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Synthesis, and crystal structure of phosphates with yavapaiite type-structure.

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Abstract.
The synthesis and structural study of three new $Ba_2SbM(PO_4)_4$ (M= Sc and Yb) phosphates, abbreviated as [Sc] and [Yb], were prepared by solid state reaction in air atmosphere and their structures has been solved ab initio by Rietveld analysis. The three phases crystallize in the Yavapaiite structure with C2/m space group (Z=2), with cell parameters a= 8.292(1) Å; b= 5.234(3) Å c= 7.878(7) Å and β= 93.81(1)° for [Sc], and a= 8.345(1) Å; b= 5.265(3) Å c= 7.977(3) Å and β= 94.22(1) ° for [Yb].

Keywords: Phosphates, solid-state reaction, Rietveld method, Yavapaiite structure.

1 Introduction

The chemistry of double $A^{II}M^{IV}(PO_4)_2$ (A^{II} =Ca, Sr, Pb, Ba; M^{IV} = Ge, Ti, Mo, Sn, Hf, Zr) phosphates have been intensively studied during the past two decades for applications including catalysts, ion conductors, optical [1-6], magnetic [7] and also as potential host matrices for minor actinide immobilization [8–9]. It should be noted that the size of the A^{2+} and M^{4+} cations has a significant effect on the crystal structure. For smaller M^{4+} ions, as in the $BaM^{IV}(PO_4)_2$ (M^{IV}= Ge, Ti, Mo, Sn, Hf, Zr) phases [10-15], the structure is monoclinic and isotypic of the archetype $KFe(SO_4)_2$ yavapaïte phase (*C2/m* space group, Z=2) [16]. For small A^{2+} and M^{4+} cations sizes, as in the case of $SrM^{IV}(PO_4)_2$ (M^{IV} = Ge Phosphates, solid-state reaction, Rietveld method, Yavapaiite structure, Ti, Sn) [11-12] and $PbM^{IV}(PO_4)_2$ (M^{IV} = Ge,Ti) [5], a distorted yavapaiite structure-type with $C2/c$ space group (Z=4) was reported. Compounds obtained from the coupled substitution of M^{IV} cations, in $A^{II}M^{IV}(PO_4)_2$ compounds, by M'^{III} and M''^{V} ions ($M^{IV}= 0.5M'^{V}+0.5M''^{III}$) as in $Ba(Nb^{V}_{0.50}M''^{III}_{0.50})(PO_4)_2$ (M''^{III} = Al, Cr, Fe, In) and $Ba(Sb^{V}_{0.50}M''^{III}_{0.50})(PO_4)_2$ (M''^{III} = Cr, Ga, Fe) have been synthesized and characterized by some of us [17-21]. The structure of these phases consists of layers of Ba^{2+} cations in tenfold coordination, alternating with dense slabs of $(M'^{V}/M''^{III})O_6$ octahedra and PO_4 tetrahedra interconnected by corner-sharing. In a continuation of our work search, in the present study, we have determined the crystal structure of [Sc] and [Yb] compounds from powder XRD data.

2 Materials and Methods

2.1 Description of the experimental

$Ba_2SbM(PO_4)_4$ (M= Sc, In and Yb) compounds was prepared from stoichiometric amounts of reagent-grade chemicals $BaCO_3$ (Riedel de Haën, 99 %), Sb_2O_3 (Riedel de Haën, 99.9 %), $NH_4H_2PO_4$ (Riedel de Haën, 99 %) and M_2O_3 (M=Sc, Yb) oxides. They were mixed in an agate mortar and putted in an alumina crucible. The mixtures were heated progressively, in a furnace at air atmosphere, with intermittent grinding at 150 °C (24 h), 300 °C (24 h), 400 °C (24 h), 600 °C (24 h), 700 °C (24 h), 800 °C (48 h), and 850°C (48 h).

2.2 X ray powder diffraction

X-ray powder diffraction data for structural determination were collected at room temperature on a Panalytical X'Pert diffractometer in Bragg–Brentano geometry using monochromatized CuKα radiation (45 kV, 40 mA). The data were collected from 10 to 90° (2θ°), in steps of 0.01. Rietveld analyses were carried out with the Fullprof suite program [22].

