

Crystallochemistry of New Isotypes of $Sr_3(PO_4)_2$

Bouchra Gourja, Malika Tridane, Abdelhamid Daoudi, Said Belaouad

Abstract: Several authors have considered the possibilities of substitution within structures $B_3(XO_4)_2$ of type $Sr_3(PO_4)_2$. Since substitutions within the phosphate of lead have never been made to our knowledge, we have proposed to do so. This allowed us to synthesize the new solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$, the average ionic radius of K^+ and Nd^{3+} being close to that of Pb^{2+} . The new phases $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10$ and 0.15 are isotypes of $\beta Pb_3(PO_4)_2$, those for $x = 0.20; 0.25; 0.50$ and 0.75 are isotypes of $Sr_3(PO_4)_2$. Substitution of Pb^{2+} with K^+ and Nd^{3+} results in a slight decrease in volume; Which is consistent with the mean value of the ionic radii of potassium and neodymium which is slightly less than the ionic radius of the lead.

Index Terms: Substitution within structures $B_3(XO_4)_2$ of type $Sr_3(PO_4)_2$, synthesize the new solid solutions, $Pb_{3-2x}K_xNd_x(PO_4)_2$.

I. INTRODUCTION

Several authors have considered the possibilities of substitution within structures $B_3(XO_4)_2$ of type $Sr_3(PO_4)_2$. Solid solutions of the formula $Sr_{3-2x}Na_xLn_x(PO_4)_2$ ($Ln = Nd, Gd$) with $0 \leq x \leq 0.90$ for Nd and $0 \leq x \leq 0.50$ for Gd, $Sr_{3-2x}K_xLn_x(VO_4)_2$ with $0 \leq x \leq 0.50$ isotypes of $Sr_3(PO_4)_2$ were thus prepared [5,10]. Some of these phases have interesting optical properties [1]. Since substitutions within the phosphate of lead have never been made to our knowledge, we have proposed to do so. This allowed us to synthesize the new solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$, the average ionic radius of K^+ and Nd^{3+} being close to that of Pb^{2+} . The substitution is done according to the scheme: $2x Pb^{2+} = xK^+ + xNd^{3+}$. The introduction of rare earth ions within the $Pb_3(PO_4)_2$ structure can lead to compounds with interesting optical properties. Similarly, the phosphate of lead with ferroelectric properties [2,3], the solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$ could present interesting ferroelectric properties.

II. RECALL OF THE STRUCTURE OF $Sr_3(PO_4)_2$

Strontium orthophosphate, $Sr_3(PO_4)_2$, crystallizes in the rhombohedral system. According to W. H. Zachariassen [4], this compound belongs to the space group $R_{3m}(D_{3d}^5)$ with the parameters $a_r = 7.294 \text{ \AA}$ and $\alpha = 43^\circ 21'$

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Its unit-cell contains 3 form groups. The phase $Sr_3(PO_4)_2$ can also be described by a hexagonal pseudo-grid whose parameters and volume are given in Table I. The parameters and the volume of the unit-cells of the synthesized $Sr_3(VO_4)_2$ and $Sr_3(AsO_4)_2$ phases by G. The Flem [5] and H. Schwartz [6] crystallizing in the same structure are also given in Table I. The projection of the structure of $Sr_3(PO_4)_2$, described by a hexagonal unit-cell, on the plane (001) is given in figure 1.

Table I: Parameters a and c and volume V of the phases $Sr_3(XO_4)_2$ (X = P, As, V)

Phase	(a ± 0,01)Å	(c ± 0,01)Å	(V ± 2)Å ³
$Sr_3(PO_4)_2$	5,39	19,79	498
$Sr_3(AsO_4)_2$	5,59	20,00	541
$Sr_3(VO_4)_2$	5,62	20,10	550

