

Disodium tetraaquabis(sulfato)iron(II)

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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)
 $T_{\text{min}} = 0.398$, $T_{\text{max}} = 0.720$
 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
 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ 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).

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

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