

Disodium tetraaquabis(sulfato)iron(II)

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Received 30 November 2007; accepted 3 January 2008

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

In the title compound, $[\text{FeNa}_2(\text{SO}_4)_2(\text{H}_2\text{O})_4]$, 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 $\text{Na}-\text{O}$ distances between 2.368 (1) and 2.612 (1) Å. The structure contains an extensive three-dimensional network of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

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

Experimental

Crystal data

$[\text{FeNa}_2(\text{SO}_4)_2(\text{H}_2\text{O})_4]$
 $M_r = 366.01$
 Monoclinic, $P2_1/c$
 $a = 5.551$ (1) Å
 $b = 8.252$ (1) Å
 $c = 11.162$ (1) Å
 $\beta = 100.20$ (1)°

$V = 503.1$ (1) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.06$ mm⁻¹
 $T = 301$ (2) K
 $0.55 \times 0.44 \times 0.17$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

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, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|----------|-------------|-------------|---------------|
| $\text{O8}-\text{H8A}\cdots\text{O5}^{\text{i}}$ | 0.78 (3) | 1.97 (3) | 2.7513 (15) | 172 (2) |
| $\text{O8}-\text{H8B}\cdots\text{O6}^{\text{ii}}$ | 0.73 (3) | 2.00 (3) | 2.7116 (15) | 165 (2) |
| $\text{O9}-\text{H9A}\cdots\text{O6}^{\text{iii}}$ | 0.74 (3) | 2.16 (3) | 2.8741 (14) | 162 (2) |
| $\text{O9}-\text{H9B}\cdots\text{O5}^{\text{i}}$ | 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).

The authors thank the Grant Agency of the Slovak Republic (grant Nos. VEGA 1/2449/05 and COSNET 545.03-P) and Structural Funds, Interreg IIIA, for financial support in purchasing the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: B12271).

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supplementary materials

Acta Cryst. (2008). E64, i10 [doi:10.1107/S1600536808000214]

Disodium tetraaquabis(sulfato)iron(II)

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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 SO₄²⁻ 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 pentaqua-(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.

Experimental

A solution of 1.0 mmol of Fe(SO₄)₂ in 2 ml water with one drop of diluted H₂SO₄(aq) and a piece of Fe metal was mixed with a solution of 2.0 mmol NaNO₂NCN in 10 ml water and a solution of 2.0 mmol of imidazole in 10 ml methanol. From this system, pale yellow crystals were isolated after a few days standing.

Refinement

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

Figures

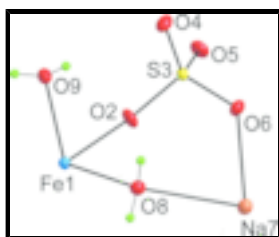


Fig. 1. The asymmetric unit of the title compound with displacement ellipsoids shown at the 30% probability level for non-H atoms.

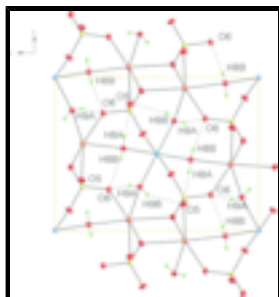


Fig. 2. Packing diagram viewed along the a axis. Hydrogen-bond interactions are indicated by dashed lines.

Disodium tetraaquabis(sulfonato)iron(II)

Crystal data

[FeNa₂(SO₄)₂(H₂O)₄]

$M_r = 366.01$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.551 (1) \text{ \AA}$

$b = 8.252 (1) \text{ \AA}$

$c = 11.162 (1) \text{ \AA}$

$\beta = 100.20 (1)^\circ$

$V = 503.1 (1) \text{ \AA}^3$

$Z = 2$

$F_{000} = 368$

$D_x = 2.416 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 17533 reflections

$\theta = 3.0\text{--}31.4^\circ$

$\mu = 2.06 \text{ mm}^{-1}$

$T = 301 (2) \text{ K}$

Block, pale yellow

$0.55 \times 0.44 \times 0.17 \text{ mm}$

Data collection

Oxford Diffraction Gemini R CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 301(2) \text{ K}$

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\text{max}} = 29.5^\circ$

$\theta_{\text{min}} = 6.6^\circ$

$h = -7 \rightarrow 7$

$k = -11 \rightarrow 11$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.047$

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 $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

| | |
|--|---|
| $S = 1.08$ | $\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$ |
| 1343 reflections | $\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$ |
| 96 parameters | Extinction correction: SHELXL97 (Sheldrick, 1997), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.062 (3) |
| 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| 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 (\AA^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) |

supplementary materials

Fe1 0.01386 (13) 0.01298 (13) 0.01206 (13) -0.00055 (8) 0.00225 (8) -0.00057 (8)

