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Supporting Information

Topochemical Synthesis of Alkali-Metal Hydroxide Layers within Double- and Triple-Layered Perovskites

Dariusz Montasserasadi,[†] Debasish Mohanty,[‡] Ashfia Huq,[‡] Luke Heroux,[‡] Edward Andrew Payzant,[‡] and John B. Wiley*,[†]

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Experimental setup for formation of hydroxide and deuterioxide compounds.

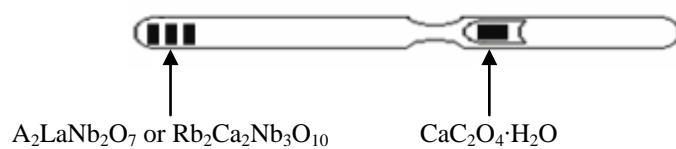


Figure S1. Sealed Pyrex tube for carrying out oxidative intercalation of $A_2\text{LaNb}_2\text{O}_7$ and $\text{Rb}_2\text{Ca}_2\text{Nb}_3\text{O}_{10}$ with water where on heating, $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ decomposes to release a stoichiometric amount of water.

X-ray diffraction data on double-layered potassium compounds KLaNb_2O_7 , $\text{K}_2\text{LaNb}_2\text{O}_7$, and $(\text{K}_2\text{OH})\text{LaNb}_2\text{O}_7$.

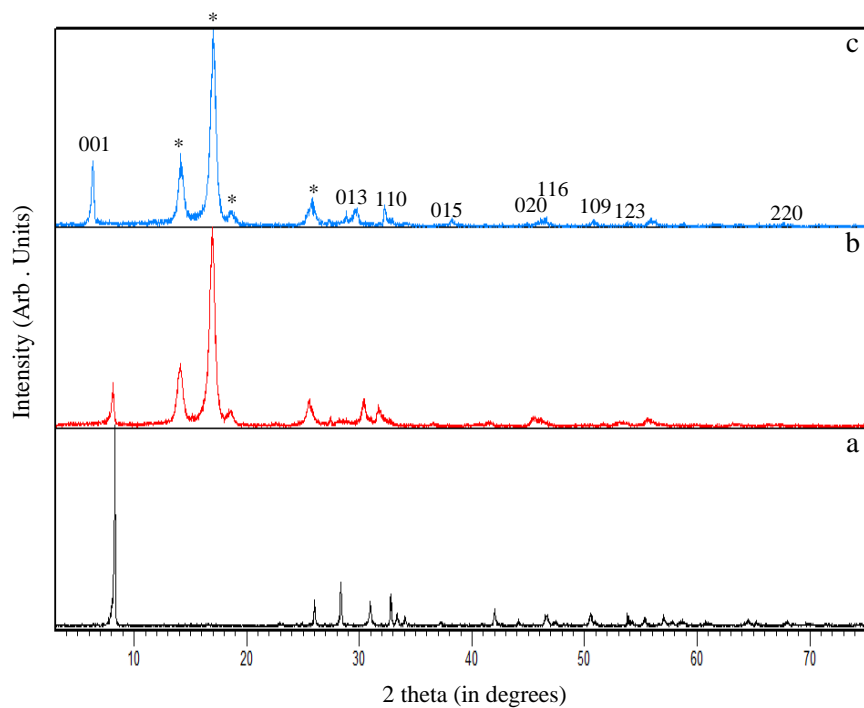


Figure S2. X-ray powder diffraction patterns of for a) KLaNb_2O_7 , b) $\text{K}_2\text{LaNb}_2\text{O}_7$, and c) $(\text{K}_2\text{OH})\text{LaNb}_2\text{O}_7$.

X-ray diffraction data on triple-layered compounds $\text{RbCa}_2\text{Nb}_3\text{O}_{10}$ and $(\text{Rb}_2\text{OH})\text{Ca}_2\text{Nb}_3\text{O}_{10}$.

