.55 (9)	C7—C8—H8	119.5
C3—O2—Na1^{vi}	127.60 (9)	C8—C9—C10	116.99 (15)
Na1^{ii}—O2—Na1^{vi}	100.48 (4)	C8—C9—H9	121.5
S1—O3—Na1^{vii}	129.47 (7)	C10—C9—H9	121.5
C4—O5—Na1	134.88 (10)	C5—C10—C9	122.33 (14)
C4—N1—S1	114.67 (10)	C5—C10—S1	109.58 (11)
C4—N1—H1	117.3 (17)	C9—C10—S1	128.06 (12)
O5—Na1—O1—C1	−141.72 (9)	Na1^{vi}—O2—C3—C1^{ii}	−147.38 (9)
O2^{ii}—Na1—O1—C1	27.46 (9)	Na1^{vi}—O2—C3—Na1^{ii}	−127.17 (13)
O2^{iii}—Na1—O1—C1	0.86 (13)	C1—C2—C3—O2	−173.24 (13)
O1^{i}—Na1—O1—C1	131.15 (10)	Cl1—C2—C3—O2	−0.03 (19)
O3^{iv}—Na1—O1—C1	−57.80 (9)	C1—C2—C3—C1^{ii}	6.5 (2)
O5—Na1—O1—Na1^{i}	87.14 (4)	Cl1—C2—C3—C1^{ii}	179.74 (9)
O2^{ii}—Na1—O1—Na1^{i}	−103.69 (4)	C1—C2—C3—Na1^{ii}	−126.4 (2)
O2^{iii}—Na1—O1—Na1^{i}	−130.29 (7)	Cl1—C2—C3—Na1^{ii}	46.8 (3)
O1^{i}—Na1—O1—Na1^{i}	0.0	Na1—O5—C4—N1	22.3 (2)
O3^{iv}—Na1—O1—Na1^{i}	171.05 (5)	Na1—O5—C4—C5	−158.35 (11)
O4—S1—O3—Na1^{vii}	164.12 (8)	S1—N1—C4—O5	−174.54 (12)
N1—S1—O3—Na1^{vii}	−68.34 (10)	S1—N1—C4—C5	5.99 (16)
C10—S1—O3—Na1^{vii}	33.61 (11)	O5—C4—C5—C10	176.99 (14)
O2^{ii}—Na1—O5—C4	−26.6 (2)	N1—C4—C5—C10	−3.55 (18)
O2^{iii}—Na1—O5—C4	−160.78 (14)	O5—C4—C5—C6	−0.2 (3)
O1—Na1—O5—C4	−5.05 (15)	N1—C4—C5—C6	179.24 (15)
O1^{i}—Na1—O5—C4	79.49 (15)	C10—C5—C6—C7	−0.7 (2)
O3^{iv}—Na1—O5—C4	−81.28 (15)	C4—C5—C6—C7	176.30 (15)
O4—S1—N1—C4	−120.06 (11)	C5—C6—C7—C8	1.6 (3)
O3—S1—N1—C4	108.99 (12)	C6—C7—C8—C9	−0.9 (3)
C10—S1—N1—C4	−5.37 (12)	C7—C8—C9—C10	−0.8 (3)

Na1—O1—C1—C2	151.68 (11)	C6—C5—C10—C9	−1.0 (2)
Na1^{i}—O1—C1—C2	−94.16 (15)	C4—C5—C10—C9	−178.39 (14)
Na1—O1—C1—C3^{ii}	−28.03 (14)	C6—C5—C10—S1	177.20 (12)
Na1^{i}—O1—C1—C3^{ii}	86.12 (13)	C4—C5—C10—S1	−0.18 (16)
Na1^{i}—O1—C1—Na1	114.16 (11)	C8—C9—C10—C5	1.7 (2)
O1—C1—C2—C3	173.81 (13)	C8—C9—C10—S1	−176.12 (13)
C3^{ii}—C1—C2—C3	−6.5 (2)	O4—S1—C10—C5	116.60 (11)
O1—C1—C2—Cl1	0.62 (19)	O3—S1—C10—C5	−110.32 (11)
C3^{ii}—C1—C2—Cl1	−179.67 (9)	N1—S1—C10—C5	3.03 (12)
Na1^{ii}—O2—C3—C2	159.56 (11)	O4—S1—C10—C9	−65.31 (16)
Na1^{vi}—O2—C3—C2	32.39 (19)	O3—S1—C10—C9	67.76 (15)
Na1^{ii}—O2—C3—C1^{ii}	−20.21 (14)	N1—S1—C10—C9	−178.89 (14)

