Supplementary data for this paper are available from the IUCr electronic archives (Reference: BM1142). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). C**53**, 870–872

Strontium Acetate Nitrate Trihydrate, [$Sr_2(CH_3COO)_2(NO_3)_2(H_2O)_3$]

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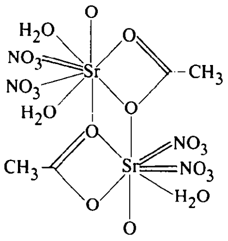
(*Received 17 September 1996; accepted 19 February 1997*)

Abstract

The structure of the title compound, di-μ-acetato-triaquadinitratodistrontium, is characterized by a band-like succession of alternating pairs comprising an Sr^{2+} cation and an acetate group along [101]. Two neighbouring strontium acetate bands are combined into sheets parallel to (010) by sharing a corner O atom of the SrO$_9$ polyhedra and by two additional bonds to intermediate NO$_3$ groups. The sheets, however, are linked only by three corresponding Sr—O bonds *via* a second NO$_3$ group. The water molecules are ligands of the Sr^{2+} cations and are further hydrogen bonded to the O atoms of the NO$_3$ groups. The centricity of the structure is in accordance with the lack of piezo-electric properties.

Comment

During the systematic search for organic crystals with interesting physical properties, we obtained the title compound, (I), which is reported to be non-centrosymmetric (Groth, 1910). However, all physical investigations have failed to confirm the proposed polar structure type. Therefore, to clarify this, the structural investigation was performed. We have established through the Cambridge Structural Database (Allen *et al.*, 1979) that only a few alkaline-earth acetate structures have been determined and that no crystallographic information is given for any acetate–nitrate compound.



(I)

The structure of the title compound consists of two Sr^{2+} cations, two acetate groups, two nitrate groups and three water molecules. It can be characterized by pairs, consisting of a Sr^{2+} ion bonded to both O atoms of the acetate group (Fig. 1). Neighbouring pairs are oriented in alternating directions and are connected laterally *via* two Sr—O bonds. All bonds between the Sr^{2+} ions and the acetate groups are arranged almost parallel to the plane (12$\bar{1}$), thus forming Sr–acetate bands along [101]. These bands are combined *via* four Sr bonds to the O atoms of the (N1)O$_3$ group establishing sheets parallel to the (010) plane (Fig. 2). In the case of Sr1—ON11—Sr2, a corner-sharing of the Sr coordination polyhedra can be observed. The second (N2)O$_3$ group located between the sheets, however, exhibits only three Sr—O bonds in this linkage along the *b* axis. This structural characteristic explains the plate-like habit and cleavage of the investigated crystals.

The Sr cations are ninefold coordinated and the Sr—O distances vary between 2.5073 (15) and 2.812 (2) Å with a mean value of 2.65 (11) and 2.64 (8) Å for Sr1—O and Sr2—O, respectively. Only the Sr1—ON22 bond which is part of the intersheet linkage exhibits a longer

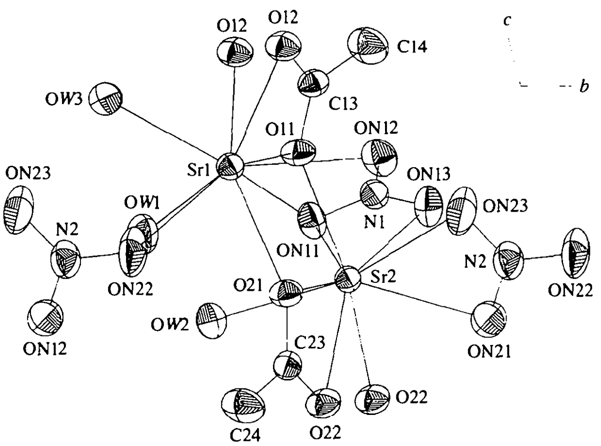


Fig. 1. A view of the stereochemistry around Sr1 and Sr2. Displacement ellipsoids are shown at the 50% probability level and H atoms have been omitted.

