ChemInform Abstract: Topochemical Synthesis of Alkali-Metal Hydroxide Layers within Double- and Triple-Layered Perovskites.

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Supporting Information

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

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

Experimental setup for formation of hydroxide and deuteroxide compounds.

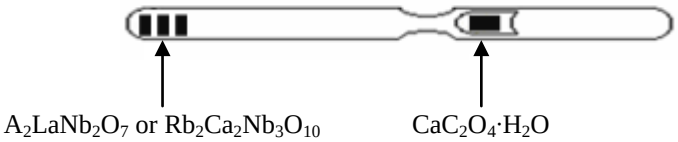

Figure S1. Sealed Pyrex tube for carrying out oxidative intercalation of $A_2LaNb_2O_7$ and $Rb_2Ca_2Nb_3O_{10}$ with water where on heating, $CaC_2O_4 \cdot H_2O$ decomposes to release a stoichiometric amount of water.

X-ray diffraction data on double-layered potassium compounds $KLaNb_2O_7$, $K_2LaNb_2O_7$, and $(K_2OH)LaNb_2O_7$.

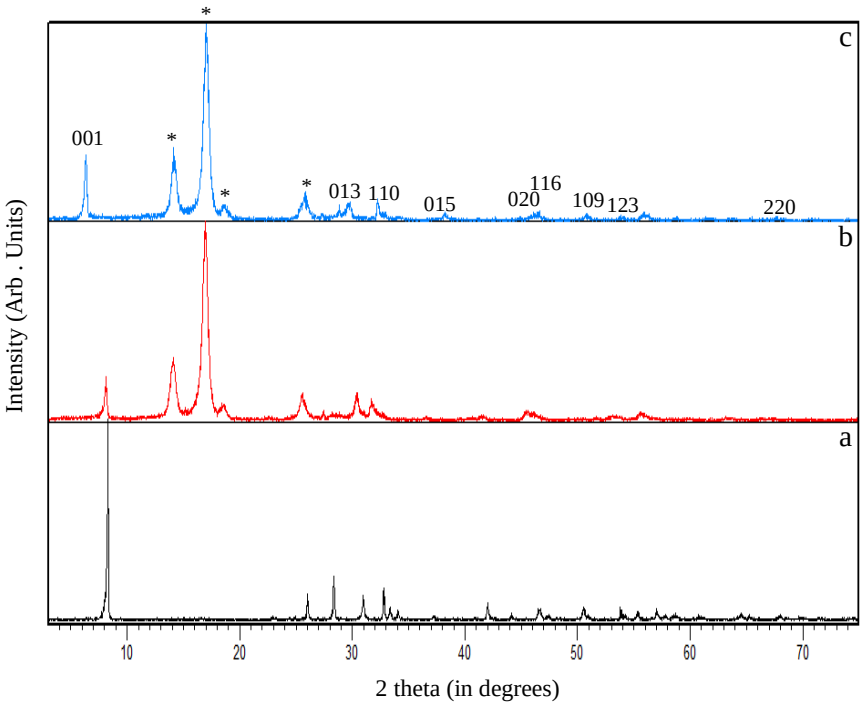

Figure S2. X-ray powder diffraction patterns of for a) $KLaNb_2O_7$, b) $K_2LaNb_2O_7$, and c) $(K_2OH)LaNb_2O_7$.

X-ray diffraction data on triple-layered compounds $RbCa_2Nb_3O_{10}$ and $(Rb_2OH)Ca_2Nb_3O_{10}$.

