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Disodium tetraaquabis(sulfato)iron(II)

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Key indicators: single-crystal X-ray study; T = 301 K; mean σ(Fe–O) = 0.001 Å; R factor = 0.018; wR factor = 0.048; data-to-parameter ratio = 14.0.

In the title compound, $[FeNa_2(SO_4)_2(H_2O)_4]$, the Fe^{2+} cation is situated on a centre of inversion and is hexacoordinated by four O atoms from water molecules and two O atoms from two sulfate anions in an octahedral geometry. The coordination environment of Na^+ comprises six O atoms in a more distorted octahedral arrangement, with Na—O distances between 2.368 (1) and 2.612 (1) Å. The structure contains an extensive three-dimensional network of O—H···O hydrogen bonds.

Related literature

For related structures, see: Held (2003); Barton *et al.* (2002).

Experimental

Crystal data

$[FeNa_2(SO_4)_2(H_2O)_4]$
M_r = 366.01
Monoclinic, $P2_1/c$
a = 5.551 (1) Å
b = 8.252 (1) Å
c = 11.162 (1) Å
β = 100.20 (1)°
V = 503.1 (1) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.06 mm^{-1}
T = 301 (2) K
0.55 × 0.44 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007), based on Clark & Reid (1995)]
T_{min} = 0.398, T_{max} = 0.720
19525 measured reflections
1343 independent reflections
1288 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.047
S = 1.07
1343 reflections
96 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8A···O5^{i}	0.78 (3)	1.97 (3)	2.7513 (15)	172 (2)
O8—H8B···O6^{ii}	0.73 (3)	2.00 (3)	2.7116 (15)	165 (2)
O9—H9A···O6^{iii}	0.74 (3)	2.16 (3)	2.8741 (14)	162 (2)
O9—H9B···O5^{i}	0.70 (3)	2.32 (3)	2.9379 (15)	150 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2271).

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supporting information

Acta Cryst. (2008). E**64**, i10 [doi:10.1107/S1600536808000214]

Disodium tetraaquabis(sulfato)iron(II)

Martin Hudák, Jesús García Díaz and Jozef Kožíšek

S1. Comment

In order to find convenient crystals as model compounds for investigation of the electronic structure of Fe^{II} complexes, the title compound was prepared. The unit cell contains two Fe^{II} cations situated on centres of inversion, four Na^+ cations, four SO_4^{2-} anions and eight water molecules. The structure contains a three-dimensional network of O—H···O hydrogen bonds.

In the title compound (Fig. 1), the Fe1—O8 [2.115 (1) Å] and Fe1—O9 [2.170 (1) Å] bond lengths are in reasonable agreement with a similar compounds in the Cambridge Structural Database (CSD; Version 5.27, 2006 release). For example, in ethylenediammonium tetra-aqua-bis(sulfato-O)-iron(II) (Held, 2003; CSD refcode WABHIR), the Fe—O(water) distances are 2.111 and 2.143 Å, respectively. The Fe1—O2 distance to the sulfate anion [2.095 (1) Å] compares to 2.126 Å in WABHIR. In the crystal structure of pentaaqua-(3-(diphenylphosphino)phenylsulfonato)-iron(II) (diphenyl(3-sulfonatophenyl)phosphine) (Barton *et al.*, 2002; CSD refcode XOHHOR), there are two symmetrically independent units with corresponding distances for Fe—O(water) in the range 2.085 to 2.125 Å and for Fe—O of the sulfonato anion between 2.10 and 2.126 Å.

S2. Experimental

A solution of 1.0 mmol of $Fe(SO_4)_2$ in 2 ml water with one drop of diluted H_2SO_4(aq) and a piece of Fe metal was mixed with a solution of 2.0 mmol $NaNO_2NCN$ in 10 ml water and a solution of 2.0 mmol of imidazole in 10 ml me thanol. From this system, pale yellow crystals were isolated after a few days standing.

S3. Refinement

H atoms were located in difference Fourier maps and refined freely with isotropic displacement parameters.

