

## References

- CHERNORUKOV, N. G., KORSHUNOV, I. A. & EGOROV, N. P. (1978). *Russ. J. Inorg. Chem.* **28**, 1306–1309.
- LECLAIRE, A., CHAHBOUN, H., GROULT, D. & RAVEAU, B. (1988). *J. Solid State Chem.* **77**, 170–179.
- LIU, K. H., TSAI, H. J. & WANG, S. L. (1990). *J. Solid State Chem.* **87**, 396–401.
- LINDE, S. A., GORBUNOVA, YU, E., LAVROV, A. V. & KUZNETSOV, V. G. (1979). *Dokl. Akad. Nauk SSSR*, **244**, 1411–1414.
- SHELDRICK, G. M. (1990). *SHELXTL-Plus*, version 4. Siemens Analytical International Inc., Madison, Wisconsin, USA.

*Acta Cryst.* (1991). **C47**, 1711–1712

## Structure of Decacstrontium Hexachromate(V) Difluoride

BY EBERHARDT HERDTWECK

Anorganisch-Chemisches Institut der Technischen Universität München, Lichtenbergstraße 4,  
D-8046 Garching bei München, Germany

(Received 28 August 1990; accepted 5 November 1990)

**Abstract.**  $\text{Sr}_{10}(\text{CrO}_4)_6\text{F}_2$ ,  $M_r = 1610.1$ , hexagonal,  $P6_3/m$ ,  $a = 9.956(1)$ ,  $c = 7.437(1)$  Å,  $V = 638.4$  Å<sup>3</sup>,  $Z = 1$ ,  $D_x = 4.188$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 22.89$  mm<sup>-1</sup>,  $F(000) = 734$ ,  $T = 296$  K. The structure was refined to  $R = 0.029$ ,  $wR = 0.035$  for 564 reflections. The title compound has an apatite-type structure with slightly distorted chromate tetrahedra (Cr—O = 1.693–1.698 Å, O—Cr—O = 106.9–114.9°).

**Experimental.**  $\text{Sr}_{10}(\text{CrO}_4)_6\text{F}_2$  was prepared by the high-temperature reaction of a stoichiometric mixture of  $\text{SrCO}_3$ ,  $\text{SrF}_2$  and  $\text{Cr}_2\text{O}_3$  at 1400 K in a corundum crucible. To avoid hydrolysis all experiments were carried out in a dry  $\text{N}_2$  atmosphere. After slowly cooling (50 K h<sup>-1</sup>), dark bluish-green needles were obtained. A crystal fragment (approximately 0.10 × 0.10 × 0.60 mm) was used for data collection on an Enraf–Nonius CAD-4 diffractometer (Mo  $K\alpha$ ,  $\lambda = 0.71073$  Å, graphite monochromator,  $T = 296$  K). Lattice parameters were refined using  $2\theta$  values of 98 reflections taken from a powder diffraction pattern (Cu  $K\alpha_1$ ,  $\lambda = 1.54051$  Å,  $10.2 \leq 2\theta \leq 114.4^\circ$ , Si as internal standard). Intensities measured for  $3 \leq \theta \leq 30^\circ$ ;  $\omega$ - $2\theta$ -scan technique, scan width  $(0.70 + 0.60 \tan \theta)^\circ$ . Three standard reflections indicated no decay throughout data collection. An experimental correction for absorption and decay was not applied. After  $L_p$  corrections (program *CADLP*; Müller, Schmidt & Massa, 1979), merging 637 data with  $I > 1.0\sigma(I)$  out of 769 collected intensities ( $0 \leq h \leq 14$ ,  $0 \leq k \leq 14$ ,  $0 \leq l \leq 10$ ) yielded 564 unique reflections ( $R_{\text{int}} = 0.029$ ) which were used for all calculations (*SHELX76*; Sheldrick, 1976).

The systematic absences ( $00l$ :  $l = 2n + 1$ ) indicated the space groups  $P6_3$  or  $P6_3/m$ . The results of the refinement confirmed the latter space group. The

atomic positions of Sr were derived from a Patterson map; the remaining atoms were found in successive difference Fourier maps. Final  $R = 0.029$ ,  $wR = 0.035$ ,  $w = 1.62/\sigma^2(F_o)$ ,  $(\Delta/\sigma)_{\text{max}} < 0.01$  for 40 variables (all atoms had anisotropic temperature factors). Maximum and minimum features in the final difference Fourier map were +0.97, -2.85 e Å<sup>-3</sup>. Atomic scattering factors,  $f'$  and  $f''$  values were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Bond distances and angles were calculated using the program *SADIAN* (Baur & Wenninger, 1969).

Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1, derived interatomic distances and angles are in Table 2.\* The structure, well known as an apatite-type structure, contains Jahn–Teller-distorted ( $d^1$ )- $\text{CrO}_4^{3-}$  tetrahedra (Fig. 1). The F atom is located in the channel position  $2(a) \{0, 0, \frac{1}{2}\}$ .

