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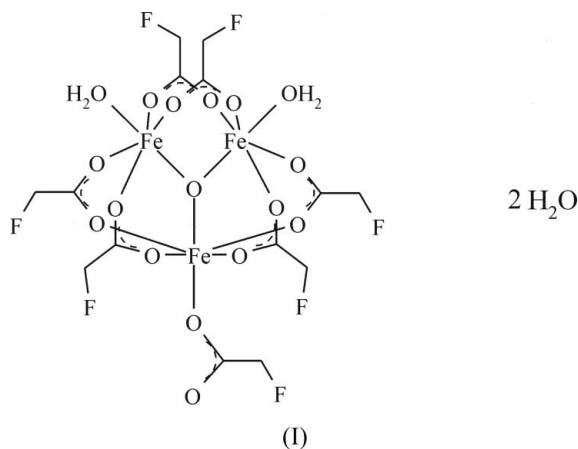
## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
Disorder in solvent or counterion  
 $R$  factor = 0.032  
 $wR$  factor = 0.085  
Data-to-parameter ratio = 13.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Diaqua-hexakis( $\mu_2$ -fluoroacetato- $\kappa^2\text{O}:\text{O}'$ )-  
(fluoroacetato- $\kappa\text{O}$ )- $\mu_3$ -oxo-triiron(III)-  
dihydrateThe title compound,  $[\text{Fe}_3(\text{C}_2\text{H}_2\text{FO}_2)_7\text{O}(\text{H}_2\text{O})_2]\cdot 2\text{H}_2\text{O}$ , was synthesized by the reaction of  $\text{Fe}(\text{NO}_3)_3\cdot 9\text{H}_2\text{O}$  with  $\text{NaC}_2\text{H}_2\text{FO}_2$  in water. The compound contains a distorted  $\text{Fe}_3$  triangle with an O atom in the centre. Each  $\text{Fe}^{3+}$  ion is surrounded by six O atoms, giving a distorted octahedron.

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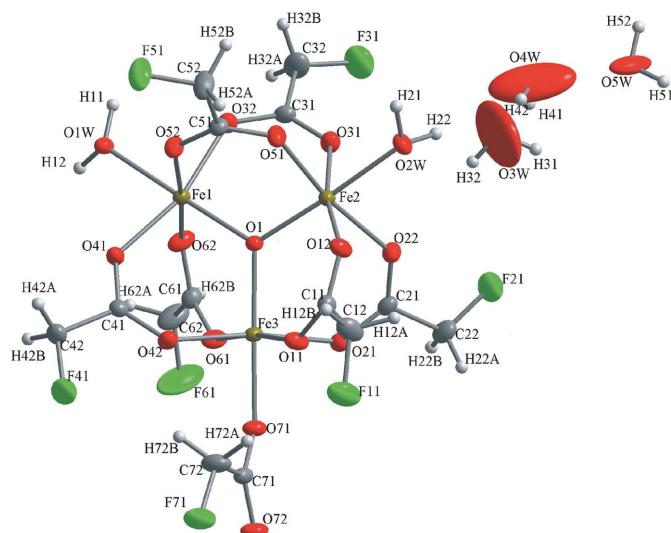
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## Comment

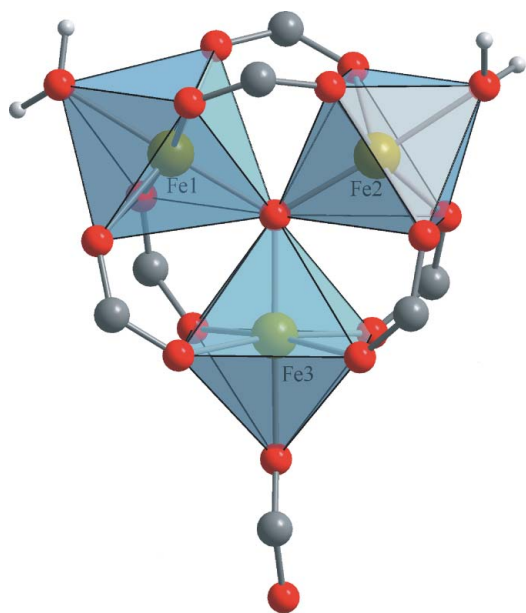
In connection with our investigations of the structural chemistry of halogenoacetates we have examined complexes with  $\text{Fe}^{3+}$ , of which, until now, only the trifluoro- (Ponomarev *et al.* 1982), trichloro- (Ponomarev *et al.* 1987), chloro- (Ren *et al.*, 2004; Overgaard *et al.*, 2003), bromo- (Sato *et al.*, 1996) and iodoacetate (Nakamoto *et al.*, 2002) were known. Here we present the crystal structure of the fluoroacetate.

The structure of (I), is shown in Fig. 1. The compound contains an  $\text{Fe}_3$  triangle [ $\text{Fe}1 \cdots \text{Fe}2 = 3.2737(6)$ ,  $\text{Fe}1 \cdots \text{Fe}3 = 3.3245(5)$  and  $\text{Fe}2 \cdots \text{Fe}3 = 3.3217(5)\text{ \AA}$ ] with an O atom in the centre. Two carboxylate groups bridge each pair of  $\text{Fe}^{III}$  ions. In addition to these bridging carboxylate groups there is a monodentate carboxylate group and two coordinated water molecules, leading to distorted oxygen octahedra around each of the  $\text{Fe}^{3+}$  ions. In the case of Fe1 and Fe2, the O atoms of the octahedra originate from four carboxylate groups, one water molecule and the central O atom. The octahedron of Fe3 is built up by O atoms from five carboxylate groups and the central O atom (Table 1 and Fig. 2). The bonds between the central O atom and the three  $\text{Fe}^{3+}$  ions are shorter than the other  $\text{Fe}-\text{O}$  bond lengths in (I). Similar results are found in related compounds (Ren *et al.*, 2004; Overgaard *et al.*, 2003).

