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Ethylenediammonium tetraaquabis(sulfato)iron(II)

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The title compound, $[(NH_3)_2(CH_2)_2][Fe(SO_4)_2(H_2O)_4]$, contains centrosymmetric $[Fe(H_2O)_4(SO_4)_2]^{2-}$ anions, with a coordination octahedron around iron(II) built up from four water molecules and two sulfate groups. The anions are linked by hydrogen bonds of medium strength, forming a three-dimensional framework. The linkage is reinforced by N—H···O bridges from the centrosymmetric $[NH_3(CH_2)_2NH_3]^{2+}$ cations, located in the centre of the interstices.

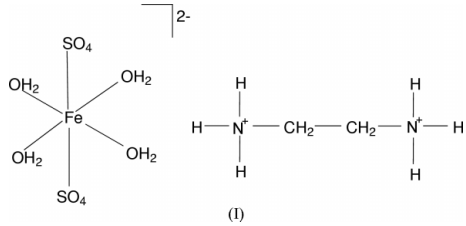
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.022
wR factor = 0.062
Data-to-parameter ratio = 21.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I), crystallizes isostructurally with the analogous manganese compound (Chaabouni *et al.*, 1996). The Fe atom is surrounded by six O atoms of four H_2O molecules and of two SO_4 groups, forming a slightly distorted octahedron. The Fe atom is placed in special Wykoff position 1*a* on an inversion centre. The structure is built of $[Fe(H_2O)_4(SO_4)_2]^{2-}$ anions, in which the SO_4 tetrahedron is vertex-linked to the central Fe^{2+} ion, sharing a common O atom (Fig. 1). Hydrogen bonds of mean strength from H_2O molecules to O atoms (O2 and O3) of the SO_4 groups interconnect neighbouring $[Fe(H_2O)_4(SO_4)_2]^{2-}$ anions, forming a three-dimensional primitive framework (Fig. 2). Placed at the centre of each interstice, $[NH_3(CH_2)_2NH_3]^{2+}$ cations form N—H···O bonds to six surrounding $[Fe(H_2O)_4(SO_4)_2]^{2-}$ anions. Every NH_3 group bonds to two O atoms (O1 and O2) of two different SO_4 groups and to one O atom (O4) coordinated to iron. The organic ethylenediammonium cation is centrosymmetric with NH_3 tails in a *trans* configuration. Both anion and cation show no deviation from the usual geometry and conformation.



(I)

Experimental

The title compound was prepared in the course of a systematic search for new 'double salts' of ethylenediammonium and divalent cations with various inorganic acids. It crystallizes from aqueous solution containing iron sulfate, ethylenediamine and sulfuric acid (in ratio 1:1:1), by slow evaporation at room temperature, in the form of yellow crystals with dimensions up to 4 mm.

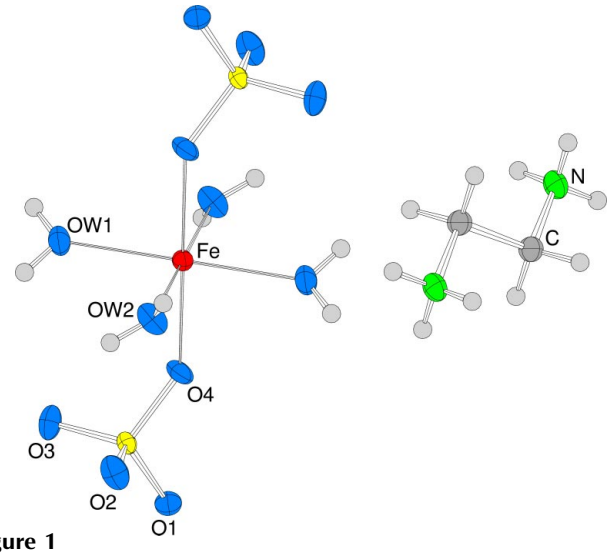


Figure 1
*ORTEP*III projection (Burnett & Johnson, 1996) of the title compound showing the atom-numbering scheme. Non-H atoms are shown as 50% probability ellipsoids and H atoms are drawn as circles of arbitrary radii.