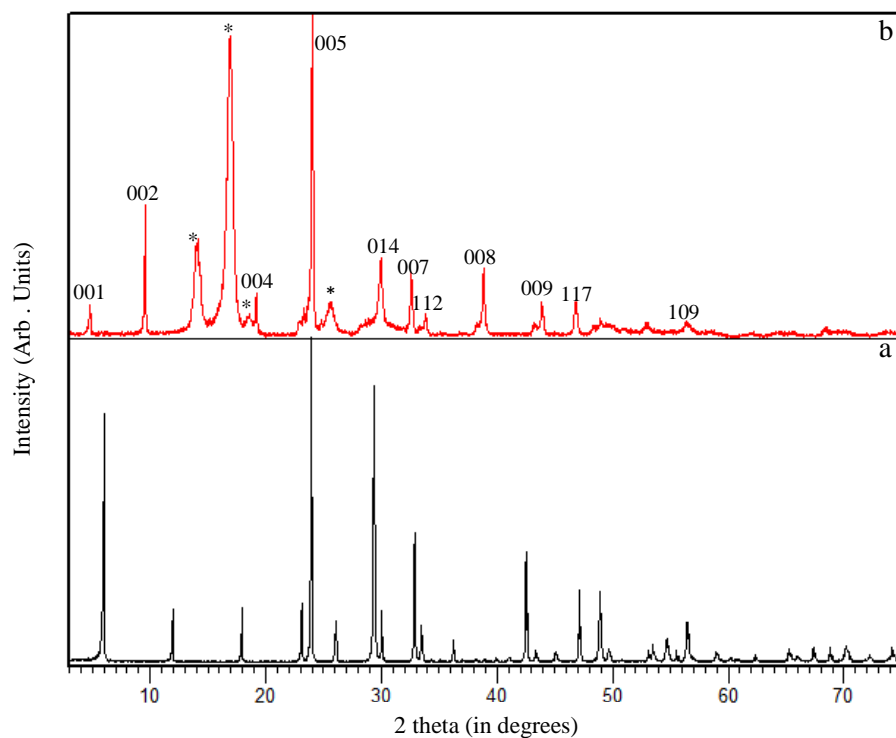


Figure S3. X-ray powder diffraction patterns for a) $\text{RbCa}_2\text{Nb}_3\text{O}_{10}$ and b) $(\text{Rb}_2\text{OH})\text{Ca}_2\text{Nb}_3\text{O}_{10}$. Asterisk (*) indicates polypropylene film peaks. Selected indices are highlighted for $(\text{Rb}_2\text{OH})\text{Ca}_2\text{Nb}_3\text{O}_{10}$.

Rietveld refinement of $(\text{Rb}_2\text{OH})\text{LaNb}_2\text{O}_7$ X-ray diffraction data

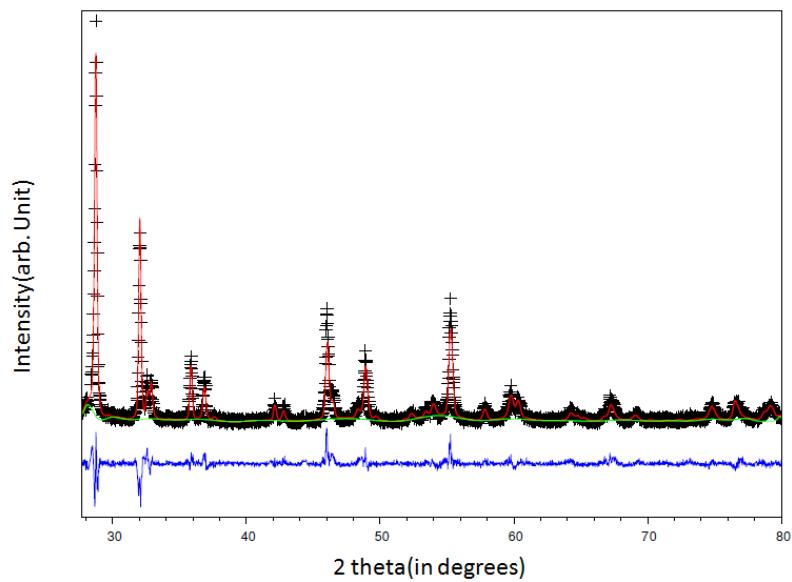


Figure S4. Observed and calculated data for the Rietveld refinement of $(\text{Rb}_2\text{OH})\text{LaNb}_2\text{O}_7$ X-ray diffraction data. Observed data are indicated by crosses, calculated pattern by a red solid line, the bottom blue curve is the difference plot and the green is the background.