Geometric parameters (Å, °)

| | | | |
|--|-------------|--|-------------|
| 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 ^{iv} —Na7—H8B | 159.2 (5) |
| O2—S3—O5 | 107.24 (6) | Na7 ^{vii} —Na7—H8B | 102.8 (5) |

| | | | |
|--|-------------|---|--------------|
| O6—S3—Na7 ⁱ | 146.99 (4) | O2 ^{viii} —Fe1—O2 | 180.0 |
| O2—S3—Na7 ⁱ | 81.15 (5) | O2 ^{viii} —Fe1—O8 | 90.43 (4) |
| O5—S3—Na7 ⁱ | 97.39 (5) | O2—Fe1—O8 | 89.57 (4) |
| O4 ^{iv} —Na7—O5 ^v | 90.76 (4) | O2 ^{viii} —Fe1—O8 ^{viii} | 89.57 (4) |
| O4 ^{iv} —Na7—O8 | 154.70 (4) | O2—Fe1—O8 ^{viii} | 90.43 (4) |
| O5 ^v —Na7—O8 | 100.26 (4) | O8—Fe1—O8 ^{viii} | 180.0 |
| O4 ^{iv} —Na7—O6 | 114.00 (4) | O2 ^{viii} —Fe1—O9 ^{viii} | 91.55 (4) |
| O5 ^v —Na7—O6 | 104.53 (4) | O2—Fe1—O9 ^{viii} | 88.45 (4) |
| O8—Na7—O6 | 85.36 (4) | O8—Fe1—O9 ^{viii} | 86.80 (4) |
| O4 ^{iv} —Na7—O4 ^{vi} | 76.41 (4) | O8 ^{viii} —Fe1—O9 ^{viii} | 93.20 (4) |
| O5 ^v —Na7—O4 ^{vi} | 90.63 (4) | O2 ^{viii} —Fe1—O9 | 88.45 (4) |
| O8—Na7—O4 ^{vi} | 80.73 (4) | O2—Fe1—O9 | 91.55 (4) |
| O6—Na7—O4 ^{vi} | 161.06 (4) | O8—Fe1—O9 | 93.20 (4) |
| O4 ^{iv} —Na7—O9 ^{iv} | 74.82 (4) | O8 ^{viii} —Fe1—O9 | 86.80 (4) |
| O5 ^v —Na7—O9 ^{iv} | 161.21 (4) | O9 ^{viii} —Fe1—O9 | 179.999 (1) |
| Na7 ⁱ —O4—S3—O6 | -164.83 (6) | Fe1—O8—Na7—O9 ^{iv} | 142.28 (6) |
| Na7 ⁱⁱ —O4—S3—O6 | -10.15 (11) | Fe1—O8—Na7—S3 ^{iv} | 129.32 (9) |
| Na7 ⁱ —O4—S3—O2 | -43.22 (8) | Fe1—O8—Na7—Na7 ^{vii} | -150.72 (5) |
| Na7 ⁱⁱ —O4—S3—O2 | 111.45 (9) | S3—O6—Na7—O4 ^{iv} | 172.17 (7) |
| Na7 ⁱ —O4—S3—O5 | 75.58 (8) | S3—O6—Na7—O5 ^v | 74.68 (8) |
| Na7 ⁱⁱ —O4—S3—O5 | -129.75 (9) | S3—O6—Na7—O8 | -24.74 (8) |
| Na7 ⁱⁱ —O4—S3—Na7 ⁱ | 154.67 (13) | S3—O6—Na7—O4 ^{vi} | -67.51 (16) |
| Na7—O6—S3—O4 | 101.13 (8) | S3—O6—Na7—O9 ^{iv} | -113.34 (8) |
| Na7—O6—S3—O2 | -21.05 (9) | S3—O6—Na7—S3 ^{iv} | 172.76 (7) |
| Na7—O6—S3—O5 | -137.70 (7) | S3—O6—Na7—Na7 ^{vii} | -166.63 (6) |
| Na7—O6—S3—Na7 ⁱ | 83.55 (10) | S3—O2—Fe1—O8 | -46.73 (10) |
| Fe1—O2—S3—O4 | -45.49 (11) | S3—O2—Fe1—O8 ^{viii} | 133.27 (10) |
| Fe1—O2—S3—O6 | 76.42 (10) | S3—O2—Fe1—O9 ^{viii} | -133.54 (10) |
| Fe1—O2—S3—O5 | -166.38 (9) | S3—O2—Fe1—O9 | 46.46 (10) |
| Fe1—O2—S3—Na7 ⁱ | -71.33 (9) | Na7—O8—Fe1—O2 ^{viii} | 150.22 (6) |
| Na7 ⁱⁱⁱ —O5—S3—O4 | 32.62 (11) | Na7—O8—Fe1—O2 | -29.78 (6) |
| Na7 ⁱⁱⁱ —O5—S3—O6 | -88.26 (10) | Na7—O8—Fe1—O9 ^{viii} | 58.69 (6) |
| Na7 ⁱⁱⁱ —O5—S3—O2 | 153.49 (9) | Na7—O8—Fe1—O9 | -121.31 (6) |
| Na7 ⁱⁱⁱ —O5—S3—Na7 ⁱ | 70.50 (9) | Na7 ⁱ —O9—Fe1—O2 ^{viii} | -152.73 (5) |
| Fe1—O8—Na7—O4 ^{iv} | -168.78 (8) | Na7 ⁱ —O9—Fe1—O2 | 27.27 (5) |
| Fe1—O8—Na7—O5 ^v | -54.28 (7) | Na7 ⁱ —O9—Fe1—O8 | 116.93 (5) |
| Fe1—O8—Na7—O6 | 49.67 (6) | Na7 ⁱ —O9—Fe1—O8 ^{viii} | -63.07 (5) |
| Fe1—O8—Na7—O4 ^{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) $-x+1, -y+1, -z+1$.