Symmetry codes: (i) −*x*+1/2, −*y*+3/2, −*z*+1; (ii) −*x*, −*y*+2, −*z*+1; (iii) *x*+1/2, *y*+1/2, *z*; (iv) *x*, *y*+1, *z*; (v) −*x*+1/2, −*y*+5/2, −*z*+1; (vi) *x*−1/2, *y*−1/2, *z*; (vii) *x*, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.84 (3)	2.01 (2)	2.7938 (16)	156 (2)

Fig. 1

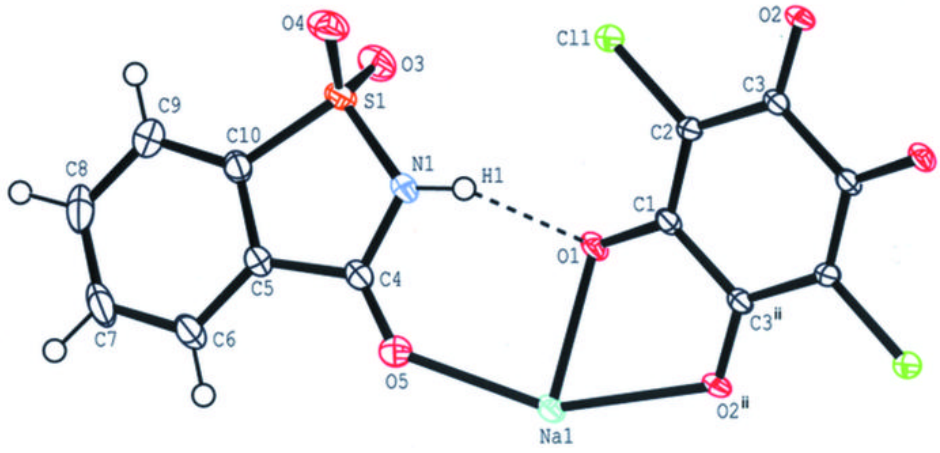
O4
O3
S1
C9
C10
C8
N1
H1
C11
O2
C3
C2
C1
O1
C5
C4
C7
C6
O5
C3ii
O2ii
Na1

Fig. 2

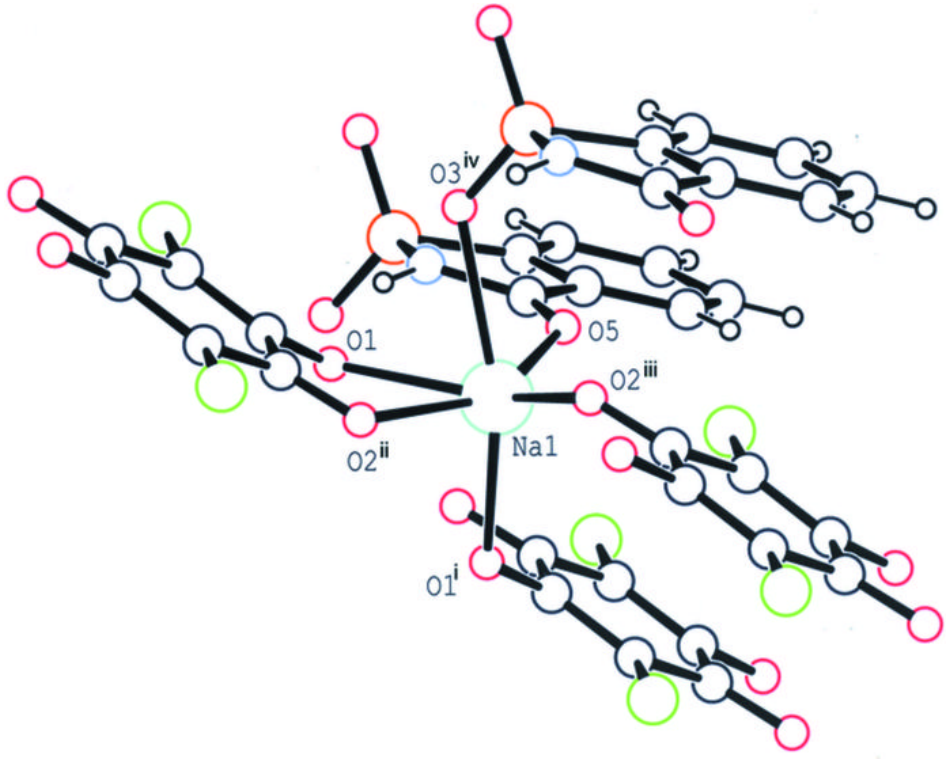

Fig. 3