IUCrData

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Di-μ-dimethylformamide-κ^4O:O-μ-tetrahydrofuran-κ^2O:O-bis[(tetrahydrofuran-κO)sodium(I)] bis(μ-3,6-dichlorobenzene-1,2-dithiolato-κ^3S,S':S)-bis[(3,6-dichlorobenzene-1,2-dithiolato-κ^2S,S')-iron(III)]

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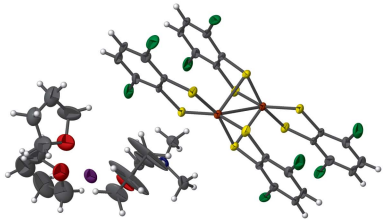
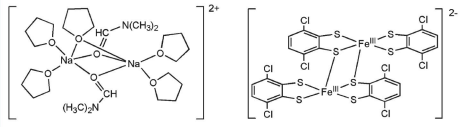
The title compound, $[Na_2(C_3H_7NO)_2(C_4H_8O)_5][Fe_2(C_6H_2Cl_2S_2)_4]$, was synthesized and its crystal structure was solved. The ionic crystal contains a $[Fe_2(S_2C_6H_2Cl_2)_4]^{2-}$ dimeric anion and a $[Na_2(THF)_4(\mu\text{-THF})(\mu\text{-DMF})_2]^{2+}$ cation, where THF is tetrahydrofuran and DMF is dimethylformamide, comprising two sodium atoms joined by one THF and two DMF molecules bridging through their O atoms. The five-coordinate environment of each Na site is completed by two terminal THF molecules. The asymmetric unit contains half a cationic unit (as the cation is placed on a twofold axis) and half an anion, as there is an inversion centre at the midpoint of the Fe—Fe vectors. The cationic and anionic moieties are linked by C—H···Cl and C—H···S interactions.

3D view



Chemical scheme



Structure description

In the title compound (Fig. 1) the $[Fe^{III}(Cl_2\text{-bdt})_2]^-$ anion (Cl_2-bdt is 3,6-dichloro-1,2-benzenedithiolate) forms a centrosymmetric dimer supported by two Fe^{III}—S bonds [Fe1—S4 = 2.4885 (16) Å] in which each iron atom shows the expected 4 + 1 square-pyramidal geometry. This is the typical coordination mode displayed by most of the iron bis(dithiolato) compounds, which is due to the strong dimerization tendency of the monoanionic $[Fe(dithiolate)_2]^-$ species (Amo-Ochoa *et al.*, 2013; Chen *et al.*, 2012;

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···Cl2^{i}	0.95	2.86	3.645 (6)	141
C16—H16A···Cl3^{ii}	0.99	2.96	3.836 (15)	148
C23—H23···Cl2^{iii}	0.95	2.92	3.787 (7)	152
C25—H25B···S4^{iv}	0.98	2.79	3.744 (6)	165
C25—H25C···S3^{iii}	0.98	2.98	3.711 (7)	132

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

Sproules & Wieghardt, 2010; Cerdeira *et al.*, 2008). The basal Fe—S bond lengths [Fe1—S1 = 2.2219 (15), Fe1—S2 = 2.2101 (16), Fe1—S3 = 2.2256 (15) and Fe1—S4 = 2.2296 (15) Å] are shorter than the axial one, 2.4885 (16) Å. On the other hand, the two sodium atoms in the cation $[Na_2(THF)_4(\mu\text{-THF})(\mu\text{-DMF})_2]^{2+}$ are bridged by one THF and two DMF molecules. To complete the pentacoordination sphere (Fig. 2), each sodium atom is additionally bonded to two terminal THF molecules, at normal distances (Benmansour *et al.*, 2015; Raja *et al.*, 2014; Thirumurugan *et al.*, 2010).

In the crystal, the supramolecular packing is determined by C—H···Cl and C—H···S interactions between anionic and cationic species (Table 1), yielding a three-dimensional network.