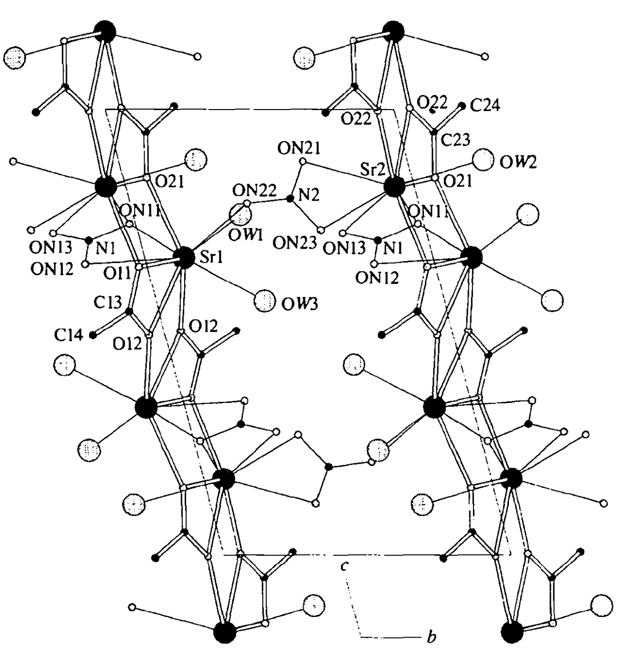


Fig. 2. A view along the *a* axis of the title compound showing the linkage between two strontium acetate bands *via* the N1 and N2 nitrate groups, and the ninefold coordination sphere of the two Sr^{2+} cations. The acetate and Sr to acetate bonds are outlined, all other bonds are shown as single lines. Atoms and groups are as follows: C (small black), Sr (large dark grey), water (large light grey), nitrate and acetate (small light grey).

interatomic distance, 2.812 (2) Å. These values are well within the range of the data given by Jones (1984). As both acetate O atoms contribute to two Sr—O bonds, no asymmetry within the distances and angles of the acetate groups can be observed.

The three water molecules are all located between the sheets and are bonded to the Sr^{2+} cations [Sr—*OW* 2.548 (2)–2.638 (2) Å], which is also reflected in the low displacement parameters. Additionally hydrogen-bonding interactions are established between the water H atoms and the O atoms of both nitrate groups except for the water–water interaction between *OW*1—*OW*2.

Experimental

The title compound was obtained by slow crystallization at room temperature from an equimolar mixture of aqueous solutions of $[Sr(NO_3)_2]$ and $[Sr(CH_3COO)_2]$. The latter was prepared from acetic acid and strontium hydroxide octahydrate. The crystal selected for measurement was sealed in a glass capillary.

Crystal data

$[Sr_2(C_2H_3O_2)_2(NO_3)_2$-
$(H_2O)_3]$
$M_r = 471.38$
Triclinic
$P\bar{1}$
$a = 7.5893\ (4)$ Å
$b = 7.9361\ (5)$ Å
$c = 12.7930\ (7)$ Å
$\alpha = 104.427\ (4)°$
$\beta = 95.662\ (4)°$
$\gamma = 90.264\ (4)°$
$V = 742.26\ (7)$ Å^3
$Z = 2$
$D_x = 2.109$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 210
reflections
$\theta = 15.5$–$20.5°$
$\mu = 7.252$ mm^{-1}
$T = 293\ (2)$ K
Prismatic
0.60 × 0.25 × 0.15 mm
Colourless

Data collection

Stoe AED-2 diffractometer
$\omega/2\theta$ scans
Absorption correction:
empirical *via* ψ scans
(*EMPIR*; Stoe & Cie,
1992)
$T_{min} = 0.107$, $T_{max} = 0.258$
8746 measured reflections
4305 independent reflections

3279 reflections with
$I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 29.93°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 17$
3 standard reflections
frequency: 180 min
intensity decay: 1.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.061$
$S = 1.043$
4305 reflections
239 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.0177P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.683$ e Å^{-3}
$\Delta\rho_{min} = -0.737$ e Å^{-3}
Extinction correction:
*SHELXL*96
Extinction coefficient:
0.0102 (5)
Scattering factors from
International Tables for Crystallography (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Sr1—O12^i	2.5416 (18)	Sr2—O22	2.6873 (17)
Sr1—*OW*3	2.548 (2)	Sr2—ON23	2.739 (2)
Sr1—O21	2.5487 (15)	Sr2—ON13^{iv}	2.749 (2)
Sr1—*OW*1	2.568 (2)	O11—C13	1.268 (2)
Sr1—O12	2.6556 (16)	O12—C13	1.245 (3)

Sr1—O11	2.686 (2)	C13—C14	1.501 (5)
Sr1—ON11	2.7331 (19)	O21—C23	1.255 (2)
Sr1—ON12	2.7881 (19)	O22—C23	1.251 (3)
Sr1—ON22^{ii}	2.813 (2)	C23—C24	1.504 (5)
Sr2—O11	2.5074 (15)	N1—ON12	1.236 (3)
Sr2—O22^{iii}	2.5238 (17)	N1—ON13	1.253 (3)
Sr2—O21	2.622 (2)	N1—ON11	1.260 (2)
Sr2—O*W*2	2.6373 (19)	N2—ON23	1.229 (3)
Sr2—ON11^{iv}	2.6557 (19)	N2—ON21	1.247 (3)
Sr2—ON21	2.6692 (19)	N2—ON22	1.248 (3)
O12—C13—O11	121.4 (2)	C24—C23—Sr2	169.2 (2)
O12—C13—C14	120.2 (2)	ON12—N1—ON13	122.5 (2)
O11—C13—C14	118.4 (3)	ON12—N1—ON11	119.2 (2)
C14—C13—Sr1	168.2 (2)	ON13—N1—ON11	118.3 (2)
O22—C23—O21	121.5 (3)	ON23—N2—ON21	118.5 (2)
O22—C23—C24	120.4 (2)	ON23—N2—ON22	121.8 (2)
O21—C23—C24	118.1 (2)	ON21—N2—ON22	119.7 (2)