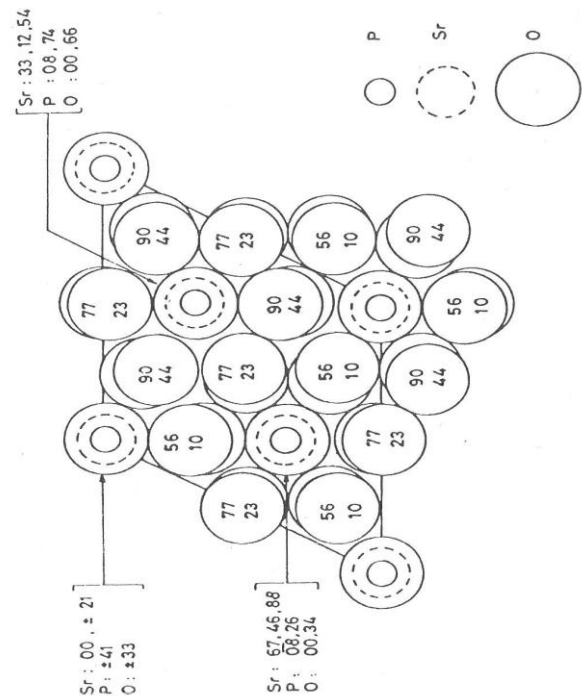


Fig. 1: Projection of the structure of $Sr_3(PO_4)_2$ on the plane (001) (hexagonal unit-cell)

In the structure of $Sr_3(PO_4)_2$, the tetrahedral groups (PO_4) are located on the ternary axis. Strontium atoms occupy two different sites:

- A site of coordination XII of symmetry D_{3d} . In this

site, the strontium atom Sr_I has 6 oxygen neighbors at the distance 2.57Å and 6 others at the distance 3.11Å substantially greater.

- A coordination site X, of symmetry C_{3v} , in which the strontium atom Sr_{II} has a neighbor oxygen at the distance 2.37Å, 3 at the distance 2.72Å and 6 others at 2.73Å.

Figure 2 shows the sites of Sr_I and Sr_{II} in $\text{Sr}_3(\text{PO}_4)_2$. The distance P-O in the group (PO_4) is 1.58Å.

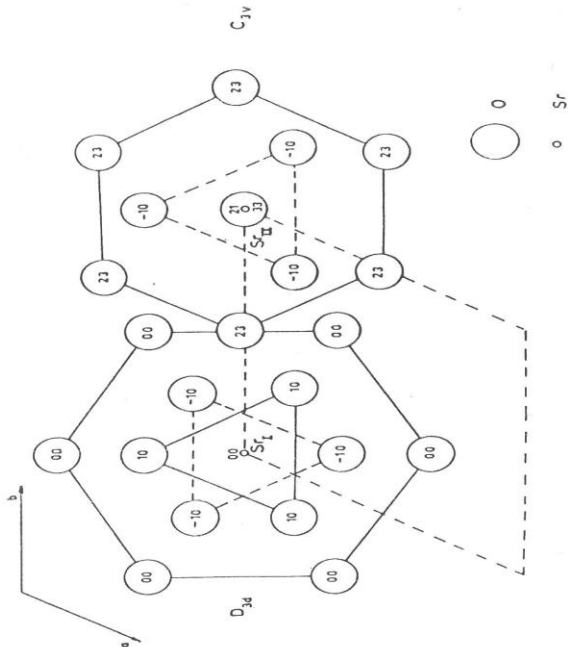


Fig. 2: Sr_I and Sr_{II} sites in the structure $\text{Sr}_3(\text{PO}_4)_2$

III. CRISTALLOCHEMISTRY OF SOLID SOLUTIONS $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$

A. Recall of the structure of $\text{Pb}_3(\text{PO}_4)_2$

$\text{Pb}_3(\text{PO}_4)_2$ has two allotropic varieties $\alpha \text{Pb}_3(\text{PO}_4)_2$ and $\beta \text{Pb}_3(\text{PO}_4)_2$. The structure of $\alpha \text{Pb}_3(\text{PO}_4)_2$ was determined by Hodenberg [7]. It has an isotype with $\text{Sr}_3(\text{PO}_4)_2$. The unit-cell is rhombohedral. This structure can also be described by a hexagonal unit-cell.