supplementary materials

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|----------|-------------|-------------|---------------|
| O8—H8A \cdots O5 ^{ix} | 0.78 (3) | 1.97 (3) | 2.7513 (15) | 172 (2) |
| O8—H8B \cdots O6 ^{vi} | 0.73 (3) | 2.00 (3) | 2.7116 (15) | 165 (2) |
| O9—H9A \cdots O6 ^x | 0.74 (3) | 2.16 (3) | 2.8741 (14) | 162 (2) |
| O9—H9B \cdots O5 ^{ix} | 0.70 (3) | 2.32 (3) | 2.9379 (15) | 150 (3) |

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

Fig. 1

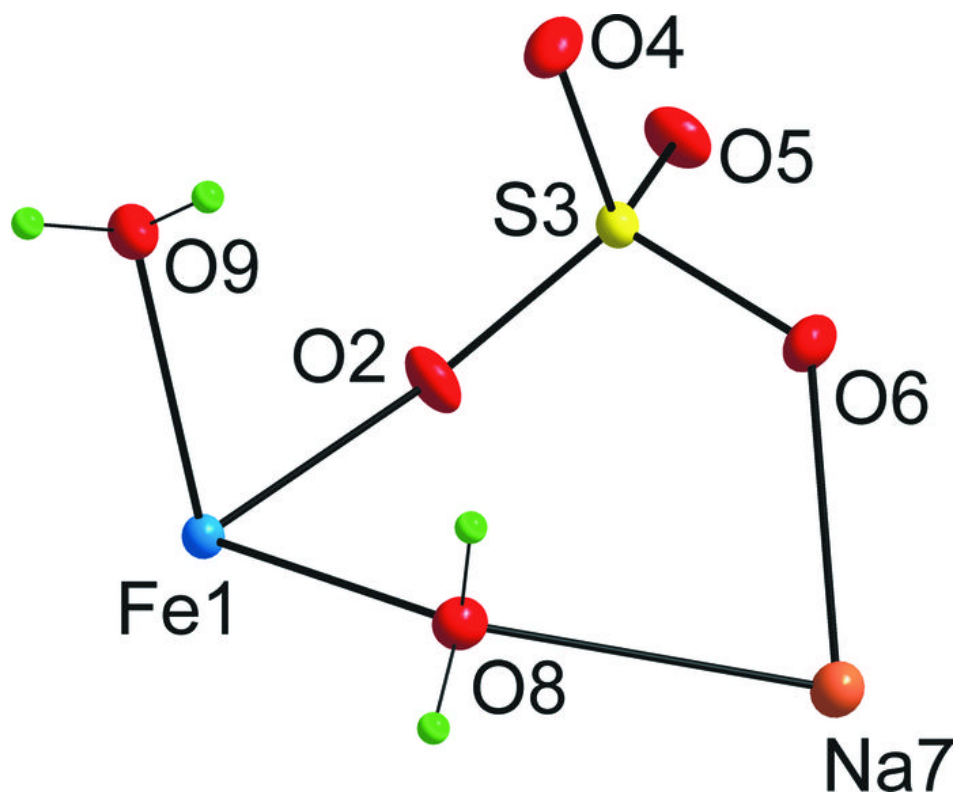


Fig. 2