Symmetry codes: (i) $-x, -y, 1-z$; (ii) $x, 1+y, z$; (iii) $1-x, -y, 2-z$; (iv) $1+x, y, z$.

The structure was solved using coordinates for the Sr atoms obtained from direct methods and subsequent full-matrix least-squares refinements on the basis of the results of the difference Fourier summations. All non-H atoms were refined anisotropically. All H atoms were located from difference maps and the H atoms were refined isotropically using an independent distance restraint for each water molecule and the CH_3 groups.

Data collection: *DIF*4 (Stoe & Cie, 1991*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1991*b*). Program(s) used to solve structure: *SHELXS*96 (Sheldrick, 1996*b*). Program(s) used to refine structure: *SHELXL*96 (Sheldrick, 1996*a*). Molecular graphics: *ATOMS*3.2 (Dowty, 1995). Software used to prepare material for publication: *SHELXL*96.

The authors thank H. Effenberger (Vienna) for her valuable help. Financial support by grant No. 90_03 (E. Tillmanns) of the JCPDS/ICDD, Newton Square, Pennsylvania, USA, is gratefully acknowledged. The crystals were grown and kindly supplied by L. Bohaty (Cologne).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: TA1134). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). C**53**, 872–874

Bis{(μ-acetato)[μ-bis(salicylidene)-1,3-propanediaminato](*N*,*N*-dimethylformamide)nickel(II)}cadmium(II)†

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(*Received 2 December 1996; accepted 3 February 1997*)

Abstract

The structure of the title compound, $[Cd(C_2H_3O_2)_2\{Ni(C_3H_7NO)(C_{17}H_{16}N_2O_2)\}_2]$, consists of a linear heterotrinuclear unit with a central Cd^{II} ion. Both this ion and the terminal Ni^{II} ions have pseudo-octahedral coordination. Each pair of metal ions is triply bridged *via* O atoms from *N*,*N*′-bis(salicylidene)-1,3-propanediaminato ($SALPD^{2-}$) ligands and acetate groups. The coordination around the Cd^{II} ion involves four O atoms from two $SALPD^{2-}$ and two acetate ligands. The coordination of the Ni^{II} ion is provided by the two O and two N atoms from a $SALPD^{2-}$ ligand and one O atom each from an acetate and a dimethylformamide ligand. The Cd···Ni distance is 3.2274 (5) Å.

Comment

Trinuclear metal complexes based on Schiff base ligands are of interest because of their magnetic super-exchange interactions between bridged metal ions. The synthesis and magnetic properties of trinuclear complexes with the general formulae $[MCu_2(CH_3CO_2)_2(SALPD)_2]$ (M = Mg, Mn, Co, Ni, Cu or Zn) and $[MNi_2(CH_3CO_2)_2(SALPD)_2]$ (M = Mg, Mn, Co, or Ni), where H_2SALPD represents *N*,*N*′-bis(salicylidene)-1,3-propanediamine, have been reported previously (Fukuhara *et al.*, 1990). From this group of compounds, only the structure of $[Zn\{(CH_3CO_2)(SALPD)Cu\}_2]$ has been determined by X-ray diffraction (Fukuhara *et al.*, 1990). Structural studies of the complexes formulated as $M_3(SALPN)_2(CH_3CO_2)_2.2dmf$ [M = Co, Fe; SALPN = *N*,*N*′-bis(salicylidene)-2,2-dimethylpropylenediamine; dmf = dimethylformamide] have also been reported (Gerli, Hagen & Marzilli, 1991). We describe

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† Alternative name: bis(μ-acetato)-1:3$\kappa^2O:O'$;2:3$\kappa^2O:O'$-bis(*N*,*N*-dimethylformamide)-1κO,2κO-bis{μ-2,2′-[1,3-propanediylbis(nitrilomethylidyne)]diphenolato}-1$\kappa^4N,N'O,O'$:3κ^2O,O';2$\kappa^4N,N'O,O'$:-3κ^2O,O'-cadmium(II)dinickel(II).