Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Pentaaqua(oxydiacetato-$\kappa^3 O,O',O''$)strontium(II) monohydrate

Gaduo, Jian-Rong Su and Duan-Jun Xu*

Department of Chemistry, Zhejiang University, People's Republic of China

Correspondence e-mail: chem@zju.edu.cn

Received 13 April 2005
Accepted 19 April 2005
Online 23 April 2005

In the title compound, $[Sr(C_4H_4O_5)(H_2O)_5]\cdot H_2O$, the Sr^{II} atom is coordinated by a tridentate oxydiacetate dianion (ODA) and five water molecules, with a distorted square antiprism coordination geometry. The ODA chelates meridionally to the Sr^{II} atom with a planar structure. The Sr—O bond distances range from 2.505 (2) to 2.688 (2) Å.

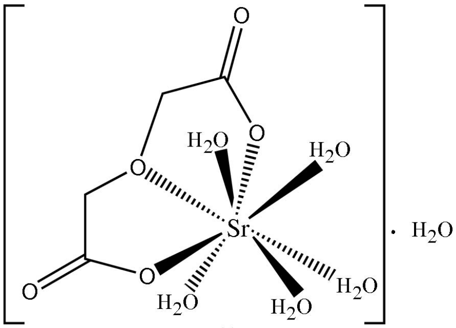
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.080
Data-to-parameter ratio = 18.4

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

Comment

The oxydiacetate dianion (ODA) usually plays the role of a tridentate chelating ligand in metal complexes, with either meridional or facial configuration for the chelating ligand (Luo *et al.*, 2004; Cao *et al.*, 2004). To study the factors affecting the configuration of ODA, the title Sr^{II} complex, (I), with a larger radius for the central atom, has been prepared and its structure has been determined.



(I)

The molecular structure of (I) is shown in Fig. 1. The eight-coordinate Sr^{II} complex assumes a distorted square antiprism coordination geometry, formed by one tridentate ODA and five coordinated water molecules. Compound (I) differs from the only other reported Sr^{II} compound with ODA, $[Sr(C_4H_4O_5)(H_2O)_3]_n.nH_2O$, which is a nine-coordinate polymeric complex (Baggio *et al.*, 1996), but is similar to the Ca^{II} analogue (Uchtman & Oertel, 1973).

The Sr—O$_{\rm carboxylate}$ bonds are longer than the Sr—O$_{\rm ether}$ bond (Table 1), which differs from that found in the reported Sr^{II} compound and also differs from those found in most of the first-row transition metal complexes incorporating chelating ODA (Li *et al.*, 2003; Luo *et al.*, 2004; Cao *et al.*, 2004;, Liu *et al.*, 2004; Shen *et al.*, 2004). A search of the Cambridge Structural Database (Version 5.26; Allen, 2002) indicates that ODA usually chelates to the transition metal ion with either meridional or facial configuration. In the facial cases, the average bond angle at the ether O atom (O3) is 110.5 (5)° (Rio *et al.*, 2003), which implies the normal sp^3 hybrid for the ether O atom. In (I), ODA chelates to the Sr^{II} atom with a planar meridional configuration, the maximum atomic deviation

