

Electronic Supplementary Information

Single-crystal microtubes of a novel apatite-type compound, (Na_{2.5}Bi_{2.5})(PO₄)₃(F,OH), with well-faceted hexagonal cross sections

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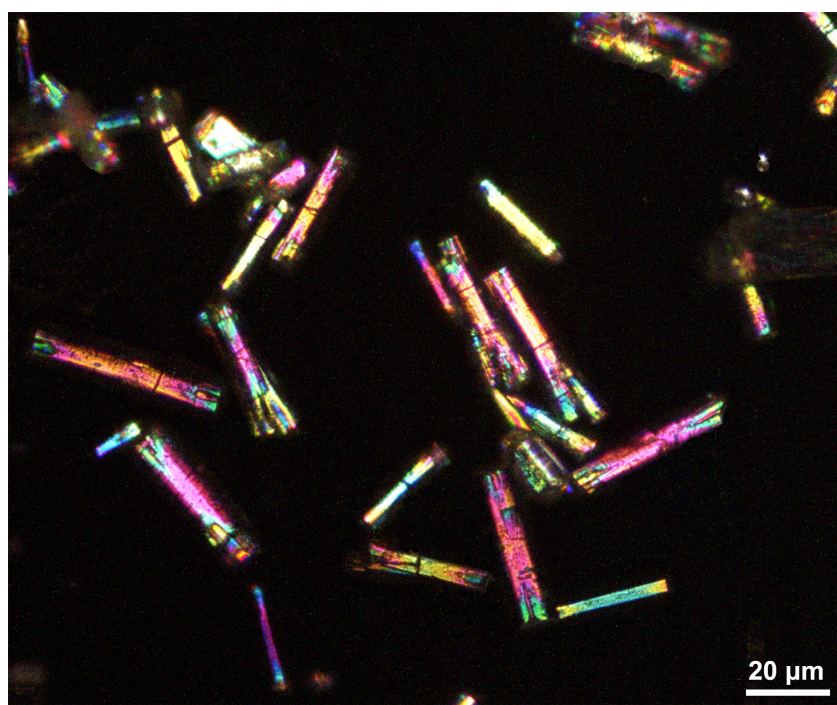
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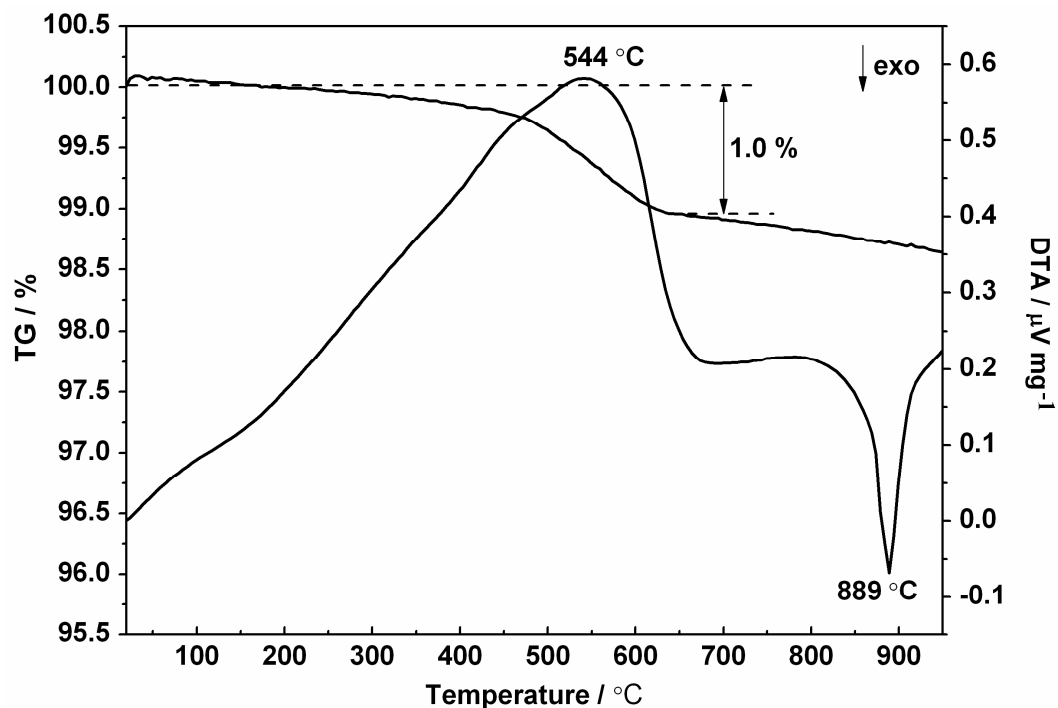
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ESI Table 1. Atomic Coordinates and Equivalent/Isotropic Displacement Parameters ($\text{\AA}^2$)
for $(\text{Na}_{2.5}\text{Bi}_{2.5})(\text{PO}_4)_3(\text{F},\text{OH})$

