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Digold(III) Strontium Octaacetate Dihydrate, Au₂Sr(C₂H₃O₂)₈.2H₂O*

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Abstract. $M_r = 989.94$, monoclinic, $C2/c$, $a = 12.332$ (4), $b = 11.487$ (4), $c = 19.496$ (8) Å, $\beta = 101.97$ (3)°, $U = 2701.7$ Å³, $Z = 4$, $D_x = 2.43$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 128$ cm⁻¹, $F(000) = 1856$, room temperature, $R = 0.065$ for 2703 observed reflections. The structure consists of isolated SrAu₂-(CH₃COO)₈ units with crystallographic symmetry 2. Coordination geometry is square planar and Archimedean antiprismatic respectively at Au and Sr. Each acetate ion bridges Au and Sr. The C–O bond lengths indicate covalent Au–O but electrostatic Sr–O interactions. The water molecules occupy 'holes' in the lattice without forming hydrogen bonds.

Introduction. Little is known about carboxylate complexes of gold; simple carboxylates of the form AuX and AuX_3 appear to be unknown, and only the triphenylphosphine complexes Ph₃PAuX (X = acetate, formate, trifluoroacetate; Nichols & Charleston, 1969) have been characterized. We have begun a systematic study of gold carboxylate complexes and I here report the structure of the strontium salt SrAu₂ac₈ (ac = acetate), which crystallizes as the dihydrate. Details of the preparation of this and other compounds of general formula MAu₂ac₈.xH₂O (M = divalent metal cation) will be reported elsewhere.

Experimental. Crystal 0.4 × 0.35 × 0.2 mm mounted in glass capillary, 4760 profile-fitted intensities (Clegg, 1981) measured on Stoe–Siemens four-circle diffractometer ($2\theta_{max}$ 60°, monochromated Mo $K\alpha$ radiation); 3 standard reflections decreased gradually in intensity by *ca* 5% and the data were scaled accordingly; empirical absorption corrections (azimuthal scans; transmissions 0.28–0.72); averaging equivalents gave 3924 unique reflections (R_{int} 0.049), 2703 with $F > 4\sigma(F)$ used for all calculations; intensity distribution corresponded to pseudo-F-centring; cell constants refined from 2θ values of 40 reflections in the range 20–23°; structure solution by heavy-atom method; refinement on F to $R = 0.065$, $R_w = 0.068$ [Au and Sr anisotropic, H not located; 83 parameters, $w^{-1} = \sigma^2(F) + 0.00055\ F^2$, $S = 1.91$], max. Δ/σ 0.001; max. and min. heights in final $\Delta\rho$ map +2 (near Au), −3 e Å⁻³;† calculations performed with *SHELXTL* (Sheldrick, 1978); atomic scattering factors from *International Tables for X-ray Crystallography* (1974).

Discussion. The atomic coordinates and bond lengths and angles are given in Tables 1 and 2. The structure is

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† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39206 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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* Carboxylate and Related Complexes of Gold. Part 1.

Table 1. *Atomic coordinates* $(\times 10^4)$ *and isotropic thermal parameters* $(\text{Å}^2 \times 10^3)$

	x	y	z	U
Au	6325 (1)	2559 (1)	4285 (1)	30 (1)*
Sr	5000	2544 (1)	2500	23 (1)*
O(11)	4969 (7)	3070 (7)	4587 (5)	43 (2)
O(12)	4091 (7)	3316 (7)	3487 (5)	43 (2)
C(11)	4144 (10)	3413 (9)	4115 (7)	35 (2)
C(12)	3168 (13)	3840 (12)	4404 (8)	56 (4)
O(21)	5930 (7)	919 (7)	4417 (5)	43 (2)
O(22)	4884 (7)	869 (6)	3338 (5)	41 (2)
C(21)	5278 (10)	403 (9)	3895 (7)	33 (2)
C(22)	5021 (11)	−838 (10)	4056 (8)	49 (3)
O(31)	7767 (7)	2015 (7)	4093 (4)	40 (2)
O(32)	6989 (8)	1754 (7)	2964 (5)	55 (2)
C(31)	7799 (10)	1713 (9)	3445 (7)	34 (2)
C(32)	8905 (11)	1337 (10)	3353 (8)	46 (3)
O(41)	6824 (7)	4186 (7)	4245 (5)	47 (2)
O(42)	6212 (7)	4224 (8)	3089 (5)	51 (2)
C(41)	6670 (9)	4689 (9)	3636 (7)	35 (2)
C(42)	7120 (11)	5920 (10)	3636 (7)	45 (3)
Ow	1537 (12)	3913 (11)	2710 (8)	107 (4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

Fig. 1. Perspective view of the $SrAu_2ac_8$ unit, showing the atom numbering scheme. The approximate (non-crystallographic) symmetry of this unit is D_{4d}.