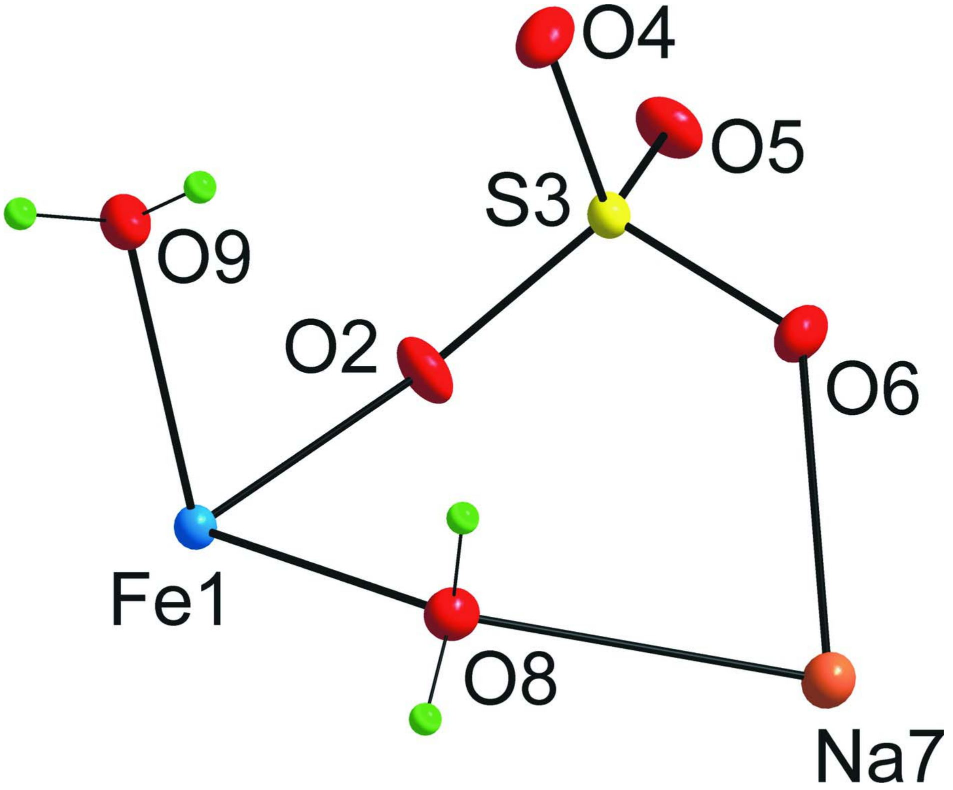

Figure 1

The asymmetric unit of the title compound with displacement ellipsoids shown at the 30% probability level for non-H atoms.