3 Results and discussion

3.1 Rietveld refinement of $Ba_2SbM(PO_4)_4$ (M= Sc and Yb)

3.1.1 Structural refinement of $Ba_2SbSc(PO_4)_4$

Barium phosphate-type has been reported in several times as fully isotypic with the yavapaiite structure phases [17-20]. Analysis of XRD spectra for the three [Sc] and [Yb] materials indicated that the principal peak positions and their intensity are similar to those observed in the $Ba_2SbFe(PO_4)_4$ XRD phase. Rietveld analysis in Le Bail's (profile matching) mode confirmed that structure of [Sc] phase is compatible with the $C2/m$ space group. So, initial starting parameters for the Rietveld refinement of [Sc] were based on those already reported by Aatiq et al. for $Ba_2SbFe(PO_4)_4$ phase in the $C2/m$ space group (Z = 2) [17]. This refinement leads to acceptable reliability factors (e.g., R_B = 3.2 %). A comparison of the experimental and calculated XRD profile of [Sc] material is given in Fig 1. Obtained crystallographic data and structural parameters are given in Tables 1. Selected interatomic distances and calculated bond valence sum BVS are gathered in Table 2

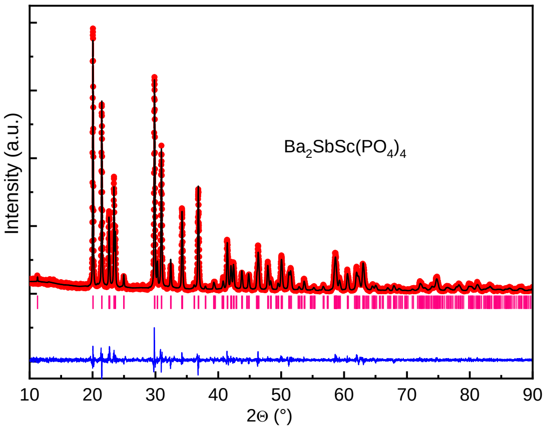

Fig.1. Rietveld refined diffraction patterns of $Ba_2SbSc(PO_4)_4$ phase.

3.1.1 Structural refinement of $Ba_2SbYb(PO_4)_4$

The atomic positions of the $Ba_2SbFe(PO_4)_4$ phase were used as starting structural parameters for the Rietveld refinements of [Yb]. In this case, the pattern indicates the presence of a secondary phase with a small amount (about 8% by weight) which is attributed to $YbPO_4$ (JCPDS PDF#83-0664). Therefore, the Rietveld refinement was carried out using a two phase model, consisting of $Ba_2SbYb(PO_4)_4$ and the $YbPO_4$ which crystallize with the $I4_1/amd$ space group. It should be noted that only high-intensity diffraction peaks of the $YbPO_4$ appear as impurity in the XRD pattern. This last refinement leads to acceptable reliability factors (R_B = 3.8%). Observed, calculated, and difference XRD patterns is shown in Fig 2. The final reliability factors and atomic parameters for [Yb] are summarised in Tables 1. Selected interatomic distances and calculated bond valence sum BVS is given in Table 2.

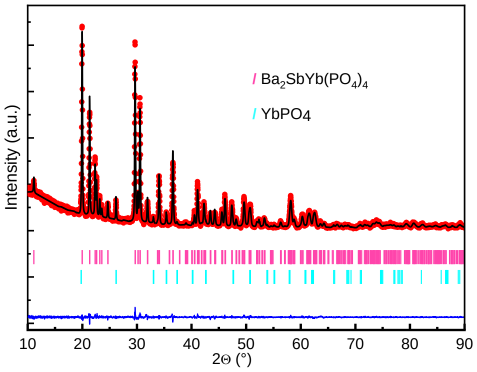

Fig.2. Rietveld refined diffraction patterns of $Ba_2SbYb(PO_4)_4$.

Table 1. Crystallographic data of $Ba_2SbM(PO_4)_4$ (M= Sc, Yb)(C2/m space group and Z=2)

$Ba_2SbM(PO_4)_4$ (M= Sc, Yb)	[Sc]	[Yb]
a(Å)	8.2924(1)	8.3451(1)
b(Å)	5.2344(3)	5.2651(3)
c(Å)	7.8787(1)	7.9772(8)
β(°)	93.8(1)	94.2(1)
V(Å^3)	340(1)	350(2)
R_P	0.086	0.074
R_{WP}	0.113	0.099
R_B	0.032	0.038
R_F	0.025	0.024

Table 2. Selected interatomic distances (Å) and calculated Bond Valence Sum (BVS) for $Ba_2SbM(PO_4)_4$.