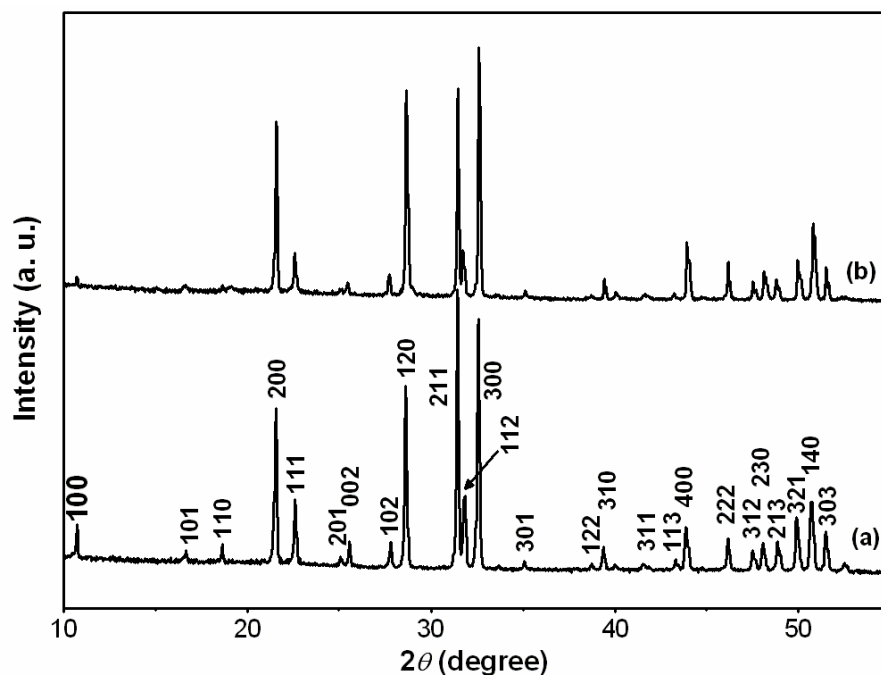
Atoms	Wyck.	x/a	y/b	z/c	U	S.O.F.
Bi1	6c	0.24806(14)	0.24318(13)	0.6490(7)	0.0238(4)	0.608(11)
Na1	6c	0.24806(14)	0.24318(13)	0.6490(7)	0.0238(4)	0.392(11)
Bi2	2b	2/3	1/3	0.4014(3)	0.0229(18)	0.447(13)
Na2	2b	2/3	1/3	0.4014(3)	0.0229(18)	0.553(13)
Bi3	2b	2/3	1/3	0.9186(8)	0.011(2)	0.231(9)
Na3	2b	2/3	1/3	0.9186(8)	0.011(2)	0.769(9)
P1	6c	0.6240(5)	0.5994(5)	0.6361(13)	0.0060(11)	1
O1	6c	0.727(3)	0.640(3)	0.459(3)	0.028(6)	1
O2	6c	0.5141(13)	0.6741(14)	0.659(4)	0.015(3)	1
O3	6c	0.5210(15)	0.4123(14)	0.631(4)	0.017(3)	1
O4	6c	0.756(2)	0.677(2)	0.819(3)	0.016(5)	1
F1	2a	0	0	0.732(4)	0.024(7)	0.1
O5	2a	0	0	0.732(4)	0.024(7)	0.9