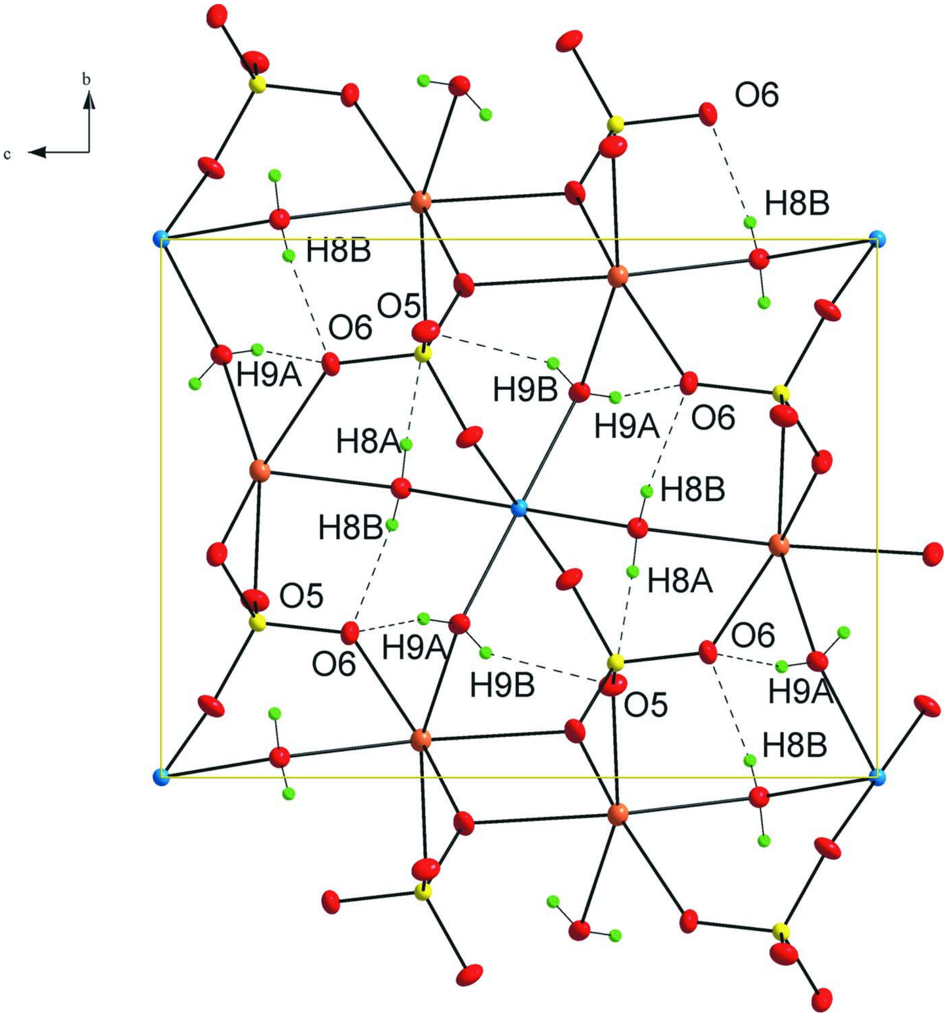

Figure 2

Packing diagram viewed along the *a* axis. Hydrogen-bond interactions are indicated by dashed lines.

Disodium tetraaquabis(sulfonato)iron(II)

Crystal data

$[FeNa_2(SO_4)_2(H_2O)_4]$
$M_r = 366.01$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.551$ (1) Å
$b = 8.252$ (1) Å
$c = 11.162$ (1) Å
$\beta = 100.20$ (1)°
$V = 503.1$ (1) Å^3
$Z = 2$
$F(000) = 368$
$D_x = 2.416$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17533 reflections
$\theta = 3.0$–31.4°
$\mu = 2.06$ mm^{-1}
$T = 301$ K
Block, pale yellow
0.55 × 0.44 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans

Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2007), based on Clark & Reid (1995)]
$T_{min} = 0.398$, $T_{max} = 0.720$
19525 measured reflections
1343 independent reflections
1288 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 29.5°$, $\theta_{min} = 6.6°$
$h = -7\rightarrow7$
$k = -11\rightarrow11$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.047$
$S = 1.08$
1343 reflections
96 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.3061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.062 (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.

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*	$U_{iso}*/U_{eq}$
O2	0.81620 (17)	0.63212 (12)	0.56957 (10)	0.0228 (2)
O4	0.70650 (19)	0.91424 (13)	0.57758 (9)	0.0234 (2)
O5	1.12799 (17)	0.82849 (12)	0.63063 (10)	0.0234 (2)
O6	0.84525 (19)	0.76778 (12)	0.76330 (9)	0.0224 (2)
O8	0.37101 (18)	0.53699 (14)	0.66515 (9)	0.01827 (19)
H8A	0.294 (4)	0.617 (3)	0.660 (2)	0.039 (6)*
H8B	0.290 (4)	0.472 (3)	0.679 (2)	0.031 (6)*
O9	0.31917 (19)	0.71528 (13)	0.41612 (10)	0.0201 (2)
H9A	0.211 (5)	0.707 (3)	0.368 (2)	0.039 (6)*
H9B	0.272 (5)	0.771 (3)	0.453 (2)	0.040 (7)*
S3	0.86989 (5)	0.78740 (3)	0.63455 (3)	0.01276 (9)
Na7	0.62761 (10)	0.56900 (7)	0.86236 (5)	0.02189 (13)
Fe1	0.5000	0.5000	0.5000	0.01297 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0175 (4)	0.0203 (5)	0.0302 (5)	−0.0039 (3)	0.0031 (4)	−0.0113 (4)