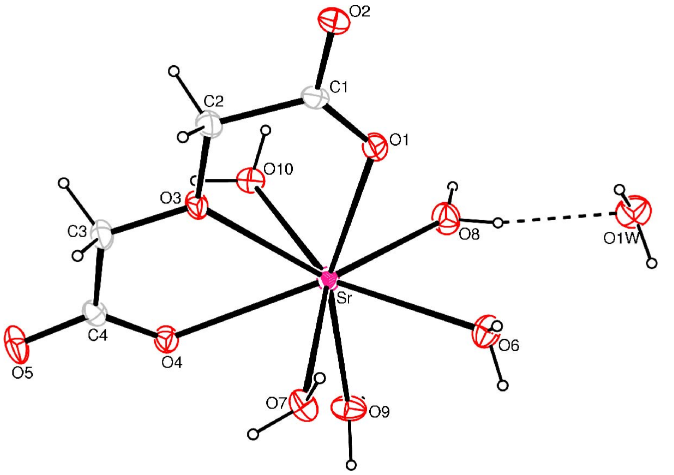


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

being 0.0737 (15) Å for atom O4. The planar configuration and the bond angles at atom O3 (Table 1) clearly suggest an sp^2 hybrid for the ether O atom in (I). This configuration of ODA is also appreciably different from the situation found in the reported complexes with a meridional ODA ligand. In these structures, the ether O atom (O3) commonly deviates from the mean plane formed by the other atoms of ODA by about 0.5 Å (Li *et al.*, 2003; Luo *et al.*, 2004), and the average bond angle at atom O3 ranges from 113.2 to 117. This may be due to the difference in the coordinate bond distances, *i.e.* the shorter metal–O coordinate bonds result in the poor planarity of the chelating ODA ligand in the first-row transition metal complexes. As expected, the O—H···O hydrogen bonds involving the water molecules lead to a hydrogen-bonded network in the crystal structure (Table 2 and Fig. 2).

Experimental

Strontium carbonate (0.15 g, 1 mmol) and oxydiacetic acid (0.13 g, 1 mmol) were dissolved in a water/ethanol mixture (20 ml, 3:1). The solution was refluxed for 3 h. After cooling to room temperature the solution was filtered. Single crystals of (I) were obtained from the filtrate after 3 d.

Crystal data

$[Sr(C_4H_4O_5)(H_2O)_5]\cdot H_2O$
$M_r = 327.79$
Monoclinic, $P2_1/n$
$a = 6.2548$ (3) Å
$b = 16.2580$ (4) Å
$c = 11.4600$ (4) Å
$\beta = 91.601$ (1)°
$V = 1164.92$ (7) Å^3
$Z = 4$
$D_x = 1.869$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8625 reflections
$\theta = 2.0$–26.0°
$\mu = 4.67$ mm^{-1}
$T = 295$ (2) K
Block, colorless
0.40 × 0.30 × 0.28 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.164$, $T_{max} = 0.278$
11 076 measured reflections
2673 independent reflections
2439 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5°$
$h = -8 \rightarrow 8$
$k = -21 \rightarrow 19$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.080$
$S = 1.25$
2673 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 1.1911P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sr—O1	2.5710 (19)	Sr—O7	2.648 (2)
Sr—O3	2.5439 (19)	Sr—O8	2.568 (2)
Sr—O4	2.5705 (18)	Sr—O9	2.505 (2)
Sr—O6	2.540 (2)	Sr—O10	2.688 (2)
O1—Sr—O3	62.78 (6)	O4—Sr—O9	77.09 (7)
O1—Sr—O4	124.27 (6)	O4—Sr—O10	72.73 (6)
O1—Sr—O6	76.63 (7)	O6—Sr—O7	70.93 (6)
O1—Sr—O7	92.35 (6)	O6—Sr—O8	71.52 (7)
O1—Sr—O8	87.35 (7)	O6—Sr—O9	81.88 (7)
O1—Sr—O9	157.53 (7)	O6—Sr—O10	142.74 (7)
O1—Sr—O10	98.80 (7)	O7—Sr—O8	141.44 (7)
O3—Sr—O4	61.51 (6)	O7—Sr—O9	86.73 (7)
O3—Sr—O6	126.60 (7)	O7—Sr—O10	146.16 (6)
O3—Sr—O7	77.34 (7)	O8—Sr—O9	79.63 (7)
O3—Sr—O8	134.32 (7)	O8—Sr—O10	71.33 (7)
O3—Sr—O9	138.17 (7)	O9—Sr—O10	94.30 (7)
O3—Sr—O10	79.63 (7)	C2—O3—C3	113.1 (2)
O4—Sr—O6	140.32 (7)	C2—O3—Sr	122.73 (15)
O4—Sr—O7	74.59 (6)	C3—O3—Sr	124.20 (15)
O4—Sr—O8	135.07 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O2^{i}	0.83	2.08	2.892 (3)	167
O1W—H1B···O10^{ii}	0.84	2.15	2.997 (3)	177
O6—H6A···O4^{ii}	0.84	2.00	2.834 (3)	173
O6—H6B···O7^{iii}	0.85	2.01	2.843 (3)	170
O7—H7A···O5^{ii}	0.89	1.82	2.706 (3)	174
O7—H7B···O2^{iv}	0.82	1.93	2.744 (3)	170
O8—H8A···O1W	0.83	2.10	2.923 (4)	171
O8—H8B···O1W^{v}	0.84	2.01	2.842 (3)	170
O9—H9A···O2^{vi}	0.88	1.96	2.812 (3)	163
O9—H9B···O4^{vii}	0.86	1.95	2.804 (3)	171
O10—H10A···O5^{viii}	0.82	1.99	2.794 (3)	166
O10—H10B···O1^{ix}	0.86	2.16	3.013 (3)	172