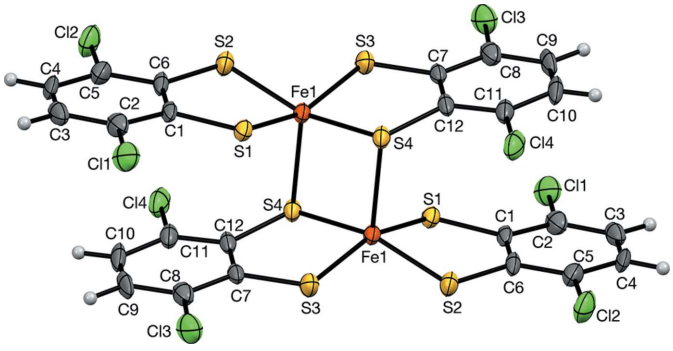


Figure 1
Ellipsoid plot (at 50% probability) of the $[Na_2(THF)_4(\mu\text{-THF})(\mu\text{-DMF})_2]^{2+}$ cation with non-hydrogen atoms labelled.

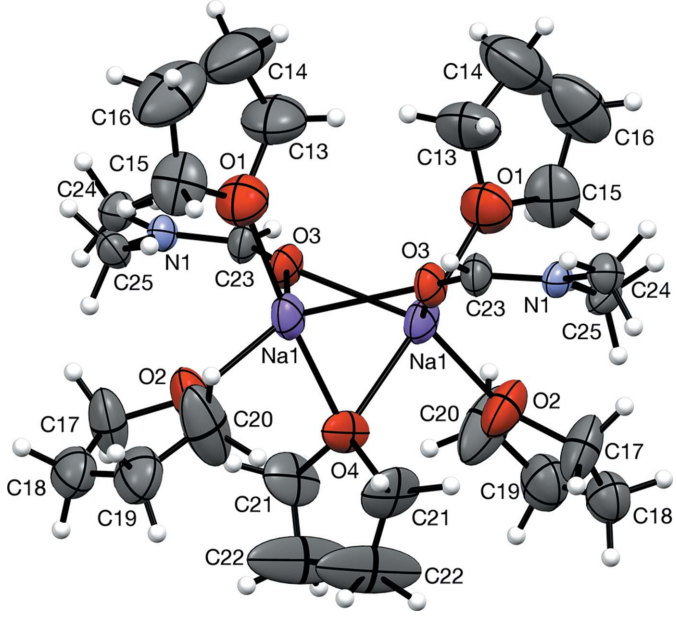


Figure 2
Ellipsoid plot (at 50% probability) of the $[Na_2(THF)_4(\mu\text{-THF})(\mu\text{-DMF})_2]^{2+}$ cation with non-hydrogen atoms labelled.

Synthesis and crystallization

An amount of 1,2-$HSC_6H_2Cl_2SH$ (238 mg, 1.1 mmol) was treated with an aqueous solution (10 ml) of NaOH, (5% by weight). Then, $FeCl_3\cdot 6H_2O$ (150 mg, 0.37 mmol) in 10 ml of ethanol/water (1:1) was slowly added. The mixture was stirred at room temperature for 30 min. The solid formed was collected by filtration and washed several times with water and *n*-hexane. Suitable crystals for X-ray analysis of the title compound were obtained from a solution in THF–DMF/*n*-hexane, at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Several C atoms from the THF molecules coordinated to the Na^+ cation (mainly for the bridging THF, see Fig. 2) present high displacement parameters. Alternative positions for disordered C atoms could not be located.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Na_2(C_3H_7NO)_2(C_4H_8O)_5]$-$[Fe_2(C_6H_2Cl_2S_2)_4]$
M_r	1500.77
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	100
a, *b*, *c* (Å)	29.063 (2), 9.9393 (6), 25.645 (3)
β (°)	121.609 (3)
V (Å^3)	6309.0 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.13
Crystal size (mm)	0.19 × 0.12 × 0.02
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.81, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43114, 5765, 3785
R_{int}	0.101
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.062, 0.169, 1.04
No. of reflections	5762
No. of parameters	359
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.26, −0.46