O4	0.0263 (5)	0.0248 (5)	0.0183 (4)	0.0113 (4)	0.0017 (4)	0.0034 (4)
O5	0.0148 (4)	0.0218 (5)	0.0342 (5)	−0.0049 (4)	0.0058 (4)	−0.0040 (4)
O6	0.0292 (5)	0.0243 (5)	0.0142 (4)	0.0024 (4)	0.0054 (4)	0.0024 (4)
O8	0.0190 (4)	0.0188 (5)	0.0182 (4)	0.0011 (4)	0.0068 (3)	0.0005 (4)
O9	0.0203 (5)	0.0178 (5)	0.0198 (5)	0.0025 (4)	−0.0030 (4)	−0.0015 (4)
S3	0.01181 (14)	0.01334 (15)	0.01272 (15)	0.00036 (9)	0.00107 (10)	−0.00092 (10)
Na7	0.0242 (3)	0.0222 (3)	0.0185 (3)	−0.0010 (2)	0.0018 (2)	0.0011 (2)
Fe1	0.01386 (13)	0.01298 (13)	0.01206 (13)	−0.00055 (8)	0.00225 (8)	−0.00057 (8)

Geometric parameters (Å, º)

O2—S3	1.4765 (10)	O9—Na7^{i}	2.6122 (12)
O2—Fe1	2.0951 (9)	O9—H9A	0.74 (3)
O4—S3	1.4553 (10)	O9—H9B	0.70 (3)
O4—Na7^{i}	2.3683 (11)	S3—Na7^{i}	3.3160 (6)
O4—Na7^{ii}	2.4413 (11)	Na7—O4^{iv}	2.3684 (11)
O5—S3	1.4805 (9)	Na7—O5^{v}	2.3974 (11)
O5—Na7^{iii}	2.3975 (11)	Na7—O4^{vi}	2.4413 (11)
O6—S3	1.4764 (10)	Na7—O9^{iv}	2.6123 (12)
O6—Na7	2.4178 (11)	Na7—S3^{iv}	3.3160 (6)
O8—Fe1	2.1146 (9)	Na7—Na7^{vii}	3.7798 (11)
O8—Na7	2.4153 (11)	Na7—H8B	2.64 (2)
O8—H8A	0.78 (3)	Fe1—O2^{viii}	2.0951 (9)
O8—H8B	0.73 (3)	Fe1—O8^{viii}	2.1146 (9)
O9—Fe1	2.1695 (10)	Fe1—O9^{viii}	2.1695 (10)

S3—O2—Fe1	135.77 (6)	O8—Na7—O9^{iv}	88.81 (4)
S3—O4—Na7^{i}	118.30 (6)	O6—Na7—O9^{iv}	92.51 (4)
S3—O4—Na7^{ii}	134.52 (6)	O4^{vi}—Na7—O9^{iv}	74.50 (4)
Na7^{i}—O4—Na7^{ii}	103.59 (4)	O4^{iv}—Na7—S3^{iv}	22.73 (2)
S3—O5—Na7^{iii}	137.19 (6)	O5^{v}—Na7—S3^{iv}	97.50 (3)
S3—O6—Na7	131.26 (6)	O8—Na7—S3^{iv}	162.20 (3)
Fe1—O8—Na7	125.04 (5)	O6—Na7—S3^{iv}	91.27 (3)
Fe1—O8—H8A	108.5 (17)	O4^{vi}—Na7—S3^{iv}	98.04 (3)
Na7—O8—H8A	102.0 (17)	O9^{iv}—Na7—S3^{iv}	73.86 (3)
Fe1—O8—H8B	113.3 (17)	O4^{iv}—Na7—Na7^{vii}	38.89 (3)
Na7—O8—H8B	99.8 (17)	O5^{v}—Na7—Na7^{vii}	90.89 (3)
H8A—O8—H8B	106 (2)	O8—Na7—Na7^{vii}	117.55 (3)
Fe1—O9—Na7^{i}	112.65 (4)	O6—Na7—Na7^{vii}	149.97 (4)
Fe1—O9—H9A	120.0 (19)	O4^{vi}—Na7—Na7^{vii}	37.52 (2)
Na7^{i}—O9—H9A	111.8 (19)	O9^{iv}—Na7—Na7^{vii}	70.32 (3)
Fe1—O9—H9B	118 (2)	S3^{iv}—Na7—Na7^{vii}	60.819 (15)
Na7^{i}—O9—H9B	91 (2)	O4^{iv}—Na7—H8B	141.4 (5)
H9A—O9—H9B	99 (3)	O5^{v}—Na7—H8B	95.4 (5)
O4—S3—O6	110.26 (6)	O8—Na7—H8B	15.9 (5)
O4—S3—O2	110.70 (6)	O6—Na7—H8B	101.2 (5)
O6—S3—O2	109.73 (6)	O4^{vi}—Na7—H8B	65.5 (5)
O4—S3—O5	110.72 (6)	O9^{iv}—Na7—H8B	88.8 (5)