The structure of $\beta \text{Pb}_3(\text{PO}_4)_2$ was determined by Keppler [8]. The unit-cell is monoclinic. The crystallographic data of the two varieties are grouped in Table II. The passage from the monoclinic variety β to the α hexagonal variety of $\text{Pb}_3(\text{PO}_4)_2$ is carried out by raising the temperature to 200°C and is accompanied by a jump of dielectric permittivity. The basic vectors of these two varieties are connected by the relation (fig. 3):

Table II: Crystallographic data of the elemental cells of the two varieties of $\text{Pb}_3(\text{PO}_4)_2$

$\alpha \text{Pb}_3(\text{PO}_4)_2$		$\beta \text{Pb}_3(\text{PO}_4)_2$
Space groups	$R_{3m} - D_{3d}^5$	$C_{2c} - C_{2h}^0$
$a_H = (5,53 \pm 0,02)$ Å	$a_R = (7,48 \pm 0,03)$ Å	$a_m = (13,82 \pm 0,04)$ Å, ($a_m \approx 2/3 c_H$)
$c_H = (20,30 \pm 0,05)$ Å	$\alpha_R = (43,40 \pm 0,03)^\circ$	$b_m = (5,69 \pm 0,02)$ Å
		$c_m = (9,42 \pm 0,02)$ Å
		$\beta = (102,36 \pm 0,05)^\circ$
$V_H = (537 \pm 5)$ Å ³	$V_R = (179 \pm 8)$ Å ³	$V_m = (724 \pm 14)$ Å ³ , ($V_m \approx 3/4 V_H$)
$Z_H = 3$		$Z_m = 4$

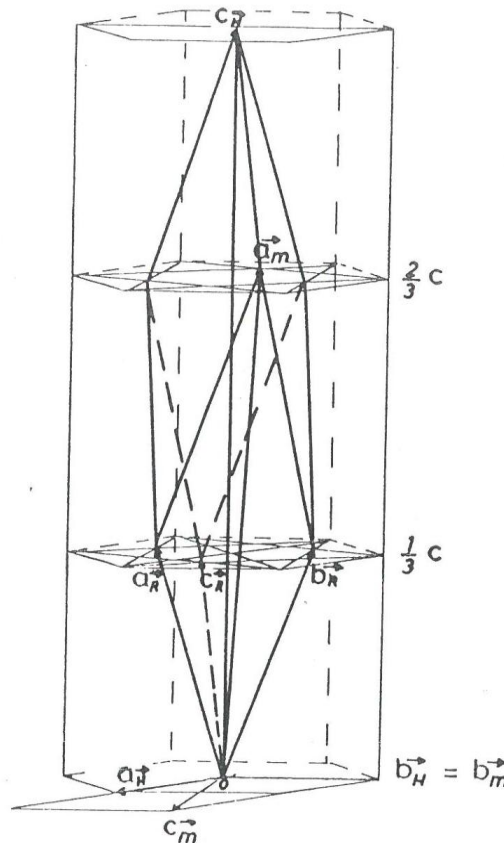
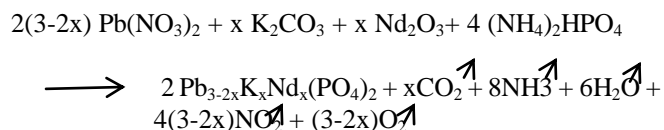


Fig. 3: Relationship between rhombohedral, hexagonal and monoclinic unit-cell of $\text{Pb}_3(\text{PO}_4)_2$

B. Preparation of the Phases $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$

We have synthesized the new $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ phases for $x = 0.05; 0.10; 0.15; 0.20; 0.25; 0.50$ and 0.75 . The starting materials required for the preparation of these compounds are $\text{Pb}(\text{NO}_3)_2$, K_2CO_3 , Nd_2O_3 and $(\text{NH}_4)_2\text{HPO}_4$. They are mixed

According to the reaction:



This stoichiometric mixture is well mixed and calcined at 400°C for 12 hours. It is then reground, pelletized

and then treated at 650 ° C for 4 days.

C. Radio crystallographic analysis

- Phase isotypes of $\alpha\text{Pb}_3(\text{PO}_4)_2$

The diffractograms of the $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ phases for $x = 0.20; 0.50; 0.75$ indicate isotype with structure $\text{Sr}_3(\text{PO}_4)_2$. The parameters a_H and c_H and the volume V_H are given in Table III. The analysis of the X spectra of these phases is recorded in appendix 1 to 4. It seems that the limit value of x (denoted x_1) for obtaining the solid solution is close to 0.75. Indeed, for values of x greater than 0.75, in particular for x equal to 1, the X-ray diffraction spectra indicate the presence of the limiting phase $\text{Pb}_{1.5}\text{K}_{0.75}\text{Nd}_{0.75}(\text{PO}_4)_2$ and phases $\text{K}_3\text{Nd}(\text{PO}_4)_2$ and NdPO_4 . When $x > 0.75$, obtaining the limiting composition $\text{Pb}_{1.5}\text{K}_{0.75}\text{Nd}_{0.75}(\text{PO}_4)_2$ can be schematized so :

