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UNIT CELL DIMENSIONS OF SOME OXOFLUOROMETALLATES OF TRANSITION METALS

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SUMMARY

Unit cell dimensions of seven oxofluorometallates of transition metals were investigated by powder X-ray diffraction method. The compounds $K_3NbO_2F_4$ and $K_3TaO_2F_4$ were found to be isomorphous with cubic (FCC) structure and having lattice parameters 8.885 and 8.942 Å respectively. Similarly, the compounds K_2NbOF_5 (a = 8.367 Å, c = 13.038 Å) and K_2TaOF_5 (a = 8.463 Å, c = 13.139 Å) were also found to be isomorphous with a tetragonal structure. The compound $K_3Zr_2O_2F_7$ (a = 9.367 Å) was found to possess a cubic (FCC) structure. Both $K_2V_2O_5F_2$ (a = 6.739 Å, c = 10.635 Å) and K_2VO_3F (a = 5.984 Å, c = 10.914 Å) have a hexagonal structure.

INTRODUCTION

It has been observed that thermal decomposition of solid fluoroperoxo compounds leads to the formation of oxidefluorides and oxofluorometallates of transition metal [1,2] Transition metal fluorides, oxidefluorides and oxofluorometallates find use as solid state materials with vast technical applications [3-7].

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Many of the chemical and physical properties are directly related to the transition metals ions in a particular anion environment predicted on the basis of crystal structure [8].

This communication reports unit cell dimensions of seven oxofluorometallates of transition metals.

EXPERIMENTAL

The oxofluorometallates $K_3MO_2F_4$ (M = Nb, Ta); $K_3Zr_2O_3F_7$; $K_2V_2O_5F_2$ and K_2VO_3F have been prepared by heating the corresponding fluoroperoxo metallates in a muffle furnace at the temperature corresponding to the flat plateau in the thermograms and characterized by the standard methods, reported earlier [1]. Powder photographs were obtained on a Phillips-1130, X-ray generator with a Debye Scherrer Camera (diameter 114.6 mm) using CuK_α radiation.

RESULTS

The lattice constants derived using Cohen's least-square method are listed below (see Table).

The compounds $K_3NbO_2F_4$ and $K_3TaO_2F_4$ were found to be isomorphous with a FCC structure. Similarly, the compounds K_2NbOF_5 and K_2TaOF_5 were also found be isomorphous and all the X-ray lines could be indexed on the basis of a tetragonal structure. All the diffraction lines in the compounds $K_2V_2O_5F_2$ and K_2VO_3F, were indexable on the basis of a hexagonal structure and, in the case of $K_3Zr_2O_2F_7$, based on a FCC Lattice.

TABLE

Compound	Structure	^{o}a (A)	^{o}c (A)	c/a
$K_3Zr_2O_2F_7$	Cubic	9.367	-	-
$K_2V_2O_5F_2$	Hexagonal	6.739	10.635	1.578
K_2VO_3F	Hexagonal	5.984	10.914	1.824
K_2NbOF_5	Tetragonal	8.367	13.038	1.558
K_2TaOF_5	Tetragonal	8.463	13.139	1.552
$K_3NbO_2F_4$	Cubic	8.885	-	-
$K_3TaO_2F_4$	Cubic	8.942	-	-

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