

## SHORT COMMUNICATIONS

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*Acta Cryst.* (1982). **B38**, 2541–2542

**The space group of  $\mu_3$ -chloro-tris(1,2-dimethoxyethane)- $\mu_3$ -sulphato-tris( $\mu$ -trifluoroacetato)-trichobalt(II).** By J. E. DAVIES, *Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

(Received 19 April 1982; accepted 7 June 1982)

### Abstract

The space group of the title complex is  $R\bar{3}$  (with  $a = 12.927$ ,  $c = 18.369$  Å,  $Z = 3$ ), not  $P1$  as originally reported [Estienne & Weiss (1972), *Chem. Commun.* pp. 862–863].

### Introduction

The crystal structure of the title complex has previously been reported (Estienne & Weiss, 1972) as triclinic, space group  $P1$ ,  $a = 9.656$ ,  $b = 9.653$ ,  $c = 12.925$  Å,  $\alpha = 132.03$ ,  $\beta = 90.02$ ,  $\gamma = 95.92^\circ$ ,  $Z = 1$ , molecular symmetry approximately  $C_{3v}$ . In fact, the structure is rhombohedral, space group  $R\bar{3}$ ,  $a = 12.927$ ,  $c = 18.369$  Å,  $Z = \bar{3}$ , molecular symmetry exactly  $C_3$ . The unique  $c$  axis of the rhombohedral cell is parallel to the  $[1\bar{2}\bar{1}]$  zone axis of the original  $P1$  cell.

### Experimental

The original reflexion data are lost (Weiss, 1981) but a set of structure factors was calculated using the original refined ( $R = 0.064$ )  $P1$  atomic coordinates. These reflexion data very clearly indicate that the Laue symmetry is  $\bar{3}$  (see Fig. 1). Reflexions  $hkl$  in the  $P1$  setting are related to reflexions  $h'k'l'$  in the  $R\bar{3}$  setting according to the following equation:

$$\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix} = \begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 1 & 1 \\ 1 & \bar{2} & \bar{1} \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}.$$

Atomic coordinates for the rhombohedral structure (Table 1) were obtained by transforming the  $P1$  coordinates to the rhombohedral setting, translating the whole structure so that atoms O(6), S(1) and Cl(1) lie on the triad axis  $[001]$ , and averaging the coordinates of the remaining 45 atoms (15 sets, each of three atoms related by the triad). The maximum deviation of any atom in a general position of the  $R\bar{3}$  structure from any of the three corresponding atoms in the  $P1$  structure is 0.20 Å for atom F(1). The average such

Table 1.  $(CF_3CO_2)_3Co_3ClSO_4(dme)_3$ : atomic coordinates for the  $R\bar{3}$  structure

$\Delta$  is the average deviation (Å) of each  $R\bar{3}$  atom from the related atoms in the  $P1$  structure.

	$x$	$y$	$z$	$\Delta$
Co(1)	-0.1919	-0.1284	0.0	0.004
S(1)	0.0	0.0	-0.1274	0
Cl(1)	0.0	0.0	0.0633	0
O(1)	-0.1774	-0.2792	-0.0027	0.013
O(2)	0.0092	-0.2427	0.0111	0.009
O(3)	-0.3667	-0.2369	-0.0476	0.089
O(4)	-0.2920	-0.2102	0.0942	0.006
O(5)	-0.1249	-0.0728	-0.1000	0.010
O(6)	0.0	0.0	-0.2063	0
C(1)	-0.0992	-0.3048	0.0072	0.013
C(2)	-0.1448	-0.4392	0.0147	0.009
C(3)	-0.4106	-0.2051	-0.1041	0.043
C(4)	-0.4557	-0.2809	0.0156	0.020
C(5)	-0.4034	-0.3059	0.0758	0.032
C(6)	-0.2300	-0.2263	0.1589	0.048
F(1)	-0.182	-0.469	0.083	0.139
F(2)	-0.240	-0.504	-0.010	0.041
F(3)	-0.075	-0.467	0.007	0.123

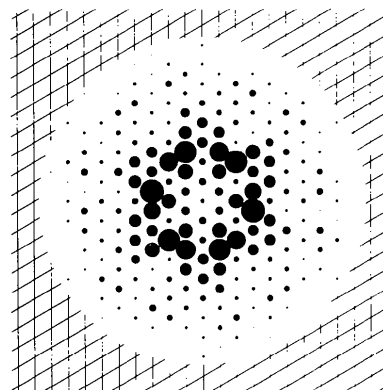


Fig. 1.  $(CF_3CO_2)_3Co_3ClSO_4(dme)_3$ : weighted reciprocal-lattice section calculated with the original  $P1$  atomic coordinates (Laue symmetry  $\bar{1}$  only assumed). Equatorial section perpendicular to the  $[1\bar{2}\bar{1}]$  zone axis in the triclinic lattice.

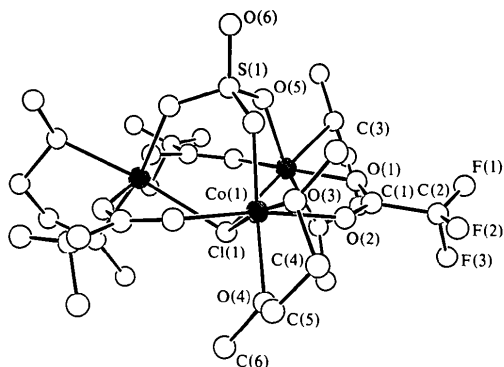


Fig. 2.  $(\text{CF}_3\text{CO}_2)_3\text{Co}_3\text{ClSO}_4(\text{dme})_3$ : molecular geometry and atom-labelling scheme.

deviation (Table 1) is 0.04 Å. These deviations indicate that the e.s.d.'s associated with the fractional coordinates in Table 1 are *ca* 0.0009 for the non-fluorine atoms and *ca* 0.003 for

the F atoms. As these e.s.d.'s are approximately the same as those obtained for the *P1* coordinates by least-squares refinement, the proposed *R3* structure does not differ significantly from the original *P1* structure. To confirm this, the *hk0* reciprocal-lattice section of the rhombohedral lattice was calculated using the coordinates in Table 1. This section is essentially identical to Fig. 1. Fig. 2 illustrates the molecular geometry and the atom-labelling scheme. Bond lengths and angles in the *R3* structure do not differ significantly from those already reported for the *P1* structure.

I thank Professor R. Weiss for very kindly providing me with a list of the original *P1* coordinates.

#### References

- ESTIENNE, J. & WEISS, R. (1972). *Chem. Commun.* pp. 862–863.  
 WEISS, R. (1981). Private communication.

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**$\text{La}_3\text{Rh}_4\text{Ge}_4$  of orthorhombic  $\text{U}_3\text{Ni}_4\text{Si}_4$  type: erratum.** By E. HOVESTREYDT, K. KLEPP and E. PARTHÉ, *Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève 4, Switzerland*

(Received 12 July 1982)

#### Abstract

An error in technical editing is corrected. The chemical name in the first line of the *Abstract* of the paper by Hovestreydt, Klepp & Parthé [*Acta Cryst.* (1982), **B38**, 1803–1805] should read: Trilanthanum tetrarhodium tetragermanide.

All relevant information is given in the *Abstract*.