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

H atoms of the water molecules were located in a difference Fourier map and were not refined. The isotropic displacement parameters were fixed at 0.05 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.97 Å, and included in the final cycles of refinement in the riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Acta Cryst. (2005). E**61**, m950–m952 Gaduo *et al.* • $[Sr(C_4H_4O_5)(H_2O)_5]\cdot H_2O$ **m951**

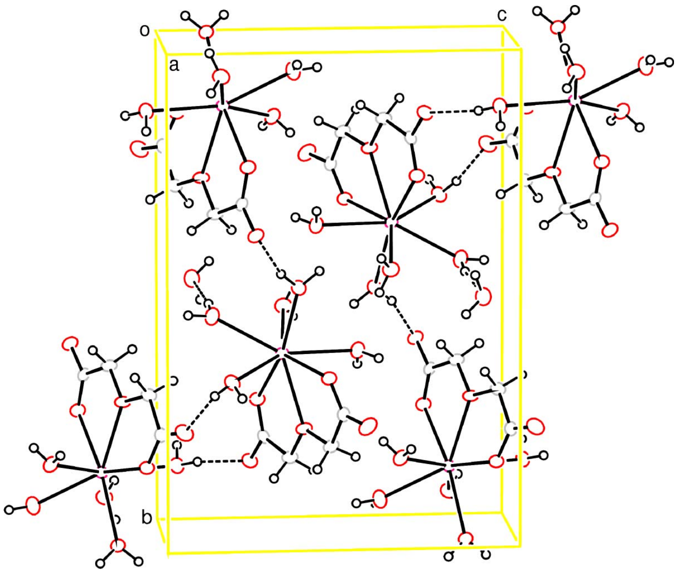


Figure 2
A packing diagram showing hydrogen bonds (dashed lines).

The project was supported by the National Natural Science Foundation of China (grant No. 20443003).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Baggio, R., Perec, M. & Garland, M. T. (1996). *Acta Cryst.* C**52**, 2996–2999.
Cao, L., Li, N. & Xu, D.-J. (2004). *Acta Cryst.* E**60**, m1066–m1067.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Higashi,, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Li, H., Luo, Y., Xu, D.-J., Wu, J.-Y. & Chiang, M. Y. (2003). *Acta Cryst.* E**59**, m622–m624.
Liu, B.-X., Tian, Y.-G. & Xu, D.-J. (2004). *Acta Cryst.* E**60**, m1453–m1455.
Luo, Y., Xu, D.-J., Wu, J.-Y. & Chiang, M. Y. (2004). *J. Coord. Chem.* **57**, 1125–1130.
Rio, D., Galindo, A., Vicente, R., Mealli, C., Ienco, A. & Masi, D. (2003). *Dalton Trans.* pp. 1813–1820.
Rigaku Corporation (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Version 3.00. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Shen, Y.-H., Liu, J.-G. & Xu, D.-J. (2004). *Acta Cryst.* E**60**, m842–m844.
Uchtman, V. A. & Oertel, R. P. (1973). *J. Am. Chem. Soc.* **95**, 1802–1811.

m952 Gaduo *et al.* • $[Sr(C_4H_4O_5)(H_2O)_5]\cdot H_2O$ *Acta Cryst.* (2005). E**61**, m950–m952