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2016). **1**, x160643 [doi:10.1107/S241431461600643X]

Di-μ-dimethylformamide-κ^4O:O-μ-tetrahydrofuran-κ^2O:O-bis[(tetrahydrofuran-κO)sodium(I)] bis(μ-3,6-dichlorobenzene-1,2-dithiolato-κ^3S,S':S)bis[(3,6-dichlorobenzene-1,2-dithiolato-κ^2S,S')iron(III)]

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Di-μ-dimethylformamide-κ^4O:O-μ-tetrahydrofuran-κ^2O:O-bis[(tetrahydrofuran-κO)sodium(I)] bis(μ-3,6-dichlorobenzene-1,2-dithiolato-κ^3S,S':S)bis[(3,6-dichlorobenzene-1,2-dithiolato-κ^2S,S')iron(III)]

Crystal data

$[Na_2(C_3H_7NO)_2(C_4H_8O)_5][Fe_2(C_6H_2Cl_2S_2)_4]$
M_r = 1500.77
Monoclinic, $C2/c$
a = 29.063 (2) Å
b = 9.9393 (6) Å
c = 25.645 (3) Å
β = 121.609 (3)°
V = 6309.0 (9) Å^3
Z = 4
$F(000)$ = 3080
D_x = 1.580 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3584 reflections
θ = 2.2–22.1°
μ = 1.13 mm^{-1}
T = 100 K
Prismatic, deep purple
0.19 × 0.12 × 0.02 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: molybdenum, x-ray tube
Graphite monochromator
θ and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.81, T_{max} = 0.98
43114 measured reflections
5765 independent reflections
3785 reflections with $I > 2\sigma(I)$
R_{int} = 0.101
θ_{max} = 25.4°, θ_{min} = 1.7°
h = −34→34
k = −11→11
l = −30→30
5765 standard reflections every 908 min
intensity decay: 0.0 (2)

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.169
S = 1.04
5762 reflections
359 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0854P)^2 + 20.9273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Refinement. There is some disorder in atoms from the coordinated THF molecules, specially in the positions occupied by C21 and C22

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1205 (2)	0.5476 (6)	0.1796 (2)	0.0255 (13)
C2	0.1666 (2)	0.6228 (6)	0.2206 (3)	0.0324 (14)
C3	0.2126 (2)	0.5608 (7)	0.2674 (3)	0.0382 (16)
H3	0.2437	0.6124	0.2942	0.046*
C4	0.2125 (2)	0.4236 (7)	0.2746 (3)	0.0370 (16)
H4	0.2438	0.38	0.3063	0.044*
C5	0.1673 (2)	0.3495 (6)	0.2359 (3)	0.0328 (14)
C6	0.1201 (2)	0.4095 (6)	0.1884 (2)	0.0257 (13)
C7	−0.1128 (2)	0.3851 (6)	−0.0270 (2)	0.0248 (13)
C8	−0.1619 (2)	0.3163 (6)	−0.0633 (3)	0.0334 (14)
C9	−0.2079 (2)	0.3846 (7)	−0.1069 (3)	0.0377 (16)
H9	−0.2406	0.3363	−0.1316	0.045*
C10	0.2067 (2)	0.4793 (7)	0.1147 (3)	0.0387 (17)
H10	0.2386	0.433	0.1437	0.046*
C11	0.1589 (2)	0.4098 (6)	0.0804 (3)	0.0314 (14)
C12	0.1114 (2)	0.4770 (6)	0.0375 (2)	0.0274 (13)
Cl1	0.16741 (7)	0.79653 (16)	0.21324 (7)	0.0429 (4)
Cl2	0.16885 (6)	0.17555 (17)	0.24562 (7)	0.0452 (4)
Cl3	−0.16552 (6)	0.14461 (18)	−0.05570 (7)	0.0456 (4)
Cl4	0.15827 (6)	0.23673 (17)	0.08984 (7)	0.0393 (4)
Fe1	0.01139 (3)	0.45371 (7)	0.06272 (3)	0.0205 (2)
S1	0.06380 (5)	0.62436 (14)	0.11780 (6)	0.0229 (3)
S2	0.06183 (5)	0.31766 (14)	0.14040 (6)	0.0267 (3)
S3	−0.05458 (5)	0.30212 (14)	0.02869 (6)	0.0265 (3)
S4	0.04882 (5)	0.39247 (14)	−0.00191 (6)	0.0231 (3)
C13	0.0826 (5)	1.1857 (10)	0.3275 (6)	0.105 (4)
H13A	0.0671	1.1971	0.283	0.126*
H13B	0.0531	1.1929	0.3359	0.126*
C14	0.1240 (7)	1.2872 (13)	0.3620 (7)	0.148 (6)
H14A	0.1343	1.332	0.3351	0.177*
H14B	0.11	1.3564	0.3779	0.177*
C15	0.1627 (3)	1.0772 (10)	0.3994 (4)	0.076 (3)
H15A	0.19	1.0432	0.3906	0.091*
H15B	0.1674	1.0287	0.4356	0.091*
C16	0.1703 (6)	1.2210 (14)	0.4120 (7)	0.121 (5)
H16A	0.1728	1.2413	0.4512	0.146*
H16B	0.2039	1.2518	0.4148	0.146*
C17	0.1423 (4)	0.6789 (11)	0.4322 (4)	0.082 (3)
H17A	0.1119	0.6231	0.4269	0.099*
H17B	0.1475	0.7541	0.4601	0.099*
C18	0.1906 (3)	0.5988 (9)	0.4591 (4)	0.069 (2)