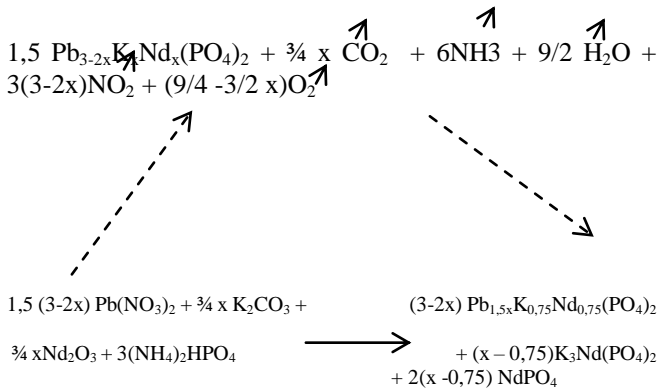


TABLE III: Parameters a_H and c_H and volume V_H of the solid solutions $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.20; 0.25; 0.50$ and 0.75

x	Phase	($a_H \pm 0,01$)Å	($c_H \pm 0,01$)Å	($V_H \pm 2$)Å ³
0,20	$\text{Pb}_{2,60}\text{K}_{0,20}\text{Nd}_{0,20}(\text{PO}_4)_2$	5,51	20,33	534
0,25	$\text{Pb}_{2,50}\text{K}_{0,25}\text{Nd}_{0,25}(\text{PO}_4)_2$	5,51	20,35	535
0,50	$\text{Pb}_{2,00}\text{K}_{0,50}\text{Nd}_{0,50}(\text{PO}_4)_2$	5,50	20,43	535
0,75	$\text{Pb}_{1,50}\text{K}_{0,75}\text{Nd}_{0,75}(\text{PO}_4)_2$	5,47	20,44	530

The evolution of the parameters a_H and c_H and the volume V_H of the phases $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.20; 0.25; 0.50$ and 0.75 is shown in fig. 4. When x increases, a_H decreases very slightly while c_H increases more substantially, V_H appears to decrease slightly. The variation of a_H is greater when x is greater than 0.50 while that of c_H is lower. The slight decrease in volume during the substitution of Pb^{2+} with K^+ and Nd^{3+} is in good agreement with the values of the ionic rays of these cations. Indeed, the mean ionic radius of K^+ and Nd^{3+} equal to 1.32 Å is slightly less than that of Pb^{2+} which is equal to 1.33 Å; $r_{\text{K}^+} = 1.55$ Å and $r_{\text{Nd}^{3+}} = 1.09$ Å [9].

$$\begin{pmatrix} a_m \\ b_m \\ c_m \end{pmatrix} \beta = \begin{pmatrix} -2/3 & -1/3 & 2/3 \\ 0 & 1 & 0 \\ 2 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_H \\ b_H \\ c_H \end{pmatrix} \alpha$$

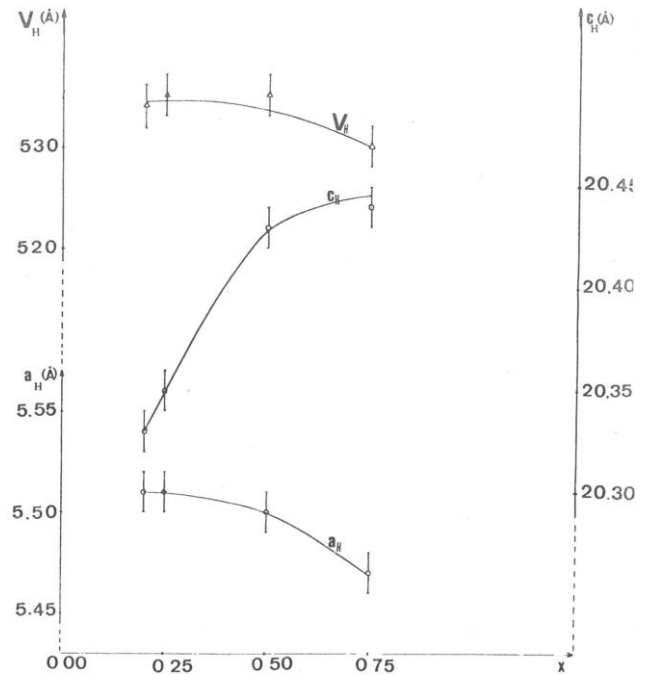


Fig. 4: The evolution of the parameters a_H and c_H and of the volume V_H of the solid solutions $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.20; 0.25; 0.50$ and 0.75 as a function of x