O6—S3—O5	108.11 (6)	S3$^{\mathrm{iv}}$—Na7—H8B	159.2 (5)
O2—S3—O5	107.24 (6)	Na7$^{\mathrm{vii}}$—Na7—H8B	102.8 (5)
O6—S3—Na7$^{\mathrm{i}}$	146.99 (4)	O2$^{\mathrm{viii}}$—Fe1—O2	180.0
O2—S3—Na7$^{\mathrm{i}}$	81.15 (5)	O2$^{\mathrm{viii}}$—Fe1—O8	90.43 (4)
O5—S3—Na7$^{\mathrm{i}}$	97.39 (5)	O2—Fe1—O8	89.57 (4)
O4$^{\mathrm{iv}}$—Na7—O5$^{\mathrm{v}}$	90.76 (4)	O2$^{\mathrm{viii}}$—Fe1—O8$^{\mathrm{viii}}$	89.57 (4)
O4$^{\mathrm{iv}}$—Na7—O8	154.70 (4)	O2—Fe1—O8$^{\mathrm{viii}}$	90.43 (4)
O5$^{\mathrm{v}}$—Na7—O8	100.26 (4)	O8—Fe1—O8$^{\mathrm{viii}}$	180.0
O4$^{\mathrm{iv}}$—Na7—O6	114.00 (4)	O2$^{\mathrm{viii}}$—Fe1—O9$^{\mathrm{viii}}$	91.55 (4)
O5$^{\mathrm{v}}$—Na7—O6	104.53 (4)	O2—Fe1—O9$^{\mathrm{viii}}$	88.45 (4)
O8—Na7—O6	85.36 (4)	O8—Fe1—O9$^{\mathrm{viii}}$	86.80 (4)
O4$^{\mathrm{iv}}$—Na7—O4$^{\mathrm{vi}}$	76.41 (4)	O8$^{\mathrm{viii}}$—Fe1—O9$^{\mathrm{viii}}$	93.20 (4)
O5$^{\mathrm{v}}$—Na7—O4$^{\mathrm{vi}}$	90.63 (4)	O2$^{\mathrm{viii}}$—Fe1—O9	88.45 (4)
O8—Na7—O4$^{\mathrm{vi}}$	80.73 (4)	O2—Fe1—O9	91.55 (4)
O6—Na7—O4$^{\mathrm{vi}}$	161.06 (4)	O8—Fe1—O9	93.20 (4)
O4$^{\mathrm{iv}}$—Na7—O9$^{\mathrm{iv}}$	74.82 (4)	O8$^{\mathrm{viii}}$—Fe1—O9	86.80 (4)
O5$^{\mathrm{v}}$—Na7—O9$^{\mathrm{iv}}$	161.21 (4)	O9$^{\mathrm{viii}}$—Fe1—O9	179.999 (1)