$Ba_2SbM(PO_4)_4$ (M= Sc, Yb)	[Sc]	[Yb]
X-O = Sb(M)-O distances (Å)		
2×X-O(2)	1.911(5)	1.930(1)
4×X-O(3)	2.038(3)	2.199(4)
Aver.<X-O>	**2.00(1)**	**2.11(1)**
BVS(X)	**4.67**	**4.19**
(should be)	(4)	(4)
P-O distances (Å)		
P-O(1)	1.561(6)	1.545(6)
P-O(2)	1.528(1)	1.544(1)
2×P-O(3)	1.571(6)	1.528(4)
Aver.<P-O>	**1.55(1)**	**1.54(1)**
BVS(P)	**4.7**	**4.98**
(should be)	(5)	(5)
Ba-O distances (Å)		
2×Ba-O(1)	2.821(6)	2.691(1)
4×Ba-O(3)	2.792(4)	2.780(2)
4×Ba-O(1)	3.170(3)	3.172(3)
Aver.<Ba-O>	**2.95(1)**	**2.92(1)**
BVS (Ba)	**1.85**	**2.08**
(should be)	(2)	(2)

3.2 Structure description of $Ba_2SbM(PO_4)_4$ (M= Sc and Yb)

The structure of $Ba_2SbM(PO_4)_4$ (M= Sc and Yb) phases is represented in Fig 3. It consists of three types of polyhedra, BaO_{10}, PO_4 and $Sb(M)O_6$. The $Sb(M)O_6$ octahedra and PO_4 tetrahedra are interconnected via corner-sharing, alternating along the c-axis with layers of Ba cations in ten-fold coordination (Figure 3). The ten oxygens in each BaO_{10} polyhedra are from six PO_4 phosphate groups. Eight of the oxygen atoms come from four bidentate PO_4 groups and the other two oxygen atoms belong to the other two mono-dentate PO_4 groups. P-O bond length within PO_4 tetrahedra are in good agreement with those found in other orthophosphates [17-21, 23]. The mean of Sb(M)–O distance in $Sb(M)O_6$ octahedra, are consistent with the crystal radii values of Sb^{5+} and M^{3+} ions in six coordination [24]. In BaO_{10} polyhedron, the Ba–O distances values can be divided to two groups (Table 3). The first group contains six relatively shortest Ba–O distances values which are around 2.80 Å for [Sc] and between 2.69 and 2.78 Å for [Yb]. The second group is formed by four longer Ba–O distances with a mean values around 3.16 Å. Therefore, the co-ordinence of Ba atoms in $Ba_2SbM(PO_4)_4$ (M= Sc,Yb) can be considered as 6 + 4.

In order to have more structural information, the bond valence sum (BVS) based on bond-strength analysis [25] for [Sc] and [Yb] were computed. The BVS values calculated for Ba, Sc, Yb, Sb, and P (Table 3) are relatively consistent with the expected formal oxidation state of Ba^{2+}, Sc^{3+}, Yb^{3+}, Sb^{5+}, and P^{5+} ions.

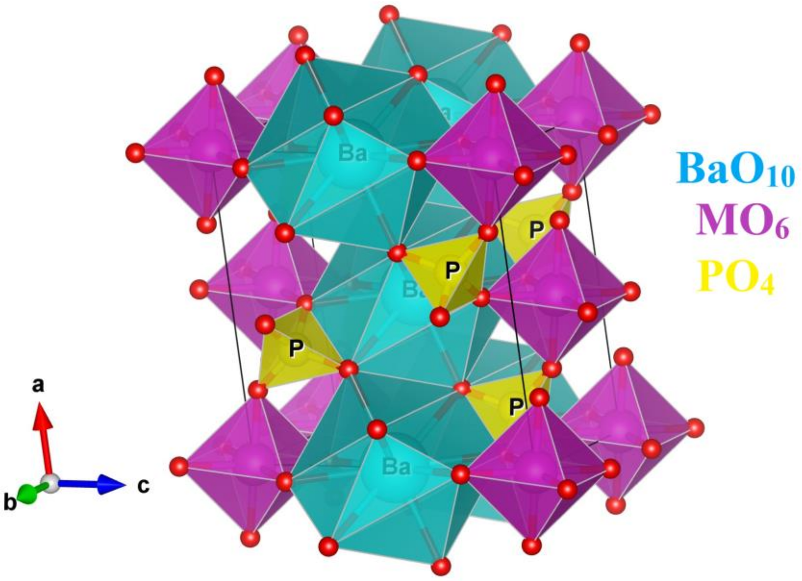

Fig.3. Crystal structure with (M= Sb(Sc) and Sb(Yb))

4 Conclusion

In conclusion, $Ba_2SbM(PO_4)_4$ (M= Sc, Yb) phosphates are prepared by solid-state reaction method and characterised by X-ray powder diffraction. The structural characterization shows that the three phases crystallize in the yavapaiite-type structure (*C2/m* space group, (Z=2)). Its structure consists of three dimensional array of dense slabs of $Sb(M)O_6$ octahedra and PO_4 tetrahedra which are interconnected via corner-sharing and alternating along the c-axis with layers of Ba cations in ten-fold coordination.

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