H18A	0.1826	0.5041	0.4635	0.083*
H18B	0.218	0.634	0.4999	0.083*
C19	0.2101 (4)	0.6087 (10)	0.4164 (4)	0.081 (3)
H19A	0.2472	0.6455	0.4377	0.098*
H19B	0.2103	0.5188	0.4	0.098*
C20	0.1741 (5)	0.6957 (13)	0.3685 (5)	0.112 (4)
H20A	0.1607	0.6507	0.3286	0.135*
H20B	0.1936	0.7782	0.3695	0.135*
C23	0.0411 (3)	0.9659 (7)	0.1732 (3)	0.0423 (16)
H23	0.0786	0.9867	0.1968	0.051*
C24	0.0492 (3)	0.9917 (7)	0.0845 (3)	0.0398 (16)
H24A	0.0869	1.011	0.1158	0.06*
H24B	0.0339	1.068	0.0563	0.06*
H24C	0.0476	0.9109	0.0617	0.06*
C25	−0.0394 (3)	0.9425 (6)	0.0737 (3)	0.0408 (16)
H25A	−0.0577	0.9574	0.0962	0.061*
H25B	−0.0447	0.849	0.0596	0.061*
H25C	−0.0546	1.0031	0.0383	0.061*
N1	0.0182 (2)	0.9694 (5)	0.1138 (2)	0.0317 (12)
Na1	0.05894 (11)	0.8688 (3)	0.30354 (12)	0.0485 (7)
O1	0.1100 (2)	1.0542 (6)	0.3483 (3)	0.0744 (17)
O2	0.1294 (2)	0.7314 (6)	0.3744 (3)	0.0757 (18)
O3	0.01874 (19)	0.9381 (4)	0.2015 (2)	0.0431 (11)
O4	0	0.6850 (7)	0.25	0.061 (2)
C21	0.0153 (4)	0.5972 (8)	0.2171 (5)	0.080 (3)
H21A	−0.0079	0.6157	0.1727	0.096*
H21B	0.0532	0.6163	0.2295	0.096*
C22	0.0109 (9)	0.4696 (10)	0.2273 (8)	0.227 (11)
H22A	0.0464	0.424	0.2462	0.272*
H22B	−0.0148	0.423	0.1886	0.272*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.014 (3)	0.049 (4)	0.010 (3)	0.001 (2)	0.004 (2)	−0.005 (2)
C2	0.026 (3)	0.048 (4)	0.021 (3)	−0.008 (3)	0.011 (3)	−0.011 (3)
C3	0.020 (3)	0.071 (5)	0.021 (3)	−0.013 (3)	0.009 (3)	−0.012 (3)
C4	0.017 (3)	0.073 (5)	0.011 (3)	0.005 (3)	0.001 (3)	0.004 (3)
C5	0.026 (3)	0.048 (4)	0.021 (3)	0.006 (3)	0.010 (3)	0.006 (3)
C6	0.014 (3)	0.045 (4)	0.012 (3)	0.006 (2)	0.003 (2)	−0.005 (2)
C7	0.013 (3)	0.044 (3)	0.015 (3)	−0.002 (2)	0.006 (2)	−0.005 (2)
C8	0.022 (3)	0.055 (4)	0.022 (3)	−0.006 (3)	0.011 (3)	−0.010 (3)
C9	0.013 (3)	0.073 (5)	0.019 (3)	−0.009 (3)	0.003 (3)	−0.018 (3)
C10	0.016 (3)	0.075 (5)	0.014 (3)	0.010 (3)	0.001 (3)	−0.007 (3)
C11	0.018 (3)	0.055 (4)	0.018 (3)	0.007 (3)	0.007 (3)	−0.002 (3)
C12	0.013 (3)	0.051 (4)	0.016 (3)	0.002 (2)	0.006 (2)	−0.006 (3)
Cl1	0.0403 (9)	0.0505 (10)	0.0307 (9)	−0.0171 (7)	0.0136 (7)	−0.0104 (7)
Cl2	0.0358 (9)	0.0544 (10)	0.0291 (9)	0.0132 (8)	0.0057 (7)	0.0141 (7)