Tabulation of Crystallographic Data for (Rb₂OH)LaNb₂O₇ from Rietveld refinement of X-ray data.

Table S1.Crystallographic Data for (Rb₂OH)LaNb₂O₇ from X-ray data.

Atom	Site	x	y	z	U _{iso} (Å ²)	g
Rb	2g	0	0	0.3313(5)	0.02(1)	1
O ₄	1d	0.5	0.5	0.5	0.02(2)	1
La	1a	0	0	0	0.0001(5)	1
Nb	2h	0.5	0.5	0.1465(4)	0.001(2)	1
O ₁	2h	0.5	0.5	0.278(2)	0.001(2)	1
O ₂	1c	0.5	0.5	0	0.003(5)	1
O ₃	4i	0	0.5	0.129(2)	0.001(4)	1

P4/mmm; Z = 1, a = 3.9303(1) Å, c = 14.9624(9) Å, Volume = 231.13(2) Å³

R_p = 15.0%, R_{wp} = 19.4%, χ^2 = 1.68, and g = occupation factor

Rietveld refinement of $(\text{Rb}_2\text{OH})\text{LaNb}_2\text{O}_7$ Neutron diffraction data

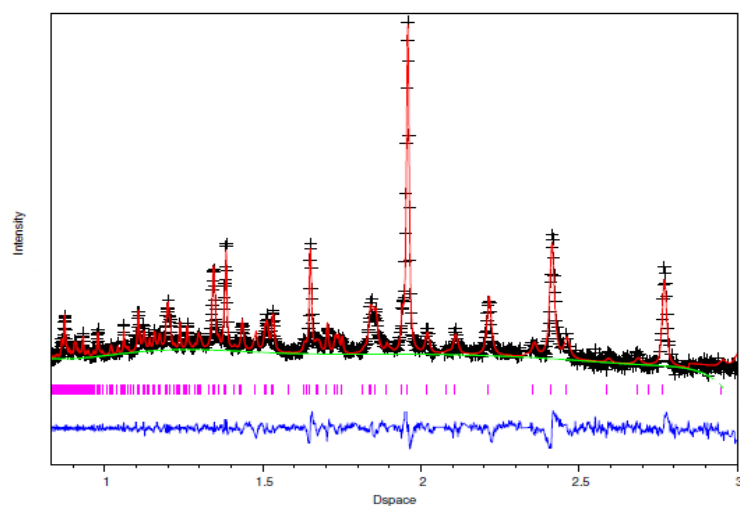


Figure S6. Observed and calculated data for the Rietveld refinement of $(\text{Rb}_2\text{OH})\text{LaNb}_2\text{O}_7$ neutron diffraction data. Observed data are indicated by crosses, calculated pattern by a red solid line, the bottom blue curve is the difference plot, and the green curve is the background. Reflection at $\sim 2.2 \text{ \AA}$ is attributed to the vanadium sample holder.

Tabulation of crystallographic data from neutron diffraction for (Rb₂OH)LaNb₂O₇

Table S2.Crystallographic Data for (Rb₂OH)LaNb₂O₇ from neutron data.

Atom	Site	x	y	z	U _{iso} (Å ²)	g
Rb	2g	0	0	0.3531(7)	0.021(1)	1
La	1a	0	0	0	0.006(2)	1
Nb	2h	0.5	0.5	0.1502(5)	0.007(2)	1
O ₁	2h	0.5	0.5	0.2651(6)	0.032(2)	1
O ₂	1c	0.5	0.5	0	0.028(4)	1
O ₃	4i	0	0.5	0.1283(4)	0.014(1)	1
O ₄	1d	0.5	0.5	0.5	0.066(7)	1
H	4o	0.25	0.5	0.5	0.026(2)	0.25

P4/mmm; Z = 1, a = 3.9132(1) Å, c = 14.757(1) Å, Volume = 225.97(1) Å³

R_p = 5.15%, R_{wp} = 3.52%, χ^2 = 4.29, and g = occupation factor