Table 2. *Bond lengths* (Å) *and angles* (°)

Au—O(11)	1·975 (9)	Au—O(21)	1·976 (8)
Au—O(31)	1·992 (9)	Au—O(41)	1·974 (8)
Sr—O(12)	2·577 (10)	Sr—O(22)	2·548 (8)
Sr—O(32)	2·596 (9)	Sr—O(42)	2·562 (9)
O(11)—C(11)	1·284 (14)	O(12)—C(11)	1·217 (16)
C(11)—C(12)	1·513 (21)	O(21)—C(21)	1·302 (14)
O(22)—C(21)	1·217 (14)	C(21)—C(22)	1·507 (16)
O(31)—C(31)	1·318 (16)	O(32)—C(31)	1·221 (14)
C(31)—C(32)	1·476 (19)	O(41)—C(41)	1·299 (16)
O(42)—C(41)	1·222 (15)	C(41)—C(42)	1·518 (16)
O(11)—Au—O(21)	89·9 (4)	O(11)—Au—O(31)	173·6 (3)
O(21)—Au—O(31)	88·8 (4)	O(11)—Au—O(41)	91·1 (4)
O(21)—Au—O(41)	174·2 (4)	O(31)—Au—O(41)	89·5 (4)
O(12)—Sr—O(22)	71·9 (3)	O(12)—Sr—O(32)	112·7 (3)
O(22)—Sr—O(32)	71·8 (3)	O(12)—Sr—O(42)	73·1 (3)
O(22)—Sr—O(42)	112·2 (3)	O(32)—Sr—O(42)	71·7 (3)
O(12)—Sr—O(12^i)	139·8 (3)	O(22)—Sr—O(12^i)	146·1 (3)
O(32)—Sr—O(12^i)	81·6 (3)	O(42)—Sr—O(12^i)	76·8 (3)
O(12)—Sr—O(22^i)	146·1 (3)	O(22)—Sr—O(22^i)	81·9 (4)
O(32)—Sr—O(22^i)	77·6 (3)	O(42)—Sr—O(22^i)	138·7 (3)
O(12)—Sr—O(32^i)	81·6 (3)	O(22)—Sr—O(32^i)	77·6 (3)
O(32)—Sr—O(32^i)	139·1 (4)	O(42)—Sr—O(32^i)	147·2 (3)
O(12)—Sr—O(42^i)	76·8 (3)	O(22)—Sr—O(42^i)	138·7 (3)
O(32)—Sr—O(42^i)	147·2 (3)	O(42)—Sr—O(42^i)	82·3 (4)
Au—O(11)—C(11)	118·1 (9)	Sr—O(12)—C(11)	147·3 (8)
O(11)—C(11)—O(12)	124·2 (12)	O(11)—C(11)—C(12)	113·9 (12)
O(12)—C(11)—C(12)	121·6 (11)	Au—O(21)—C(21)	117·4 (7)
Sr—O(22)—C(21)	147·0 (7)	O(21)—C(21)—O(22)	124·4 (10)
O(21)—C(21)—C(22)	112·9 (10)	O(22)—C(21)—C(22)	122·7 (10)
Au—O(31)—C(31)	117·9 (7)	Sr—O(32)—C(31)	147·6 (9)
O(31)—C(31)—O(32)	122·9 (12)	O(31)—C(31)—C(32)	113·9 (10)
O(32)—C(31)—C(32)	123·2 (12)	Au—O(41)—C(41)	118·0 (7)
Sr—O(42)—C(41)	147·4 (9)	O(41)—C(41)—O(42)	123·8 (10)
O(41)—C(41)—C(42)	115·5 (10)	O(42)—C(41)—C(42)	120·7 (11)

Symmetry operator: (i) $1 - x, y, 0·5 - z$.

shown in Fig. 1. The gold atom exhibits the usual square-planar coordination of Au^{III}; each of the four independent acetate ions is coordinated to gold through one oxygen atom. The second oxygen of each acetate is coordinated to strontium; this lies on a cryst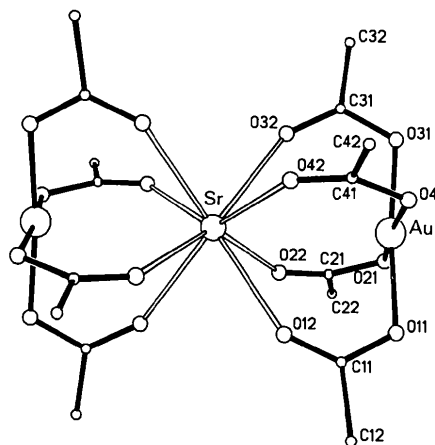allographic twofold axis and thus forms the centre of an isolated $SrAu_2ac_8$ unit with AuO_4 moieties as end 'faces'. The coordination geometry at strontium is that of an Archimedian antiprism.

There are no unusually short contacts between the $SrAu_2ac_8$ units; neighbouring 'faces' show Au···Au 3·58 (1) Å (corresponding symmetry operator $1·5 - x$, $0·5 - y$, $1 - z$). The water molecule is not involved in obvious H-bonding interactions; the shortest Ow···O contact is 3·27 (2) Å to O(12) at x, y, z. The high temperature factor of Ow is consistent with this lack of secondary interactions.

The Au—O bond lengths, 1·97–1·99 Å, are similar to those in other gold(III)–oxyanion complexes, *e.g.* $Au(NO_3)_4^-$ 1·99, 2·02 Å (Gardner & Wallwork, 1970), $Au_2(SeO_3)_2(Se_2O_5)$ 1·97–2·01 Å (Jones, Schwarzmann, Sheldrick & Timpe, 1981). The acetate ligands show a marked asymmetry of C—O bond lengths; for O bonded to Au, the average is 1·30 Å, *cf.* 1·22 Å for O···Sr. This is consistent with regarding the Au—O interaction as covalent but the Sr—O interaction as primarily electrostatic.

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