The diffractograms of the solid solutions $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.05; 0.10$ and 0.15 were indexed in the monoclinic system by isotype with $\beta \text{Pb}_3(\text{PO}_4)_2$. The parameters a_m, b_m, c_m and β and the volume V_m of their elementary meshes as well as those of the $\beta \text{Pb}_3(\text{PO}_4)_2$ phase are given in Table IV. The scans of the X spectra of these phases are shown in appendices 5 to 7.

TABLE IV: Parameters a_m, b_m, c_m and β and the volume V_m of the phases $\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.05; 0.10$ and 0.15

x	Phase	($a_m \pm 0,01$)Å	($b_m \pm 0,01$)Å	($c_m \pm 0,01$)Å	($\beta \pm 0,01$)°	($V_m \pm 4$)Å ³
0	$\text{Pb}_3(\text{PO}_4)_2$	13,82	5,69	9,43	102,36	724
0,05	$\text{Pb}_{2,90}\text{K}_{0,05}\text{Nd}_{0,05}(\text{PO}_4)_2$	13,82	5,66	9,44	102,54	721
0,10	$\text{Pb}_{2,80}\text{K}_{0,10}\text{Nd}_{0,10}(\text{PO}_4)_2$	13,86	5,63	9,47	102,70	722
0,15	$\text{Pb}_{2,70}\text{K}_{0,15}\text{Nd}_{0,15}(\text{PO}_4)_2$	13,88	5,56	9,52	102,81	716

The evolution of the parameters and the volume as a function of x is represented in figs. 5, 6 and 7. The parameters b_m, c_m and β increase slightly when x increases while a_m decreases. The volume decreases slightly as x increases; This fact is in agreement with the ionic rays of $\text{K}^+, \text{Nd}^{3+}$ and Pb^{2+} . Thus, the new phases

$\text{Pb}_{3-2x}\text{K}_x\text{Nd}_x(\text{PO}_4)_2$ for $x = 0.05; 0.10$ and 0.15 are isotypes of $\beta \text{Pb}_3(\text{PO}_4)_2$, while those for $x = 0.20; 0.25; 0.50$ and 0.75 are isotypes of $\alpha \text{Pb}_3(\text{PO}_4)_2$. The transition from $\beta \text{Pb}_3(\text{PO}_4)_2$ to $\alpha \text{Pb}_3(\text{PO}_4)_2$, which was only possible by raising the temperature up to 200 ° C, also became possible by substituting lead for potassium and neodymium from O_f x close to 0.20.

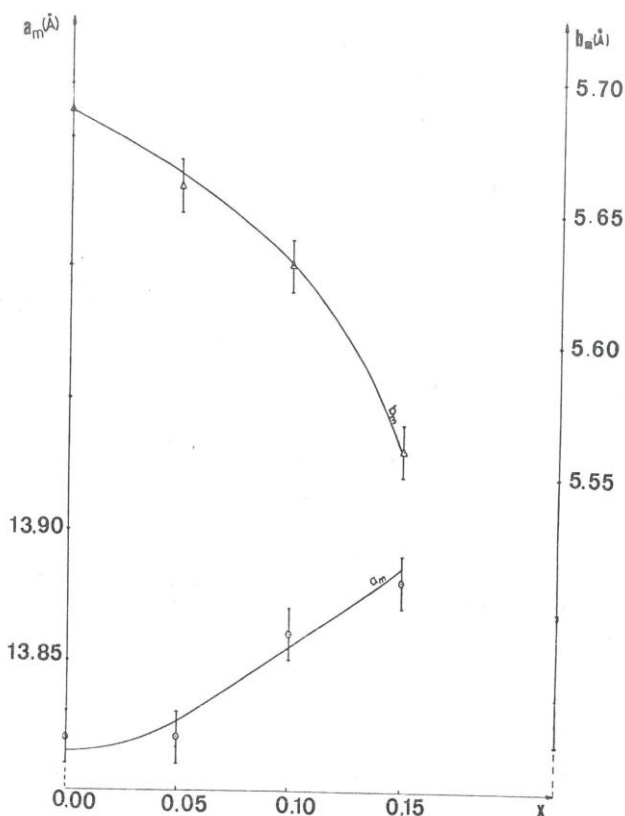


Fig. 5: Evolution of the parameters a_m and b_m of the solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10$ and 0.15 as a function of x