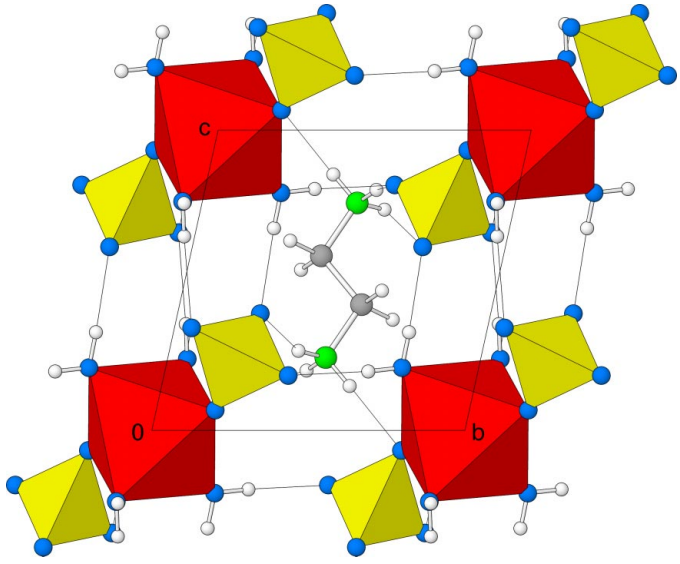


Figure 2
Projection along [100] of the title compound, showing $[SO_4]$ tetrahedra (yellow), $[Mn(H_2O)_4O_2]$ octahedra (red), oxygen (blue), nitrogen (green), carbon (grey) and hydrogen (white) atoms. Hydrogen bonds (grey lines) interlink ethylenediammonium cations to different polyhedra.

Crystal data

$(C_2H_{10}N_2)[Fe(SO_4)_2(H_2O)_4]$	$Z = 1$
$M_r = 382.15$	$D_x = 1.974$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.8350$ (3) Å	Cell parameters from 25 reflections
$b = 7.1253$ (3) Å	$\theta = 12.3$–$19.3°$
$c = 7.2235$ (4) Å	$\mu = 1.56$ mm^{-1}
$\alpha = 75.012$ (4)°	$T = 293$ (2) K
$\beta = 72.355$ (4)°	Parallelepiped, pale yellow
$\gamma = 79.185$ (4)°	0.25 × 0.23 × 0.21 mm
$V = 321.55$ (3) Å^3	

Data collection

Nonius MACH3 diffractometer	$\theta_{max} = 34.2°$
$\omega/2\theta$ scans	$h = -10 \rightarrow 10$
Absorption correction: ψ scan (*MolEN*; Fair, 1990)	$k = -11 \rightarrow 10$
$T_{min} = 0.686$, $T_{max} = 0.721$	$l = -11 \rightarrow 11$
4830 measured reflections	3 standard reflections
2660 independent reflections	every 100 reflections
2393 reflections with $I > 2\sigma(I)$	frequency: 60 min
$R_{int} = 0.040$	intensity decay: −4.9%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0214P)^2 + 0.0617P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.022$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.063$	$\Delta\rho_{max} = 0.74$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.43$ e Å^{-3}
2660 reflections	Extinction correction: *SHELXL*97
125 parameters	Extinction coefficient: 0.190 (6)
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å).

Fe—*OW*1	2.1111 (9)	S—O1	1.4782 (8)
Fe—O4	2.1260 (7)	S—O4	1.4899 (7)
Fe—*OW*2	2.1430 (8)	C—N	1.476 (1)
S—O3	1.4649 (8)	C—C^{i}	1.513 (2)
S—O2	1.4699 (8)		

Symmetry code: (i) $1-x, 1-y, -1-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
*OW*1—H1*W*1···O2^{ii}	0.82 (2)	1.94 (2)	2.759 (1)	174 (2)
*OW*1—H2*W*1···O1^{iii}	0.83 (2)	1.91 (3)	2.741 (1)	176 (2)
*OW*2—H1*W*2···O3^{iv}	0.82 (2)	2.06 (2)	2.862 (1)	166 (2)
*OW*2—H2*W*2···O3^{v}	0.80 (2)	1.96 (2)	2.727 (1)	162 (2)
N—H1N···O1^{vi}	0.87 (2)	2.08 (2)	2.887 (1)	154 (2)
N—H2N···O4	0.88 (2)	1.94 (2)	2.818 (1)	177 (2)
N—H3N···O2^{vii}	0.89 (2)	1.98 (2)	2.835 (1)	159 (2)

Symmetry codes: (ii) $-x, -y, 1-z$; (iii) $x, y-1, z$; (iv) $x, y, z-1$; (v) $1-x, -y, -z$; (vi) $1-x, 1-y, -z$; (vii) $-x, 1-y, -z$.

Data collection: *MACH*3 (Enraf–Nonius, 1993); cell refinement: *MACH*3; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2002) and *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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