Na7$^{\mathrm{i}}$—O4—S3—O6	−164.83 (6)	Fe1—O8—Na7—O9$^{\mathrm{iv}}$	142.28 (6)
Na7$^{\mathrm{ii}}$—O4—S3—O6	−10.15 (11)	Fe1—O8—Na7—S3$^{\mathrm{iv}}$	129.32 (9)
Na7$^{\mathrm{i}}$—O4—S3—O2	−43.22 (8)	Fe1—O8—Na7—Na7$^{\mathrm{vii}}$	−150.72 (5)
Na7$^{\mathrm{ii}}$—O4—S3—O2	111.45 (9)	S3—O6—Na7—O4$^{\mathrm{iv}}$	172.17 (7)
Na7$^{\mathrm{i}}$—O4—S3—O5	75.58 (8)	S3—O6—Na7—O5$^{\mathrm{v}}$	74.68 (8)
Na7$^{\mathrm{ii}}$—O4—S3—O5	−129.75 (9)	S3—O6—Na7—O8	−24.74 (8)
Na7$^{\mathrm{ii}}$—O4—S3—Na7$^{\mathrm{i}}$	154.67 (13)	S3—O6—Na7—O4$^{\mathrm{vi}}$	−67.51 (16)
Na7—O6—S3—O4	101.13 (8)	S3—O6—Na7—O9$^{\mathrm{iv}}$	−113.34 (8)
Na7—O6—S3—O2	−21.05 (9)	S3—O6—Na7—S3$^{\mathrm{iv}}$	172.76 (7)
Na7—O6—S3—O5	−137.70 (7)	S3—O6—Na7—Na7$^{\mathrm{vii}}$	−166.63 (6)
Na7—O6—S3—Na7$^{\mathrm{i}}$	83.55 (10)	S3—O2—Fe1—O8	−46.73 (10)
Fe1—O2—S3—O4	−45.49 (11)	S3—O2—Fe1—O8$^{\mathrm{viii}}$	133.27 (10)
Fe1—O2—S3—O6	76.42 (10)	S3—O2—Fe1—O9$^{\mathrm{viii}}$	−133.54 (10)
Fe1—O2—S3—O5	−166.38 (9)	S3—O2—Fe1—O9	46.46 (10)
Fe1—O2—S3—Na7$^{\mathrm{i}}$	−71.33 (9)	Na7—O8—Fe1—O2$^{\mathrm{viii}}$	150.22 (6)
Na7$^{\mathrm{iii}}$—O5—S3—O4	32.62 (11)	Na7—O8—Fe1—O2	−29.78 (6)
Na7$^{\mathrm{iii}}$—O5—S3—O6	−88.26 (10)	Na7—O8—Fe1—O9$^{\mathrm{viii}}$	58.69 (6)
Na7$^{\mathrm{iii}}$—O5—S3—O2	153.49 (9)	Na7—O8—Fe1—O9	−121.31 (6)
Na7$^{\mathrm{iii}}$—O5—S3—Na7$^{\mathrm{i}}$	70.50 (9)	Na7$^{\mathrm{i}}$—O9—Fe1—O2$^{\mathrm{viii}}$	−152.73 (5)
Fe1—O8—Na7—O4$^{\mathrm{iv}}$	−168.78 (8)	Na7$^{\mathrm{i}}$—O9—Fe1—O2	27.27 (5)
Fe1—O8—Na7—O5$^{\mathrm{v}}$	−54.28 (7)	Na7$^{\mathrm{i}}$—O9—Fe1—O8	116.93 (5)
Fe1—O8—Na7—O6	49.67 (6)	Na7$^{\mathrm{i}}$—O9—Fe1—O8$^{\mathrm{viii}}$	−63.07 (5)
Fe1—O8—Na7—O4$^{\mathrm{vi}}$	−143.24 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8*A*···O5$^{\mathrm{ix}}$	0.78 (3)	1.97 (3)	2.7513 (15)	172 (2)

O8—H8*B*···O6^{vi}	0.73 (3)	2.00 (3)	2.7116 (15)	165 (2)
O9—H9*A*···O6^{x}	0.74 (3)	2.16 (3)	2.8741 (14)	162 (2)
O9—H9*B*···O5^{ix}	0.70 (3)	2.32 (3)	2.9379 (15)	150 (3)

Symmetry codes: (vi) −*x*+1, *y*−1/2, −*z*+3/2; (ix) *x*−1, *y*, *z*; (x) *x*−1, −*y*+3/2, *z*−1/2.