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Synthesis and structure of the new layered potassium sodiostannate

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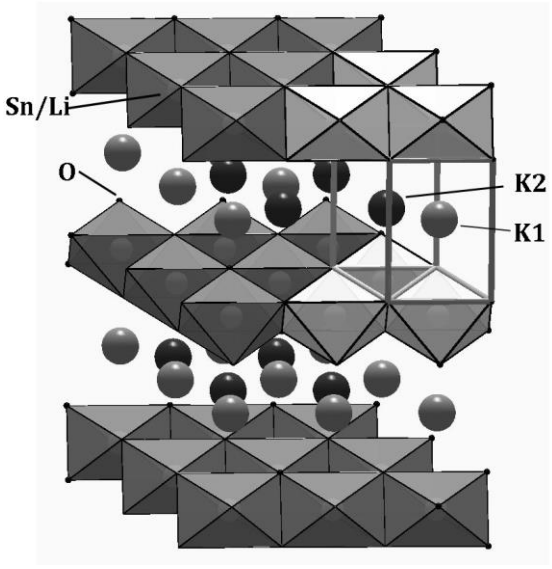

Figure S1 Model of $K_{0.72}Li_{0.24}Sn_{0.76}O_2$. Octahedra are $Sn(Li)O_6$ groups. Ions K positions between layers are shown as spheres: dark spheres represent ions in the "main" prisms, light ones – in the "additional".

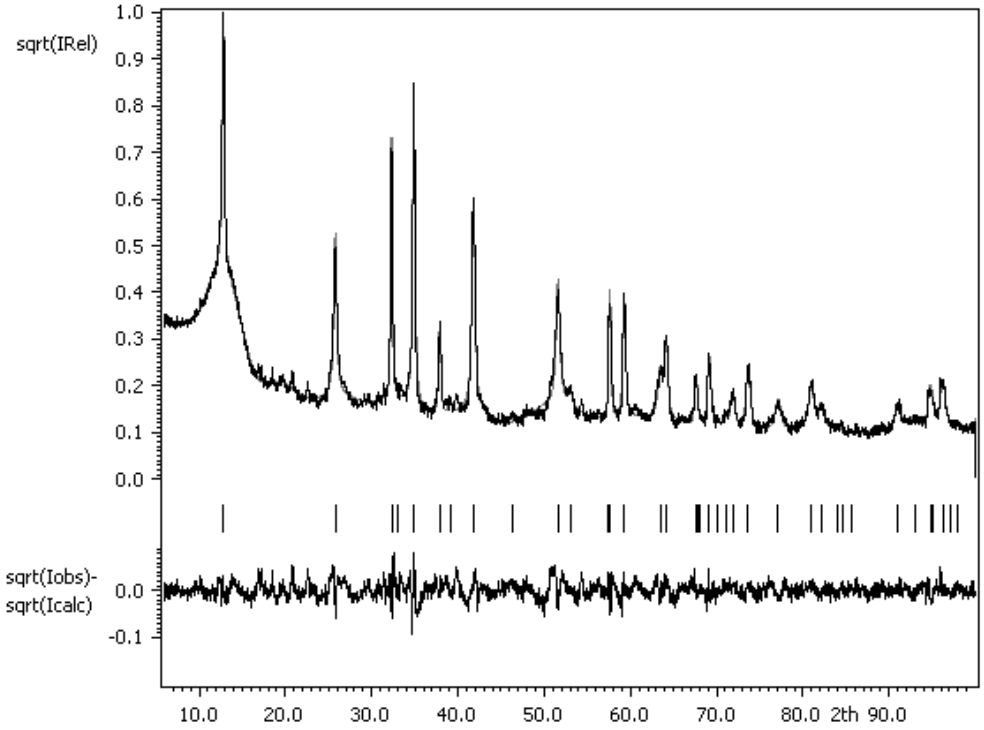

Figure S2 Calculated and observed powder XRD patterns of $K_{0.72}Na_{0.24}Sn_{0.76}O_2$. The difference is plotted.