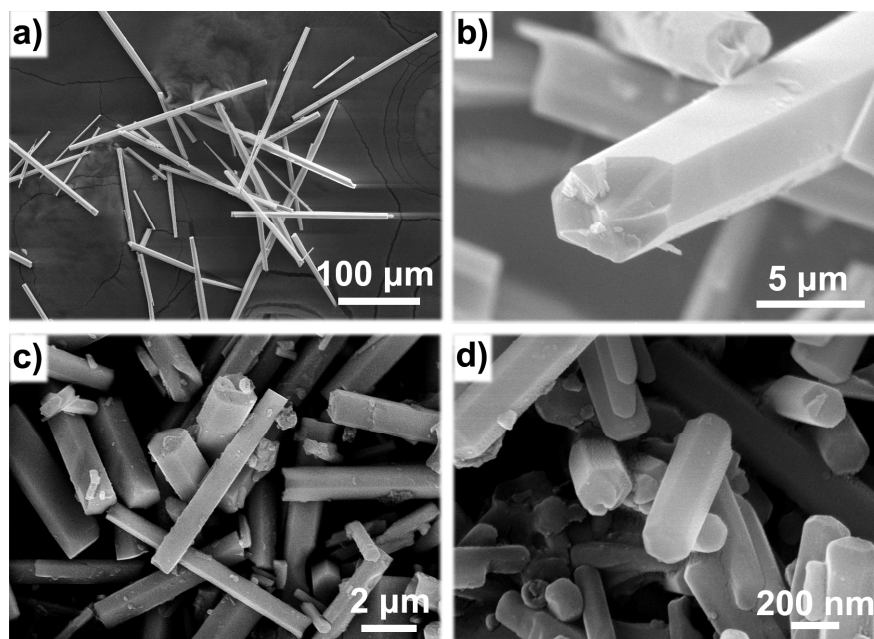
ESI Figure 1 Optical micrograph of the $(\text{Na}_{2.5}\text{Bi}_{2.5})(\text{PO}_4)_3(\text{F},\text{OH})$ (NBPF) microtubes under the microscope with polarized light. Optical continuity and extinction every 90° of rotation indicate that they are single crystals.



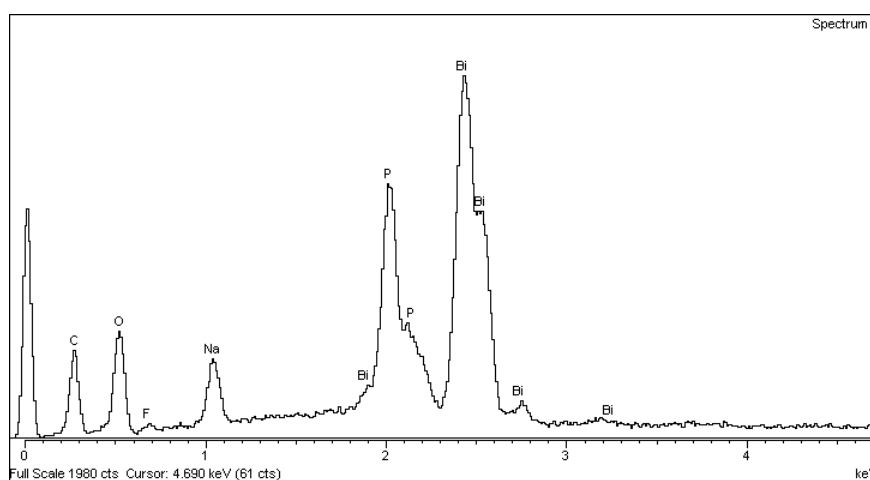
ESI Figure 2 TG-DTA curve of NBPF (heating rate $10\text{ }^{\circ}\text{C min}^{-1}$; atmosphere: argon). 1.0 % weight loss associated with the endothermic peak at 544 °C in the DTA curve is in agreement with the calculated weight loss of one H_2O per $(\text{Na}_{2.5}\text{Bi}_{2.5})(\text{PO}_4)_3(\text{F},\text{OH})$ unit. The exothermic peak at 889 °C accounts for a phase transition.



ESI Figure 3 PXRD patterns of the $(\text{Na}_{2.5}\text{Bi}_{2.5})(\text{PO}_4)_3(\text{F},\text{OH})$ microtubes (NBPF) (a) non-annealed sample, (b) after thermal treatment at 650 °C.



ESI Figure 4 SEM images of $(\text{Na}_{2.5}\text{Bi}_{2.5})(\text{PO}_4)_3(\text{OH})$ (a, b, c) microrods without addition of any fluoride as reactants, and NBPF submicrorods (d), synthesized at the pH range of 6.5-7.0 at 180 °C for 48h: (a) needles; the reactants including Bi_2O_3 , $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$ and $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ with a reaction concentration (Bi^{3+} for example) about $0.05 \text{ mol} \cdot \text{L}^{-1}$ (b) microrods; the reactants including Bi_2O_3 and $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ with a reaction concentration (Bi^{3+} for example) about $0.05 \text{ mol} \cdot \text{L}^{-1}$ (c) microrods; the reactants including Bi_2O_3 , $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$, $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ and polyacrylamide, with a reaction concentration (Bi^{3+} for example) about $0.05 \text{ mol} \cdot \text{L}^{-1}$ (d) submicrorods; the reactants including Bi_2O_3 , $\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$, $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ and NaBF_4 with a reaction concentration (Bi^{3+} for example) about $0.20 \text{ mol} \cdot \text{L}^{-1}$



ESI Figure 5 EDS spectrum from the Figure 3c microrod carried out at the cross section of hexagonal morphology shows the characteristic peaks of Na, Bi, P, O and F.