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Diaquabis(7-iodo-8-oxidoquinolinium-5-sulfonato)-strontium(II) monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.075
wR factor = 0.230
Data-to-parameter ratio = 22.0

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

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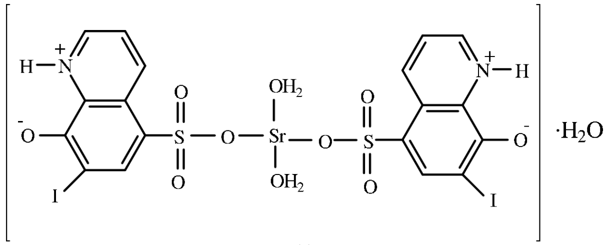
The title compound, $[Sr(C_9H_5INO_4S_2)_2(H_2O)_2]\cdot H_2O$, is isomorphous with the corresponding calcium complex of ferron (8-hydroxy-7-iodoquinoline-5-sulfonic acid). The asymmetric unit consists of one Sr^{II} ion, two organic ligands, two coordinated water molecules and one uncoordinated water molecule. The Sr^{II} ion has a pentagonal–bipyramidal coordination geometry made up of O atoms of three different sulfonate groups, deprotonated quinolinol O atoms of two different oxine rings and two water molecules. In the ligands of type I, two O atoms of the sulfonate group are involved in coordination, whereas in type II ligands, only one O atom is involved. Ligands of type I are stacked on top of one another, each pair of adjacent members of the stack being related by an inversion centre. Ligands of type II are also stacked in a similar manner. These molecular stacks are cross-linked by Sr—O(sulfonate) and Sr—O(quinolinol) bonds, leading to an extended framework. This architecture is further stabilized by a number of O—H···O and N—H···O hydrogen bonds.

Comment

Derivatives of 8-hydroxyquinoline (oxine) are known for their anti-amoebic, antibacterial and antifungal activities, which are correlated to their metal-chelating ability (Banerjee & Saha, 1986). The biological activities of oxine derivatives have been correlated with their capacity for metal chelation. Oxine and its derivatives have long been extensively used in analytical chemistry (Hollingshead, 1954–1956), and oxine derivatives are fluorogenic ligands for many metal ions (Launay *et al.*, 2001). The investigation of three-dimensional networks constructed by metal sulfonates through various modes of coordination is of current interest (Cai *et al.*, 2001; Onoda *et al.*, 2001; Cote *et al.*, 2002). The crystal structures of copper complexes of HQS (8-hydroxyquinoline-5-sulfonic acid) have also been investigated (Petit, Coquerel & Perez, 1993; Petit, Ammor *et al.*, 1993). From our laboratory, the crystal structures of 7-iodo-8-hydroxyquinoline-5-sulfonic acid (ferron; Balasubramanian & Muthiah, 1996), lithium (Murugesan & Muthiah, 1997), sodium (Raj *et al.*, 2003), nickel (Raj *et al.*, 2001) and potassium (Francis, Muthiah, Bocelli & Cantoni, 2003*b*) complexes of HQS, and nickel (Raj *et al.*, 2003), copper (Francis, Muthiah, Bocelli & Cantoni, 2003*c*), calcium (Francis, Muthiah, Rychlewska & Warzajtis, 2003), cobalt (Balasubramanian, 1995), zinc (Francis, Muthiah, Bocelli & Cantoni, 2003*a*) and barium (Muthiah *et al.*, 2003) complexes of ferron have been reported. We now present the crystal structure of the title Sr–ferron complex, (I).

The crystal structure of (I) is isomorphous with the calcium complex of ferron (Francis, Muthiah, Rychlewska & Warzajtis, 2003). The asymmetric unit contains one Sr^{2+} ion, two

8-hydroxy-7-iodoquinoline-5-sulfonate (ferron) anions and three water molecules, as shown in Fig. 1. The metal–ferron ratio is 1:2. The coordination geometry around Sr is seven-coordinate pentagonal bipyramidal, made up of two deprotonated quinolinol O atoms (O4 and O24), the O atoms (O1, O2 and O23) of three different sulfonate groups of the ferron anions, and two water molecules (Fig. 2). In ligands of type I, containing atom N1, two O atoms of the sulfonate groups are involved in coordination, whereas in type II ligands (containing atom N2), only one O atom is involved. Ligands of type I are stacked above one another, each pair of adjacent members of the stack being related by an inversion centre, and type II ligands are stacked in a similar manner. These stacks are cross-linked by Sr—O(sulfonate) and Sr—O(quinolinol) bonds, leading to a metallo-organic framework (Fig. 3).



(I)

Atoms O1*W* and O2*W* of the coordinated water molecules donate H atoms to the O atoms (O21 and O3) of two sulfonate groups to form six-membered hydrogen-bonded rings on either side of the Sr atom (Table 2). The non-coordinated water molecule donates H atoms to the O atoms (O3 and O22) of the sulfonate groups to form a 16-membered ring. It also acts as an acceptor for one of the coordinated water molecules (O2*W*), to produce an eight-membered ring, and bridges two complexes, through hydrogen bonding, as shown in Fig. 4.