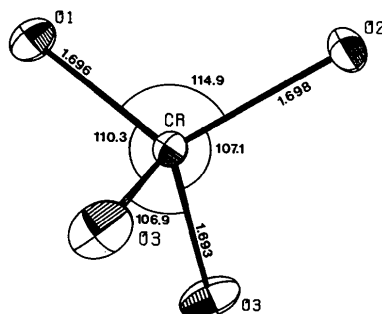
**Related literature.** Isomorphous replacements in compounds of the general formula  $A_{10}(\text{BO}_4)_6X_2$  provide an immense variety of apatite-type and apatite-like structures. Many apatites, both natural and synthetic, contain a high proportion of carbonate; others show cation or anion deficiency (Wyckoff, 1965). Single-crystal data, only available for a small number of these compounds, often proved a lower symmetry than indicated by powder data. A typical example is the doubling of the  $c$  axis in oxypyromorphite  $\text{Pb}_{10}(\text{PO}_4)_6\text{O}$  (Fischer, 1988). Finally, the relationship of all these different

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53725 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates and equivalent isotropic temperature factors ( $\text{\AA}^2 \times 10^4$ )

$U_{eq}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U_{eq}$
Sr(1)	$\frac{1}{3}$	$\frac{2}{3}$	-0.0007 (1)	169 (1)
Sr(2)	0.0105 (1)	0.2491 (1)	$\frac{1}{3}$	152 (2)
Cr	0.3986 (1)	0.3693 (1)	$\frac{1}{3}$	90 (3)
O(1)	0.3136 (6)	0.4804 (5)	$\frac{1}{3}$	163 (16)
O(2)	0.5956 (5)	0.4700 (5)	$\frac{1}{3}$	158 (14)
O(3)	0.3423 (4)	0.2523 (4)	0.0671 (5)	197 (10)
F	0	0	$\frac{1}{3}$	330 (20)

Fig. 1. Jahn-Teller-distorted ( $d^1$ )- $\text{CrO}_4^{3-}$  tetrahedron.

structures to  $\text{Mn}_5\text{Si}_3$ -( $D_{8h}$ ) types (Wondratschek, Merker & Schubert, 1964) and even  $\text{AlB}_2$  or WC types can be described by the useful tool *non-characteristic orbits* (Engel, Matsumoto, Steinmann & Wondratschek, 1984).

*Acta Cryst.* (1991). C47, 1712-1714

## Structure of the Anti-Cancer Drug Complex Tetrakis( $\mu$ -acetato)-bis(1-methyladenosine)dirhodium(II) Monohydrate

BY JOHN R. RUBIN

NCI-FCRF, PO Box B, Frederick, MD 21701, USA

AND TULI P. HAROMY AND M. SUNDARALINGAM\*

Department of Biochemistry, College of Agricultural and Life Sciences, University of Wisconsin-Madison, Madison, WI 53706, USA

(Received 19 July 1990; accepted 2 January 1991)

**Abstract.**  $[\text{Rh}_2(\text{C}_2\text{H}_3\text{O}_2)_4(\text{C}_{11}\text{H}_{16}\text{N}_5\text{O}_4)_2] \cdot \text{H}_2\text{O}$ ,  $M_r = 1024.6$ , triclinic,  $P1$ ,  $a = 7.808$  (3),  $b = 11.469$  (4),  $c =$

$12.091$  (2)  $\text{\AA}$ ,  $\alpha = 69.55$  (2),  $\beta = 79.46$  (2),  $\gamma = 76.61$  (3) $^\circ$ ,  $V = 980.7$  (6)  $\text{\AA}^3$ ,  $Z = 1$ ,  $D_x = 1.735$   $\text{g cm}^{-3}$ ,  $\lambda(\text{Cu } K\alpha) = 1.5418$   $\text{\AA}$ ,  $\mu = 77.6$   $\text{cm}^{-1}$ ,  $F(000) = 522$ , room temperature,  $R = 0.053$  for 3638 unique reflections. Structure consists of two rhodium(II) ions in a metal-metal bond bridged by

\* To whom correspondence should be addressed. Present address: Department of Chemistry, The Ohio State University, 120 West 18th Avenue, Columbus, OH 43210, USA.

Table 2. Selected bond distances ( $\text{\AA}$ ) and angles ( $^\circ$ )

Sr(1)—O(1)	2.567 (3) $3 \times$	Sr(2)—O(1)	2.732 (4)
Sr(1)—O(2)	2.598 (3) $3 \times$	Sr(2)—O(2)	2.514 (3)
Sr(1)—O(3)	2.952 (3) $3 \times$	Sr(2)—O(3)	2.513 (4) $2 \times$
		Sr(2)—O(3)	2.657 (3) $2 \times$
Cr—O(1)	1.696 (4)	Sr(2)—F	2.430 (1)
Cr—O(2)	1.698 (3)		
Cr—O(3)	1.693 (4)		
O(1)—Cr—O(2)	114.9 (2)	O(2)—Cr—O(3)	107.1 (1)
O(1)—Cr—O(3)	110.3 (1)	O(3)—Cr—O(3)	106.9 (2)

I am grateful to Professor Dr H. Wondratschek for his kindness and help.

### References

- BAUR, W. H. & WENNINGER, G. (1969). *SADIAN. Program for Calculation of Atomic Distances and Angles in Crystal Structures*. Univ. of Illinois, Chicago, USA.
- ENGEL, P., MATSUMOTO, T., STEINMANN, G. & WOND RATSCHEK, H. (1984). *The Non-Characteristic Orbits of the Space Groups*. *Z. Kristallogr.* Supplement, Issue No. 1. München: R. Oldenbourg Verlag.
- FISCHER, U. E.-M. (1988). PhD Thesis, Univ. Karlsruhe, Germany.
- MÜLLER, U., SCHMIDT, R. E. & MASSA, W. (1979). *CADLP. Ein Programm zur LP-Korrektur von Diffraktometerdaten*. FB Chemie, Marburg, Germany.
- SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.
- WOND RATSCHEK, H., MERKER, L. & SCHUBERT, K. (1964). *Z. Kristallogr.* pp. 393-394.
- WYCKOFF, R. W. G. (1965). *Crystal Structures*, 2nd ed., Vol. 3, pp. 228 ff. New York: Interscience.