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catena-Poly[[tetraaquairon(II)]-μ-succinato-κ^2O:O']

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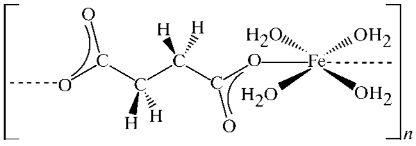
The title complex, {[Fe($C_4H_4O_4$)(H_2O)$_4$]}$_n$, is an infinite polymeric compound bridged by the succinate dianion. Two carboxylate groups coordinate in a monodentate manner to the Fe^{II} atom, in a *trans* fashion, with an O—Fe—O bond angle of 175.72 (6)° and Fe—O distances of 2.0886 (14) and 2.1008 (15) Å. One of the uncoordinated carboxylate O atom forms an intramolecular hydrogen bond with a coordinated water molecule. Extensive hydrogen bonding between parallel polymeric complex chains results in a three-dimensional supramolecular structure.

Comment

The succinate dianion has been used as a bridging ligand in the preparation of multinuclear metal complexes. A variety of bridging modes, including μ_2, μ_3 and μ_4, has been found (Ng, 1998; Rastsvetaeva *et al.*, 1996; Ng & Kumar Das, 1993). Some recent structure determinations have shown that the coordination mode of the succinate dianion is affected by hydrogen bonding between water molecules and one of the carboxylate groups (Liu *et al.*, 2002).



(I)

A section of the structure of the title compound, (I), is shown in Fig. 1. Two succinate O atoms, related by translation symmetry, and four water molecules coordinate to the Fe^{II} center with normal octahedral coordination geometry. The succinate carbon skeleton assumes a *trans*-planar conformation, with a C1—C2—C3—C4 torsion angle of −173.67 (18)°. This skeleton is approximately coplanar with the coordination plane formed by atoms O1, O3^i, O6 and O8 [dihedral angle 6.08 (11)°; symmetry code: (i) $1+x$, y, $1+z$] and perpendicular to the coordination plane formed by atoms O1, O3^i, O5 and O7 [dihedral angle 89.84 (19)°]. The two carboxylate groups of the same succinate dianion are nearly perpendicular to one another [dihedral angle 75.98 (17)°]. One of the carboxylate groups is nearly coplanar with the carbon skeleton [dihedral angle 4.5 (3)°], while the other is nearly perpendicular to it [dihedral angle 79.5 (2)°]. A search of the Cambridge Structural Database (Allen, 2002) showed that this perpendicular arrangement of the two carboxylate groups is different from the situation in μ_2-succinate–metal complexes, including the similar Ni^{II} complex tetraaqua(μ_2-succinato)nickel(II) (Gupta *et al.*, 1983). Two separate intramolecular hydrogen bonds are observed between the carboxylate groups and coordinated water molecules (Fig. 1), which may be responsible for the nearly perpendicular arrangement of the carboxylate groups.

The succinate dianions act as bridging ligands in the structure, linking neighboring Fe^{II} atoms related by translational

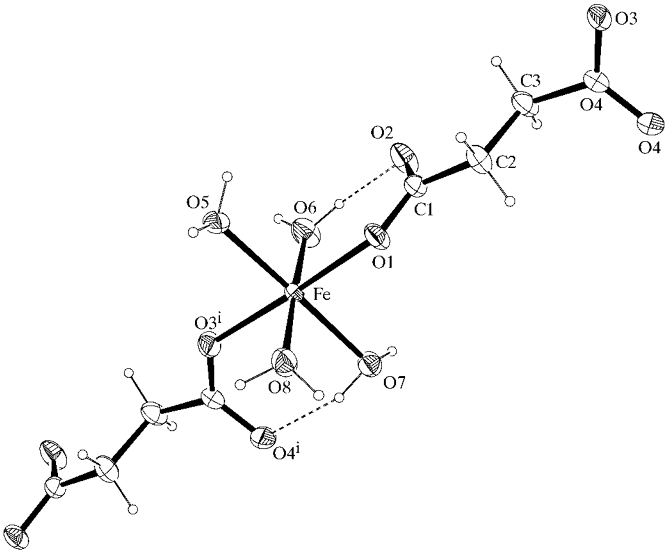


Figure 1
A section of the structure of the title polymeric compound, shown with 50% probability displacement ellipsoids [symmetry code: (i) $1+x$, y, $1+z$].