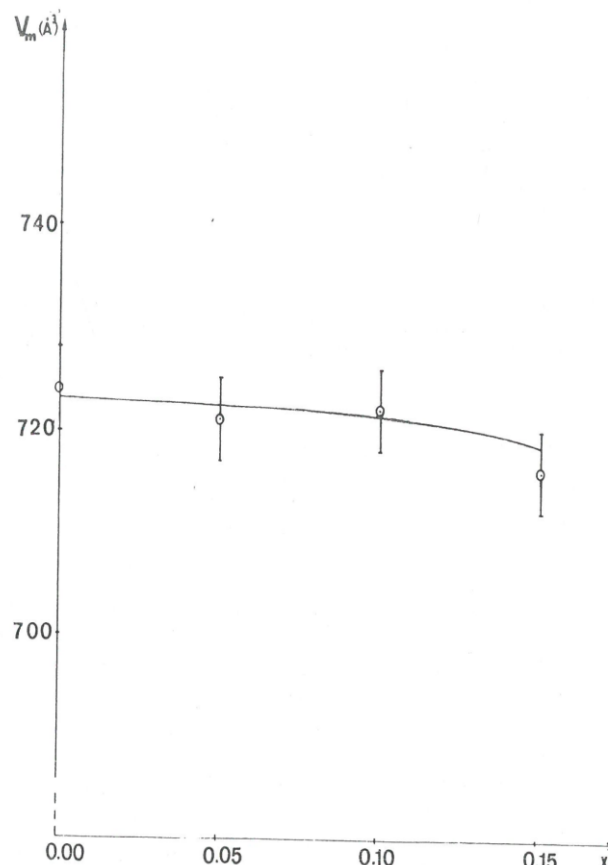


Fig. 7: Evolution of the volume V_m of the solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10$ and 0.15 as a function of x

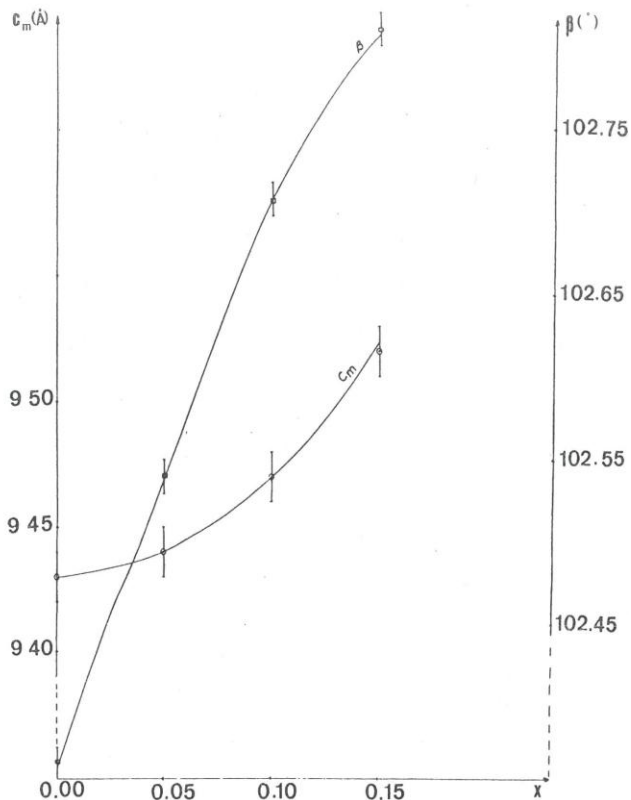


Fig. 6: Evolution of the parameters c_m and β of the solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10$ and 0.15 as a function of x

IV. CONCLUSION

We have synthesized the new solid solutions $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10; 0.15; 0.20; 0.25; 0.50$ and 0.75 . These were obtained from $Pb_3(PO_4)_2$ according to the substitution scheme: $2xPb^{2+} = xK^+ + xNd^{3+}$

The new phases $Pb_{3-2x}K_xNd_x(PO_4)_2$ for $x = 0.05; 0.10$ and 0.15 are isotypes of $\beta Pb_3(PO_4)_2$, those for $x = 0.20; 0.25; 0.50$ and 0.75 are isotypes of $Sr_3(PO_4)_2$. Substitution of Pb^{2+} with K^+ and Nd^{3+} results in a slight decrease in volume; Which is consistent with the mean value of the ionic rays of potassium and neodymium which is slightly less than the ionic radius of the lead.