Cl3	0.0338 (9)	0.0593 (11)	0.0357 (9)	−0.0211 (8)	0.0127 (8)	−0.0123 (8)
Cl4	0.0278 (8)	0.0548 (10)	0.0284 (9)	0.0184 (7)	0.0100 (7)	0.0074 (7)
Fe1	0.0155 (4)	0.0280 (4)	0.0147 (4)	0.0012 (3)	0.0056 (3)	−0.0010 (3)
S1	0.0184 (7)	0.0303 (7)	0.0161 (7)	−0.0007 (5)	0.0063 (6)	−0.0019 (6)
S2	0.0203 (7)	0.0322 (7)	0.0187 (7)	0.0009 (6)	0.0041 (6)	0.0020 (6)
S3	0.0206 (7)	0.0329 (8)	0.0195 (7)	−0.0050 (6)	0.0059 (6)	−0.0009 (6)
S4	0.0163 (7)	0.0303 (8)	0.0179 (7)	0.0036 (5)	0.0057 (6)	−0.0008 (6)
C13	0.132 (10)	0.066 (7)	0.118 (10)	−0.026 (7)	0.066 (8)	−0.010 (6)
C14	0.221 (19)	0.094 (10)	0.165 (16)	−0.054 (11)	0.127 (15)	−0.058 (10)
C15	0.045 (5)	0.109 (8)	0.082 (7)	−0.018 (5)	0.039 (5)	−0.006 (6)
C16	0.118 (11)	0.127 (12)	0.143 (13)	−0.065 (9)	0.085 (10)	−0.055 (10)
C17	0.073 (6)	0.129 (9)	0.046 (5)	0.035 (6)	0.032 (5)	0.030 (5)
C18	0.067 (6)	0.075 (6)	0.054 (5)	−0.008 (5)	0.023 (5)	−0.004 (4)
C19	0.073 (7)	0.091 (7)	0.061 (6)	−0.017 (5)	0.022 (5)	−0.006 (5)
C20	0.114 (9)	0.175 (12)	0.091 (8)	0.075 (9)	0.084 (8)	0.061 (8)
C23	0.048 (4)	0.050 (4)	0.027 (4)	−0.001 (3)	0.019 (3)	0.002 (3)
C24	0.045 (4)	0.044 (4)	0.040 (4)	−0.001 (3)	0.029 (3)	0.002 (3)
C25	0.050 (4)	0.039 (4)	0.036 (4)	−0.012 (3)	0.024 (3)	−0.010 (3)
N1	0.042 (3)	0.035 (3)	0.028 (3)	−0.001 (2)	0.024 (3)	−0.002 (2)
Na1	0.0597 (18)	0.0594 (17)	0.0355 (16)	0.0062 (14)	0.0313 (14)	0.0059 (13)
O1	0.074 (4)	0.073 (4)	0.075 (4)	−0.015 (3)	0.038 (4)	−0.007 (3)
O2	0.086 (4)	0.097 (4)	0.055 (4)	0.029 (4)	0.045 (3)	0.030 (3)
O3	0.054 (3)	0.054 (3)	0.034 (3)	−0.001 (2)	0.032 (2)	0.003 (2)
O4	0.115 (7)	0.047 (4)	0.072 (5)	0	0.084 (5)	0
C21	0.129 (9)	0.074 (6)	0.102 (8)	0.003 (6)	0.105 (7)	−0.016 (5)
C22	0.55 (3)	0.060 (7)	0.36 (2)	0.010 (12)	0.44 (3)	0.004 (10)

