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SUPPLEMENTARY MATERIAL TO

Search for new apatite-like phases for lead utilization based on crystal structure and thermal expansion

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TABLE S-I. X-ray fluorescence analysis data for synthesized compounds.

Compound	PbO / wt%		SiO_2 / wt%		GeO_2 / wt%		P_2O_5 / wt%		SO_3 / wt%		CrO_3 / wt%	
	found	calc	found	calc	found	calc	found	calc	found	calc	found	calc
$Pb_5(SiO_4)(PO4)_2$	84.68	84.67	4.54	4.56			10.78	10.77				
$Pb_5(GeO_4)(PO4)_2$	81.92	81.91			7.66	7.68	10.42	10.42				
$Pb_5(GeO_4)_2(SO_4)$	79.42	79.41			14.82	14.89			5.76	5.70		
$Pb_5(GeO_4)_2(CrO_4)$	78.3	78.3			14.7	14.68					7.00	7.02

Standard uncertainties u are u(wt) = 0.02%.

TABLE S-II. Assignment of lines in IR spectra of mixed-tetrahedral apatites under study

Assignment	$Pb_5(SiO_4)(PO4)_2$	$Pb_5(GeO_4)(PO4)_2$	$Pb_5(GeO_4)_2(SO_4)$	$Pb_5(GeO_4)_2(CrO_4)$
ν (SiO_4)	850 s 827 m			
δ (SiO_4)	514 m 475 m			
ν (GeO_4)		724 m 703 m	730 m 708 sh	728 m 699 sh
δ (GeO_4)		416 m	411 m	412 m
ν (PO_4)	1097 sh 1056 sh 1021 s 970 s 932 sh 888 sh 870 sh 852 s 832 sh	1104 w 1061 sh 1015 s 964 s 932 sh 870 m 827 sh		
δ (PO_4)	572 s 550 m 538 m	570 s 549 m 538 m		
ν (SO_4)			1128 m 1026 m 963 m 896 w	
δ (SO_4)			876 w 617 m 602 m 520 w	
ν (CrO_4)				1126 m 1100 sh 1085 sh 1030 w
δ (CrO_4)				622 w 527 sh

s – strong, m – medium, w – weak, sh - shoulder

TABLE S-III. Temperature dependencies of linear thermal expansion coefficients for "classical" apatites (column 1-5), mixed-tetrahedral apatites (column 6-9), solid solutions in $(Ca_xPb_{1-x})_5(PO_4)_3Cl$ (column 10-12) and $(Ca_xPb_{1-x})_4Bi_2(PO_4)_6O$ (column 13-15) systems

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
T (K)	PbPF	PbPCl	PbPI	PbVF	PbVCl	PbSiP2	PbGeP2	PbGe2S	PbGe2Cr	Ca3.5Pb1.5	Ca2.5Pb2.5	Ca1.25Pb3.75	Ca6Pb2Bi2	Ca4Pb4Bi2	Ca2Pb6Bi2
									α_a (K^{-1})·10^6						
298	9.7	13.5	-1.0	15.3	12.2	15.2	14.3	16.4	17.3	13.0	6.4	11.7	11.0	12.5	12.5
373	10.9	13.8	1.6	15.3	12.5	15.6	14.7	17.1	17.8	13.6	9.6	12.2	11.6	13.1	13.1
473	12.5	14.2	5.0	15.4	13.0	16.2	15.3	18.0	18.4	14.5	13.9	12.8	12.3	13.8	13.9
573	14.0	14.6	8.5	15.4	13.4	16.7	15.8	18.9	19.0	15.5	18.2	13.4	13.0	14.6	14.6
673	15.6	15.0	11.9	15.5	13.9	17.3	16.3	19.8	19.6	16.4	22.4	14.0	13.8	15.3	15.4
773	17.1	15.4	15.3	15.5	14.3	17.8	16.8	20.7	20.1	17.2	26.6	14.7	14.5	16.1	16.1
873	18.7	15.8	18.7	15.6	14.8	18.3	17.3	21.6	20.7	18.1	30.8	15.3	15.2	16.8	16.9
									α_c (K^{-1})·10^6						
298	10.5	12.0	3.1	9.9	22.1	16.0	15.1	16.3	19.5	9.7	3.3	11.2	10.1	9.6	13.0
373	13.0	13.9	6.4	11.8	23.0	17.4	16.4	17.8	20.7	11.0	8.8	12.7	11.4	11.7	14.5
473	16.3	16.5	10.9	14.4	24.2	19.2	18.1	19.8	22.4	12.8	16.0	14.7	13.3	14.6	16.5
573	19.5	19.0	15.4	16.9	25.3	21.0	19.8	21.9	24.0	14.6	23.2	16.7	15.1	17.4	18.5
673	22.8	21.5	19.8	19.5	26.5	22.8	21.5	23.9	25.6	16.3	30.4	18.7	16.9	20.2	20.4
773	26.0	24.0	24.2	22.0	27.6	24.6	23.2	25.9	27.2	18.1	37.5	20.7	18.7	23.0	22.4
873	29.2	26.5	28.6	24.5	28.8	26.3	24.9	27.9	28.8	19.8	44.5	22.7	20.5	25.8	24.3

Standard uncertainties u are u(wt) = 0.02%.