The monoclinic-rhombohedral transition takes place at $200^\circ C$. for the $Pb_3(PO_4)_2$ phase. For the solid solution $Pb_{3-2x}K_xNd_x(PO_4)_2$, the rhombohedral phase is stable at room temperature for values of $x \geq 0.20$. The monoclinic-rhombohedral transition temperature should decrease continuously when the substitution rate x of lead ranges from 0 to 0.15. This should be confirmed by X-ray diffraction study at high temperature. Similarly, we can imagine that the rhombohedral phases corresponding to $x \geq 0.20$ at ambient temperature will become monoclinic below ambient temperature at lower temperatures as x is high.

APPENDIX: THE ANALYSIS OF THE X SPECTRA OF THE PHASES

1) The analysis of the X spectra of the $Pb_{2.6}K_{0.2}Nd_{0.2}(PO_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
15	4,650	4,646	1 0 1
<5	4,317	4,139	0 1 2
40	3,479	3,479	1 0 4
100	3,096	3,095	0 1 5
50	2,758	2,755	1 1 0
<5	2,484	2,481	1 0 7
<5	2,374	2,370	0 2 1
<5	2,328	2,323	2 0 2
30	2,258	2,259	0 0 9
10	2,165	2,160	0 2 4
<5	2,139	2,137	1 1 6
20	2,060	2,058	2 0 5
30	1,871	1,870	1 0 10
<5	1,799	1,796	2 1 1
15	1,748	1,747	1 1 9
<5	1,739	1,739	2 0 8
<5	1,702	1,700	2 1 4
10	1,649	1,649	1 2 5
5	1,590	1,590	3 0 0

2) The analysis of the X spectra of the $Pb_{2.50}K_{0.25}Nd_{0.25}(PO_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
25	4,649	4,646	1 0 1
5	4,232	4,320	0 1 2
50	3,480	3,480	1 0 4
100	3,097	3,097	0 1 5
70	2,757	2,755	1 1 0
5	2,482	2,483	1 0 7
5	2,370	2,370	0 2 1
5	2,321	2,323	2 0 2
40	2,260	2,261	0 0 9
17	2,161	2,160	0 2 4
5	2,139	2,138	1 1 6
35	2,059	2,058	2 0 5
40	1,872	1,872	1 0 10
5	1,797	1,796	2 1 1
25	1,748	1,748	1 1 9
5	1,738	1,740	2 0 8
5	1,701	1,700	2 1 4
15	1,648	1,649	1 2 5
5	1,592	1,591	3 0 0

3) The analysis of the X spectra of the $Pb_{2.0}K_{0.5}Nd_{0.5}(PO_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
25	4,644	4,639	1 0 1
<5	4,315	4,317	0 1 2
33	3,485	3,483	1 0 4
100	3,102	3,101	0 1 5
70	2,749	2,750	1 1 0
<5	2,488	2,488	1 0 7
<5	2,364	2,365	0 2 1
7	2,320	2,319	2 0 2
20	2,270	2,270	0 0 9

15	2,158	2,158	0 2 4
5	2,139	2,139	1 1 6
30	2,057	2,057	2 0 5
25	1,877	1,877	1 0 10
<5	1,790	1,793	2 1 1
20	1,750	1,751	1 1 9
<5	1,746	1,742	2 0 8
15	1,698	1,698	2 1 4
8	1,647	1,647	1 2 5
5	1,587	1,588	3 0 0
5	1,550	1,551	0 2 10

4) The analysis of the X spectra of the $Pb_{1.50}K_{0.75}Nd_{0.75}(PO_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
24	4,605	4,607	1 0 1
<5	4,294	4,291	0 1 2
40	3,470	3,470	1 0 4
100	3,092	3,092	0 1 5
92	2,732	2,730	1 1 0
<5	2,484	2,484	1 0 7
<5	2,347	2,348	0 2 1
7	2,305	2,303	2 0 2
20	2,271	2,271	0 0 9
20	2,148	2,146	0 2 4
8	2,132	2,130	1 1 6
36	2,048	2,047	2 0 5
30	1,877	1,876	1 0 10
<5	1,784	1,780	2 1 1
20	1,747	1,746	1 1 9
10	1,738	1,735	2 0 8
5	1,688	1,687	2 1 4
18	1,637	1,637	1 2 5
10	1,578	1,576	3 0 0
5	1,547	1,546	0 2 10