In this crystal structure, π–π stacking interactions are also observed between the oxine rings. For the type I ligand, the interplanar and centroid–centroid distances are 3.373 and 3.942 (5) Å, respectively, and the slip angle (defined as the angle between the plane normal and the line joining the centroids) is 32.3°. The corresponding values for the type II ligand are 3.347 and 3.725 (5) Å and 19.3°, respectively. Similar stacking has also been observed in the nickel (Raj *et al.*, 2003) and zinc complexes (Francis, Muthiah, Bocelli & Cantoni, 2003*a*) of ferron.

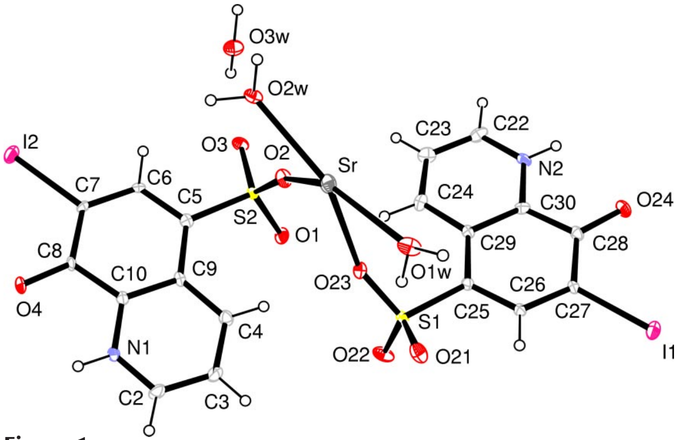


Figure 1
A view of the asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

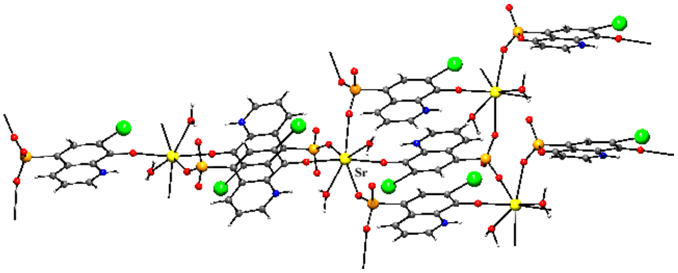


Figure 2
The coordination geometry of Sr in (I).

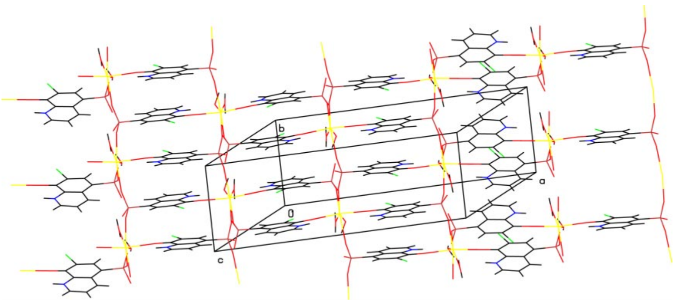


Figure 3
The supramolecular architecture of (I).

Some I···O interactions that are significantly shorter than the van der Waals separation of these atoms (3.5 Å) are observed in (I) (Table 3). Halogen···O interactions have been recognized in the literature and widely used in crystal engineering (Thalladi *et al.*, 1996). This type of I···O interaction has also been observed in ferron (Balasubramanian & Muthiah, 1996) and its nickel complex (Raj *et al.*, 2003).

Experimental

Hot aqueous solutions of ferron (88 mg; Riedel de Haen) and salicylic acid (35 mg; Merck) were mixed in a 1:1 molar ratio. The resultant solution was added to $SrCO_3$ (37 mg; SISCO CHEM) in a 1:1:1 molar ratio and warmed in a water bath for 90 min. The red solution was filtered and allowed to evaporate slowly. After a few days, red block-shaped crystals of (I) separated from the solution.