Table S1 Atomic coordinates and displacement parameters for $K_{0.72}Na_{0.24}Sn_{0.76}O_2$

* U22=U11, U12=0.5U11, U13=U23=0
**U 12=0.5U22, U13=U23=0
*** Formula from occupation values: $K_{0.78}Na_{0.221}Sn_{0.755}O_2$

position (site)	x	y	z	occup.***	displacement parameters, Å^2	
Sn(2a)	0	0	0	0.742(3)	U11*	0.0065(19)
					U33	0.020(3)
Na(2a)	0	0	0	0.206(4)	U11*	0.029(8)
					U33	0.031(13)
Na21 (6h)	0.706(4)	0.413(8)	1/4	0.0163(8)	U11	0.037(7)
					U22**	0.026(10)
					U33	0.03(2)
K1(4e)	0	0	0.2026(17)	0.092(3)	U11*	0.065(7)
					U33	0.07(2)
K11 (6h)	0.7857(4)	0.5714(8)	1/4	0.0485(5)	U11	0.070(2)
					U22**	0.0373(13)
					U33	0.045(5)
K21 (6h)	0.2199(4)	0.4397(7)	3/4	0.1278(12)	U11	0.0613(19)
					U22**	0.0562(14)
					U33	0.024(4)
O(4f)	1/3	2/3	0.0744(7)	1	Uiso	0.015(2)

Table S2 Selected interatomic distances (Å) in $K_{0.72}Na_{0.24}Sn_{0.76}O_2$

	interatomic distances	ionic radii sum, CN(metal) = 6; CN(O) = 4
Sn – O	2.12	0.83+1.24=2.07
Na – O	2.12	1.16+1.24=2.40
K2 (Na1) – O	4 · 2.89 2 · 3.46	1.52 (1.16)+1.24=2.76 (2.4)
K1 – O	3 · 2.51 3 · 3.60	1.52+1.24=2.76
K11 – O	2 · 2.70 4 · 3.26	

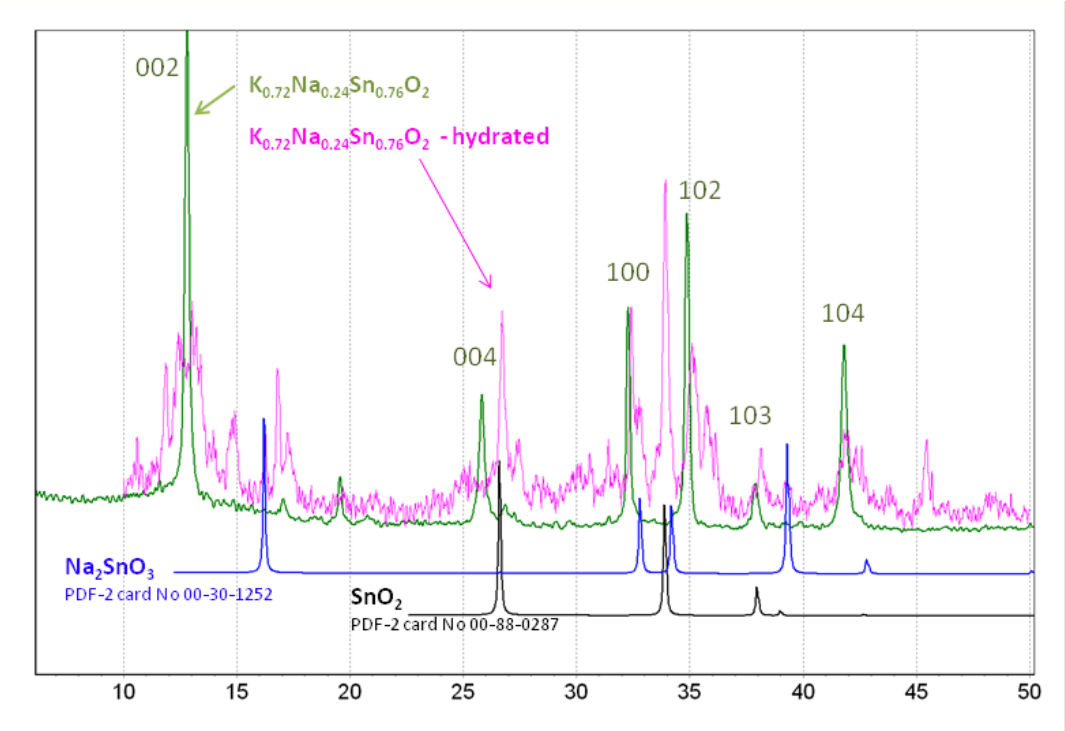

Figure S3 Powder profiles revealing phase changes with $K_{0,72}Na_{0,24}Sn_{0,76}O_2$ after hydration process. Green profile – fresh obtained sample, pink placed in water and dried in air, blue and black profiles of sodium stannate and tin oxide from database, respectively.