Geometric parameters (Å, º)

C1—C6	1.393 (8)	S4—Fe1^{i}	2.2296 (15)
C1—C2	1.407 (8)	C13—C14	1.461 (16)
C1—S1	1.753 (5)	C13—O1	1.477 (12)
C2—C3	1.388 (8)	C14—C16	1.442 (18)
C2—Cl1	1.739 (7)	C15—O1	1.419 (10)
C3—C4	1.376 (9)	C15—C16	1.456 (15)
C4—C5	1.374 (8)	C17—O2	1.425 (9)
C5—C6	1.402 (7)	C17—C18	1.436 (11)
C5—Cl2	1.745 (6)	C18—C19	1.473 (12)
C6—S2	1.742 (5)	C19—C20	1.416 (12)
C7—C12^{i}	1.402 (8)	C20—O2	1.428 (10)
C7—C8	1.407 (8)	C23—O3	1.236 (7)
C7—S3	1.746 (5)	C23—N1	1.303 (8)
C8—C9	1.390 (9)	C24—N1	1.462 (7)
C8—Cl3	1.727 (7)	C25—N1	1.458 (8)
C9—C10^{i}	1.371 (9)	Na1—O1	2.265 (6)
C10—C9^{i}	1.372 (9)	Na1—O3^{ii}	2.298 (5)
C10—C11	1.377 (8)	Na1—O2	2.336 (6)
C11—C12	1.403 (8)	Na1—O3	2.341 (5)

C11—Cl4	1.739 (7)	Na1—O4	2.385 (6)
C12—C7^{i}	1.402 (8)	Na1—Na1^{ii}	3.069 (5)
C12—S4	1.764 (6)	O3—Na1^{ii}	2.298 (5)
Fe1—S2	2.2101 (16)	O4—C21^{ii}	1.438 (7)
Fe1—S1	2.2219 (15)	O4—C21	1.438 (7)
Fe1—S3	2.2256 (15)	O4—Na1^{ii}	2.385 (6)
Fe1—S4^{i}	2.2296 (15)	C21—C22	1.315 (11)
Fe1—S4	2.4885 (16)	C22—C22^{ii}	1.593 (17)