Crystal data

$[Sr(C_9H_5INO_4S)_2(H_2O)_2]\cdot H_2O$
$M_r = 841.89$
Monoclinic, $P2_1/c$
$a = 20.539$ (3) Å
$b = 7.012$ (2) Å
$c = 19.243$ (3) Å
$\beta = 116.95$ (3)°
$V = 2470.4$ (11) Å^3
$Z = 4$
$D_x = 2.264$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
$\theta = 3.1$–30.2°
$\mu = 4.91$ mm^{-1}
$T = 293$ (2) K
Block, red
0.33 × 0.27 × 0.18 mm

Data collection

Philips *PW*1100 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.257$, $T_{\max} = 0.413$
7400 measured reflections
7228 independent reflections
4772 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.091$
$\theta_{\max} = 30.2°$
$h = 0 \rightarrow 28$
$k = 0 \rightarrow 9$
$l = -27 \rightarrow 24$
1 standard reflection every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.075$
$wR(F^2) = 0.230$
$S = 1.00$
7228 reflections
328 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1552P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 3.22$ e Å^{-3}
$\Delta\rho_{\min} = -3.81$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sr—O1*W*	2.582 (7)	Sr—O4$^{\rm iii}$	2.314 (7)
Sr—O2	2.500 (6)	N1—C2	1.324 (10)
Sr—O2*W*	2.551 (5)	N1—C10	1.361 (11)
Sr—O23	2.475 (6)	N2—C30	1.357 (11)
Sr—O24$^{\rm i}$	2.331 (7)	N2—C22	1.306 (11)
Sr—O1$^{\rm ii}$	2.521 (6)		
O1*W*—Sr—O2	141.14 (18)	O2—Sr—O23	71.18 (18)
O1*W*—Sr—O2*W*	149.59 (19)	O2—Sr—O24$^{\rm i}$	98.9 (2)
O1*W*—Sr—O23	70.39 (19)	O2*W*—Sr—O23	139.88 (19)
O1*W*—Sr—O24$^{\rm i}$	77.2 (2)	O2*W*—Sr—O24$^{\rm i}$	99.7 (2)
O2—Sr—O2*W*	69.21 (18)	O23—Sr—O24$^{\rm i}$	92.3 (2)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···O24	0.86	2.35	2.696 (9)	104
N2—H1···O1*W*$^{\rm i}$	0.86	2.10	2.943 (13)	167
O1*W*—H1*W*···O22$^{\rm ii}$	0.95	2.02	2.719 (9)	129
O1*W*—H2*W*···O21	0.95	1.99	2.893 (9)	159
O2*W*—H3*W*···N1$^{\rm iii}$	0.95	2.11	2.880 (10)	137
O2*W*—H4*W*···O3$^{\rm ii}$	0.96	1.99	2.807 (8)	143
O3*W*—H5*W*···O22$^{\rm iv}$	0.96	1.99	2.856 (12)	149
N1—H6···O4	0.86	2.33	2.678 (9)	105
N1—H6···O2*W*$^{\rm v}$	0.86	2.05	2.880 (10)	161
O3*W*—H6*W*···O3	0.97	1.93	2.819 (8)	152
C24—H4···O23	0.93	2.35	2.951 (11)	122
C26—H5···O21	0.93	2.45	2.850 (11)	106
C3—H8···O3*W*$^{\rm vi}$	0.93	2.39	3.317 (10)	174
C4—H9···O1	0.93	2.45	3.024 (11)	120
C6—H10···O3	0.93	2.44	2.851 (11)	106

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

Table 3
Short halogen···O contact geometry (Å).

I1···O24	3.230 (6)	I2···O4	3.208 (6)
I1···O22$^{\rm vii}$	3.315 (7)		

Symmetry code: (vii) $-x, \frac{1}{2}+y, \frac{1}{2}-z$.

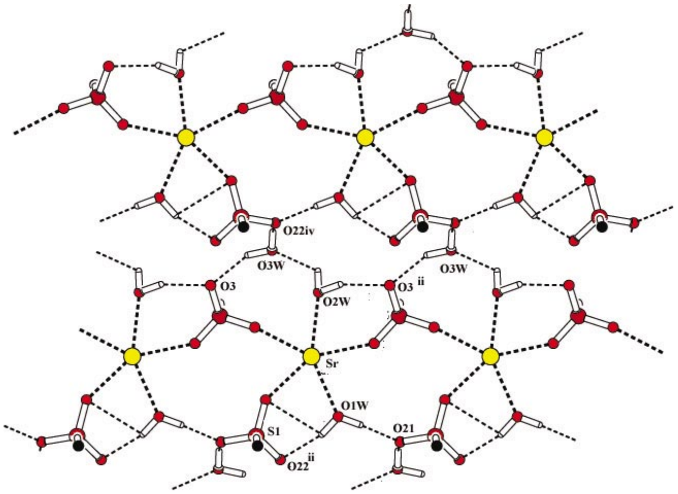


Figure 4
Detail of the hydrogen-bonded network (dashed lines) in the structure of (I). Symmetry codes as in Table 2.

H atoms were located in a difference map and treated as riding atoms, with C—H, O—H and N—H distances of 0.93, 0.95–0.97 and 0.86 Å, respectively; $U_{\rm iso}$ values were set at $1.2U_{\rm eq}$ of the carrier atom. The positions of the water H atoms are less certain, as reflected in a short H3*W*···H6 intermolecular contact of 1.39 Å. The highest residual electron-density peak is located 0.87 Å from atom I2.

Data collection: *FEBO* (Belletti, 1996); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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