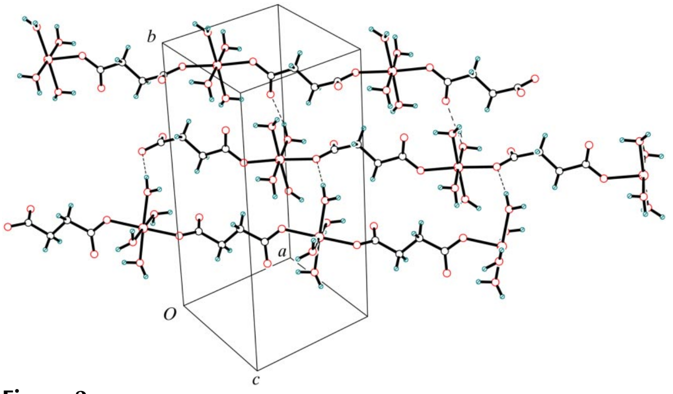


Figure 2
A packing diagram, showing the intermolecular hydrogen bonding between neighboring polymeric chains.

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symmetry to form infinite polymeric complex chains along the [101] direction. Each carboxylate group of the succinate dianion acts is monodentate, perhaps owing to the intramolecular hydrogen bonding between the coordinated carboxylate groups and coordinated water molecules.

An extensive hydrogen-bonding network exists in the crystal structure of (I), involving all carboxylate O atoms (Fig. 2). The uncoordinated carboxylate atoms, O2 and O4, are involved in intramolecular hydrogen bonding to neighboring coordinated water molecules, as mentioned above, and in intermolecular hydrogen bonding to adjacent polymeric chains. Water atoms O5 and O7 act as both donors and acceptors of hydrogen bonds. The polymeric chains are interlinked *via* hydrogen bonding, resulting in a three-dimensional supramolecular structure.

Experimental

An acetonitrile solution (20 ml) containing succinic acid (0.12 g, 1 mmol), $FeCl_3\cdot 6H_2O$ (0.27 g, 1 mmol) and NaOH (0.08 g, 2 mmol) was refluxed for 1 h. The resulting dark-yellow solution was cooled to room temperature and filtered. Orange crystals were obtained from the filtrate after one week.

Crystal data

$[Fe(C_4H_4O_4)(H_2O)_4]$
$M_r = 243.99$
Monoclinic, $P2_1/c$
$a = 7.4046\ (10)$ Å
$b = 14.7960\ (13)$ Å
$c = 7.7788\ (11)$ Å
$\beta = 99.727\ (12)^\circ$
$V = 839.98\ (18)$ Å^3
$Z = 4$
$D_x = 1.929$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
$\theta = 4.5$–10.0°
$\mu = 1.81$ mm^{-1}
$T = 298\ (2)$ K
Prism, orange
0.45 × 0.40 × 0.35 mm

Data collection

Rigaku AFC-7*S* diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.443$, $T_{max} = 0.509$
1778 measured reflections
1651 independent reflections
1496 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 26.0^\circ$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 18$
$l = -9 \rightarrow 9$
3 standard reflections every 150 reflections intensity decay: 0.1%

Table 1
Selected geometric parameters (Å, °).

Fe—O5	2.0821 (15)	Fe—O7	2.1424 (16)
Fe—O1	2.0886 (14)	O1—C1	1.273 (3)
Fe—O6	2.0951 (16)	O2—C1	1.245 (3)
Fe—O3^i	2.1008 (15)	O3—C4	1.269 (3)
Fe—O8	2.1074 (15)	O4—C4	1.254 (2)
O5—Fe—O1	92.17 (6)	O1—Fe—O8	89.55 (6)
O1—Fe—O6	91.22 (6)	O3^i—Fe—O8	88.32 (6)
O5—Fe—O3^i	84.21 (6)	O1—Fe—O7	89.06 (6)
O1—Fe—O3^i	175.72 (6)	O3^i—Fe—O7	94.54 (6)
O6—Fe—O3^i	91.10 (6)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H51···O1^i	0.91	1.80	2.706 (2)	172
O5—H52···O4^{ii}	0.88	1.84	2.692 (2)	163
O6—H61···O2	0.90	1.74	2.620 (2)	165
O6—H62···O5^{iii}	0.85	2.20	2.996 (2)	157
O7—H71···O2^{iv}	0.87	1.84	2.697 (2)	169
O7—H72···O4^v	0.91	1.78	2.655 (2)	161
O8—H81···O7^i	0.91	1.95	2.847 (2)	173
O8—H82···O3^{vi}	0.93	1.91	2.823 (2)	169

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

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.076$
$S = 1.04$
1651 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 0.3528P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.025 (2)

The methylene H atoms were placed in calculated positions (C—H = 0.97 Å) and included in the final cycles of refinement as riding, with U_{iso}(H) values equal to $1.2U_{eq}$ of the carrier atom. The H atoms of the coordinated water molecules were located in a difference Fourier map and were allowed for with fixed positional parameters and U_{iso}(H) values of 0.08 Å^2.

Data collection: *MSC*/*AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC*/*AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1400). Services for accessing these data are described at the back of the journal.

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