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Note on the symmetry and cell of calcium orthovanadate

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The structures of the orthophosphates of Ba and Sr were determined by ZACHARIASEN[1] using the powder method. Their cells and symmetry are listed in Table 1 and their structures are described in Table 2. Later the arsenates and vanadates of Ba and Sr were studied by DURIF[2] using the powder method and assigned the same structures. More recently single crystals of calcium orthovanadate were examined by BRIXNER, FLOURNOY and BABCOCK[3] and found to have a different symmetry, $C2c$, and a different cell.

Table 1. *Symmetries and cells*

Compound	Symmetry	Cell dimensions			
		Rhombohedral cell		Hexagonal cell	
		a_r	α	a_h	c_h
$Sr_3(PO_4)_2$	$R\bar{3}m$	7.280 Å	43°21′	5.621 Å	20.14 Å
$Ba_3(PO_4)_2$	$R\bar{3}m$	7.696	42°35′	5.783	21.34
$Sr_3(AsO_4)_2$	$R\bar{3}m$	7.399	44°19′	5.581	19.98
$Ba_3(AsO_4)_2$	$R\bar{3}m$	7.804	43°15′	5.753	21.18
$Sr_3(VO_4)_2$	$R\bar{3}m$	7.458	44°17′	5.621	20.14
$Ba_3(VO_4)_2$	$R\bar{3}m$	7.859	43°10′	5.783	21.34
$Ca_3(VO_4)_2$	$R3c$ or $R\bar{3}c$	14.02	45°19′	10.80	37.65

[1] W. H. ZACHARIASEN, The crystal structure of the normal orthophosphates of barium and strontium. Acta Crystallogr. **1** (1948) 263—265.

[2] ANDRÉ DURIF, Structure cristalline des orthovanadates et orthoarseniates de baryum et de strontium. Acta Crystallogr. **12** (1959) 420—421.

[3] L. H. BRIXNER, P. A. FLOURNOY and KEITH BABCOCK, Note on calcium orthovanadate. Journ. Electrochem. Soc. **111** (1964) 873.

Table 2. *Structure data*

Atom	Equipoint	Coordinates	Parameters	
			$Sr_2(PO_4)$	$Ba_2(PO_4)$
1 Sr(1)	1*a*	000		
2 Sr(2)	2*c*	xxx, $\bar{x}\bar{x}\bar{x}$	$x = .208$	$x = .208$
2 P	2*c*	xxx, $\bar{x}\bar{x}\bar{x}$	$x = .412$	$x = .412$
2 O(1)	2*c*	xxx, $\bar{x}\bar{x}\bar{x}$	$x = .333$	$x = .337$
6 O(2)	6*h*	xxz, $\bar{x}\bar{x}\bar{z}$ xzx, $\bar{x}\bar{z}\bar{x}$ zxx, $\bar{z}\bar{x}\bar{x}$	$x = .279$ $z = .753$	$x = .285$ $z = .742$

This failure of $Ca_3(VO_4)_2$ to conform with the rest of the chemically similar substances presented an anomaly. Accordingly fragments of a $Ca_3(VO_4)_2$ single crystal, grown by this Czochralski method, were examined with the aid of a petrographic microscope. Since it proved to give a uniaxial interference figure it seemed likely that the assignment to monoclinic symmetry was in error. Further study by the precession method showed that the cell was rhombohedral and related to these published for the strontium and barium phosphates, arsenates and vanadates as shown in Table 1. The calcium orthovanadate has a_r doubled and a *c* glide in place of mirror.

The structure of $Ca_3(VO_4)_2$ is being investigated in this laboratory.

Errata

Zeitschrift für Kristallographie **128** (1969) 300–314: « Les colonnes cylindriques unicolores » par TIBERIU ROMAN.

P. 300, Abstract, 3e ligne
au lieu de: seventy-five cylinder groups
lire: seventy-five crystallographic cylinder groups

P. 301, 12e ligne *au lieu de:* simples *lire:* simple)
13e ligne *au lieu de:* 17 type) *lire:* 17 types
14e ligne *au lieu de:* déduites *lire:* déduits

P. 302, 8e ligne d'en bas et P. 310, 11e ligne
au lieu de: colonne *lire:* colonnes

Il faut ajouter aux « Travaux cités » (P. 314):

N. V. BELOV (1956), [Sur les groupes cristallographiques unidimensionels]. Kristallografiya **1**, 474–476 [en russe].

N. N. NERONOVA and N. V. BELOV (1961), A single scheme for the classical and black-and-white crystallographic symmetry groups. Kristallografiya **6**, 3–12 [en russe]; Soviet Physics–Crystallography **6**, 1–9.

E. I. GALYARSKII and A. M. ZAMORZAEV (1965), A complete derivation of crystallographic stem groups of symmetry and different types of antisymmetry. Kristallografiya **10**, 147–154 [en russe]; Soviet Physics–Crystallography **10**, 109–115.