In the crystal structure of (I) there are two non-coordinated water molecules, one of which is disordered over two sites. These water molecules and the cluster molecule are connected



**Figure 1**  
View of the asymmetric unit of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Both components of the disordered water molecule are shown.



**Figure 2**  
Coordination environments of atoms Fe1, Fe2 and Fe3.

through a complicated pattern of hydrogen-bonding interactions involving numerous O—H...O and O—H...F links giving a three-dimensional network (Table 2). The shortest inter-cluster Fe...Fe distance is 5.6297 (6) Å.

### Experimental

The title compound was prepared by the reaction of Fe(NO<sub>3</sub>)<sub>3</sub>·9H<sub>2</sub>O (3 mmol, 1.2 g; Fluka, >98%) with sodium fluoroacetate (10 mmol, 1.0 g; Fluka, >90%) in water (8 ml) at room temperature. After a few weeks, red crystals suitable for X-ray structural analysis were formed.

### Crystal data

[Fe<sub>3</sub>(C<sub>2</sub>H<sub>2</sub>FO<sub>2</sub>)<sub>7</sub>O(H<sub>2</sub>O)<sub>2</sub>]·2H<sub>2</sub>O  
*M<sub>r</sub>* = 794.87  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 17.9617 (15) Å  
*b* = 10.6921 (5) Å  
*c* = 15.5496 (13) Å  
 β = 111.329 (9)°  
*V* = 2781.7 (4) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.898 Mg m<sup>-3</sup>  
 Mo Kα radiation  
 μ = 1.67 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Block, red  
 0.48 × 0.35 × 0.30 mm

### Data collection

Stoe IPDS area-detector diffractometer  
 φ scans  
 Absorption correction: multi-scan (Blessing, 1995)  
*T<sub>min</sub>* = 0.552, *T<sub>max</sub>* = 0.606

38802 measured reflections  
 5450 independent reflections  
 4281 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.048  
 θ<sub>max</sub> = 26.1°

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.032  
*wR*(*F*<sup>2</sup>) = 0.085  
*S* = 0.98  
 5450 reflections  
 410 parameters

H atoms treated by a mixture of independent and constrained refinement  
*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0589*P*)<sup>2</sup>]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δσ)<sub>max</sub> = 0.001  
 Δρ<sub>max</sub> = 0.66 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.52 e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Fe1—O1	1.9134 (17)	Fe2—O31	2.0386 (19)
Fe1—O41	1.9871 (19)	Fe2—O12	2.0461 (19)
Fe1—O62	2.009 (2)	Fe2—O2W	2.054 (2)
Fe1—O32	2.011 (2)	Fe3—O1	1.9244 (17)
Fe1—O52	2.0288 (19)	Fe3—O71	1.9847 (19)
Fe1—O1W	2.0702 (18)	Fe3—O42	2.0199 (19)
Fe2—O1	1.8896 (17)	Fe3—O61	2.0245 (19)
Fe2—O51	2.003 (2)	Fe3—O21	2.030 (2)
Fe2—O22	2.018 (2)	Fe3—O11	2.033 (2)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H11...O12 <sup>i</sup>	0.922 (18)	1.993 (19)	2.901 (3)	168 (3)
O1W—H12...O72 <sup>ii</sup>	0.946 (17)	1.74 (2)	2.654 (3)	160 (3)
O1W—H12...F71 <sup>ii</sup>	0.946 (17)	2.46 (3)	3.091 (3)	124 (2)
O2W—H21...O72 <sup>iii</sup>	0.959 (18)	1.81 (2)	2.739 (3)	161 (3)
O2W—H22...O3W	0.935 (18)	1.70 (2)	2.611 (6)	164 (3)
O3W—H31...F31 <sup>iv</sup>	0.85	2.34	3.192 (9)	178
O3W—H32...O22	0.85	2.50	3.349 (8)	178
O4W—H41...O71 <sup>v</sup>	0.85	2.27	3.018 (7)	147
O4W—H42...O3W	0.85	1.77	2.620 (12)	178
O5W—H51...F61 <sup>vi</sup>	0.85	2.43	2.869 (13)	113
O5W—H51...F11	0.85	2.61	3.279 (16)	137
O5W—H52...O51 <sup>vii</sup>	0.85	2.34	3.157 (13)	161
O5W—H52...O31 <sup>vii</sup>	0.85	2.64	3.195 (11)	124

Symmetry codes: (i) *x*, -*y* - ½, *z* + ½; (ii) *x*, -*y* - ¾, *z* + ½; (iii) *x*, *y* + 1, *z*; (iv) -*x* + 1, -*y*, -*z* + 1; (v) -*x* + 1, -*y* - 1, -*z* + 1; (vi) *x*, -*y* - ¾, *z* - ½; (vii) *x*, -*y* - ½, *z* - ½.

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The H atoms on the water atoms O1W and O2W were located in a Fourier map and refined with the restraints O—H = 0.99 (2) Å and H...H = 1.55 (4) Å, and with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(O). The positions of H atoms attached to the water atoms O3W, O4W and O5W were not observed directly in Fourier maps. To include them and construct the hydrogen-

bond network, the method of Nardelli (1999), as implemented in *WinGX* software (Farrugia, 1999), was adopted. These H atoms were refined with  $O-H = 0.85(1) \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . The fractional site occupancies of the disordered atom pair O4W/O5W were constrained to sum to unity, resulting in refined occupancies of 0.748(10)/0.252(10).

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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