C6—C1—C2	119.2 (5)	C14—C13—O1	106.0 (11)
C6—C1—S1	119.5 (4)	C16—C14—C13	108.2 (12)
C2—C1—S1	121.4 (5)	O1—C15—C16	109.1 (9)
C3—C2—C1	121.3 (6)	C14—C16—C15	106.8 (11)
C3—C2—Cl1	118.2 (5)	O2—C17—C18	111.1 (7)
C1—C2—Cl1	120.5 (5)	C17—C18—C19	105.4 (8)
C4—C3—C2	119.2 (6)	C20—C19—C18	106.8 (8)
C5—C4—C3	120.1 (6)	C19—C20—O2	111.0 (8)
C4—C5—C6	122.0 (6)	O3—C23—N1	126.0 (7)
C4—C5—Cl2	119.0 (5)	C23—N1—C25	121.0 (5)
C6—C5—Cl2	119.1 (5)	C23—N1—C24	121.9 (6)
C1—C6—C5	118.2 (5)	C25—N1—C24	117.0 (5)
C1—C6—S2	119.3 (4)	O1—Na1—O3^{ii}	98.5 (2)
C5—C6—S2	122.5 (5)	O1—Na1—O2	90.4 (3)
C12^{i}—C7—C8	117.9 (5)	O3^{ii}—Na1—O2	130.9 (2)
C12^{i}—C7—S3	120.5 (4)	O1—Na1—O3	97.9 (2)
C8—C7—S3	121.6 (5)	O3^{ii}—Na1—O3	87.03 (19)
C9—C8—C7	120.7 (6)	O2—Na1—O3	139.6 (2)
C9—C8—Cl3	118.9 (5)	O1—Na1—O4	175.4 (2)
C7—C8—Cl3	120.4 (5)	O3^{ii}—Na1—O4	79.00 (16)
C10^{i}—C9—C8	120.8 (6)	O2—Na1—O4	94.2 (2)
C9^{i}—C10—C11	119.7 (6)	O3—Na1—O4	78.16 (15)
C10—C11—C12	120.7 (6)	O1—Na1—Na1^{ii}	125.53 (17)
C10—C11—Cl4	119.2 (5)	O3^{ii}—Na1—Na1^{ii}	49.18 (13)
C12—C11—Cl4	120.1 (5)	O2—Na1—Na1^{ii}	143.93 (18)
C11—C12—C7^{i}	120.1 (5)	O3—Na1—Na1^{ii}	47.98 (13)
C11—C12—S4	121.2 (5)	O4—Na1—Na1^{ii}	49.97 (12)
C7^{i}—C12—S4	118.7 (4)	C15—O1—C13	107.9 (7)
S2—Fe1—S1	89.09 (6)	C15—O1—Na1	134.7 (6)
S2—Fe1—S3	88.13 (6)	C13—O1—Na1	116.8 (6)
S1—Fe1—S3	158.23 (7)	C17—O2—C20	105.1 (6)
S2—Fe1—S4^{i}	163.07 (7)	C17—O2—Na1	132.0 (5)
S1—Fe1—S4^{i}	86.93 (6)	C20—O2—Na1	122.6 (5)
S3—Fe1—S4^{i}	89.48 (6)	C23—O3—Na1^{ii}	147.1 (4)
S2—Fe1—S4	97.79 (6)	C23—O3—Na1	128.0 (4)
S1—Fe1—S4	102.52 (6)	Na1^{ii}—O3—Na1	82.83 (18)
S3—Fe1—S4	99.25 (6)	C21^{ii}—O4—C21	105.3 (8)
S4^{i}—Fe1—S4	99.13 (5)	C21^{ii}—O4—Na1^{ii}	116.9 (4)
C1—S1—Fe1	104.4 (2)	C21—O4—Na1^{ii}	118.5 (4)

C6—S2—Fe1	104.9 (2)	C21^{ii}—O4—Na1	118.5 (4)
C7—S3—Fe1	105.5 (2)	C21—O4—Na1	116.9 (4)
C12—S4—Fe1^{i}	105.7 (2)	Na1^{ii}—O4—Na1	80.1 (2)
C12—S4—Fe1	100.46 (18)	C22—C21—O4	112.1 (7)
Fe1^{i}—S4—Fe1	80.87 (5)	C21—C22—C22^{ii}	105.3 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···Cl2^{iii}	0.95	2.86	3.645 (6)	141
C16—H16*A*···Cl3^{iv}	0.99	2.96	3.836 (15)	148
C23—H23···Cl2^{v}	0.95	2.92	3.787 (7)	152
C25—H25*B*···S4^{i}	0.98	2.79	3.744 (6)	165
C25—H25*C*···S3^{v}	0.98	2.98	3.711 (7)	132

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