5) The analysis of the X spectra of the $Pb_{2.85}K_{0.05}Nd_{0.05}(PO_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
20	4,712	4,714	-1 1 1
15	4,608	4,607	0 0 2
5	4,380	4,386	1 1 1
<5	4,262	4,260	-2 0 2
10	3,606	3,608	-1 1 2
20	3,519	3,521	3 1 0
65	3,490	3,493	-3 1 1
40	3,478	3,470	2 0 2
<5	3,313	3,318	1 1 2
100	3,117	3,117	3 1 1
65	3,056	3,056	-4 0 2
25	2,828	2,830	0 2 0
85	2,752	2,750	-1 1 3
15	2,703	2,705	0 2 1
5	2,570	2,568	-2 2 1
10	2,480	2,477	4 0 2
5	2,410	2,411	0 2 2
5	2,354	2,357	-2 2 2

Crystallochemistry of New Isotypes of $\text{Sr}_3(\text{PO}_4)_2$

<5	2,344	2,341	-2 0 4
<5	2,307	2,304	0 0 4
50	2,250	2,248	6 0 0
15	2,193	2,193	2 2 2
10	2,174	2,176	-1 1 4
5	2,141	2,141	3 1 3
10	2,130	2,130	-4 0 4
30	2,076	2,076	-4 2 2

<5	2,362	2,362	-2 2 2
<5	2,331	2,334	-2 0 4
5	2,321	2,321	0 0 4
75	2,256	2,256	6 0 0
10	2,185	2,185	2 2 2
7	2,173	2,173	-1 1 4
10	2,148	2,149	3 1 3
10	2,145	2,143	-4 0 4
20	2,063	2,063	-4 2 2

6) The analysis of the X spectra of the $\text{Pb}_{2,80}\text{K}_{0,10}\text{Nd}_{0,10}(\text{PO}_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
15	4,700	4,703	-1 1 1
10	4,627	4,620	0 0 2
<5	4,378	4,374	1 1 1
<5	4,280	4,277	-2 0 2
<5	3,606	3,607	-1 1 2
15	3,519	3,518	3 1 0
45	3,490	3,493	-3 1 0
25	3,475	3,475	-3 1 1
<5	3,315	3,316	2 0 2
100	3,116	3,115	1 1 2
50	3,069	3,068	3 1 1
15	2,816	2,815	-4 0 2
55	2,756	2,753	0 2 0
<5	2,691	2,693	-1 1 3
<5	2,560	2,559	0 2 1
10	2,481	2,480	-2 2 1
<5	2,402	2,404	4 0 2
<5	2,350	2,351	0 2 2
<5	2,348	2,349	-2 2 2
<5	2,310	2,309	-2 0 4
70	2,254	2,253	0 0 4
10	2,189	2,187	6 0 0
10	2,181	2,180	2 2 2
10	2,174	2,176	-1 1 4
10	2,144	2,142	3 1 3
10	2,139	2,138	-4 0 4
20	2,074	2,074	-4 2 2

7) The analysis of the X spectra of the $\text{Pb}_{2,70}\text{K}_{0,15}\text{Nd}_{0,15}(\text{PO}_4)_2$ phase

I/I_0	dobs (Å)	dcal (Å)	h k l
15	4,669	4,668	-1 1 1
<5	4,640	4,641	0 0 2
5	4,348	4,346	1 1 1
<5	4,296	4,298	-2 0 2
		3,600	-1 1 2
30	3,502	3,503	3 1 0
50	3,482	3,482	-3 1 1
		3,484	2 0 2
5	3,310	3,310	1 1 2
100	3,106	3,106	3 1 1
50	3,081	3,078	-4 0 2
20	2,781	2,780	0 2 0
50	2,757	2,756	-1 1 3
<5	2,664	2,663	0 2 1
5	2,539	2,533	-2 2 1
7	2,480	2,484	4 0 2
<5	2,385	2,385	0 2 2

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