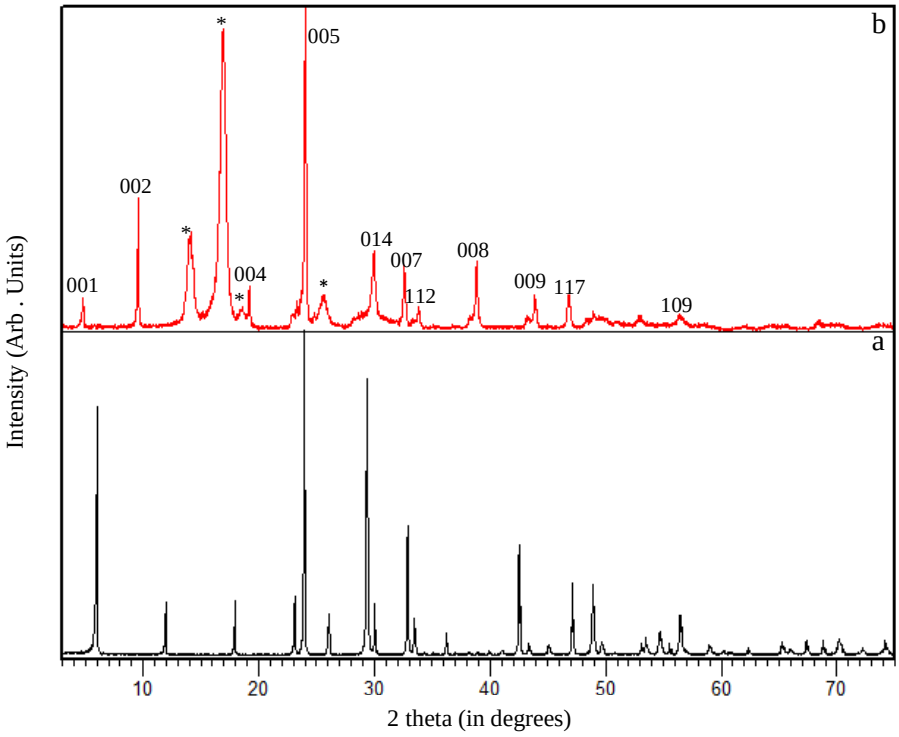

Figure S3. X-ray powder diffraction patterns for a) $RbCa_2Nb_3O_{10}$ and b) $(Rb_2OH)Ca_2Nb_3O_{10}$. Asterisk (*) indicates polypropylene film peaks. Selected indices are highlighted for $(Rb_2OH)Ca_2Nb_3O_{10}$.

Rietveld refinement of $(Rb_2OH)LaNb_2O_7$ X-ray diffraction data

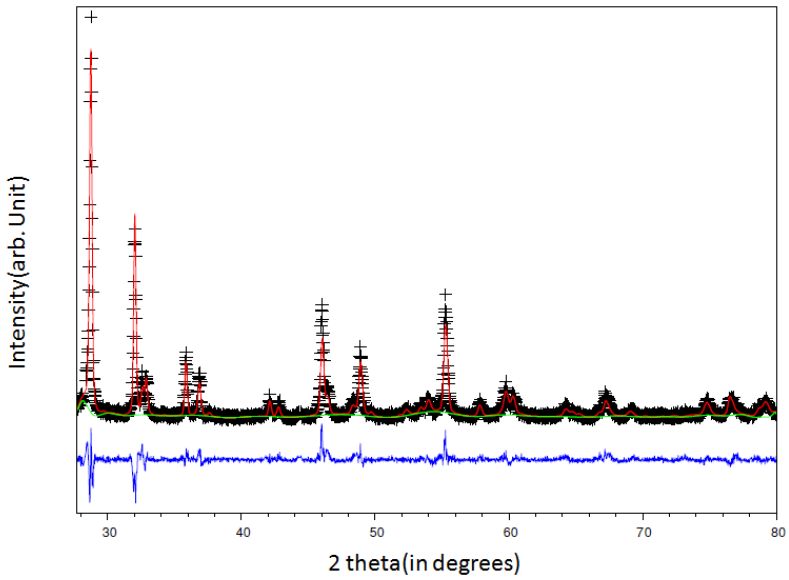

Figure S4. Observed and calculated data for the Rietveld refinement of $(Rb_2OH)LaNb_2O_7$ X-ray diffraction data. Observed data are indicated by crosses, calculated pattern by a red solid line, the bottom blue curve is the difference plot and the green is the background.

Tabulation of Crystallographic Data for $(Rb_2OH)LaNb_2O_7$ from Rietveld refinement of X-ray data.

Table S1. Crystallographic Data for $(Rb_2OH)LaNb_2O_7$ 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

*P*4/*mmm*; Z = 1, a = 3.9303(1) Å, c =14.9624(9) Å, Volume = 231.13(2) $Å^3$

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

Rietveld refinement of $(Rb_2OH)LaNb_2O_7$ Neutron diffraction data

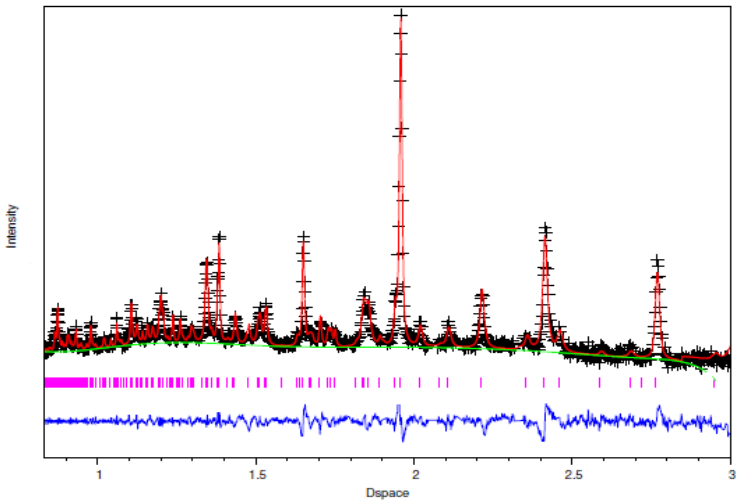

Figure S6. Observed and calculated data for the Rietveld refinement of $(Rb_2OH)LaNb_2O_7$ neutron diffraction data. Observed data are indicated by crosses, calculated pattern by a red solid line, the bottom blue curve is the difference plot, and the green curve is the background. Reflection at ~ 2.2 Å is attributed to the vanadium sample holder.

Tabulation of crystallographic data from neutron diffraction for $(Rb_2OH)LaNb_2O_7$

Table S2. Crystallographic Data for $(Rb_2OH)LaNb_2O_7$ 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

*P*4/*mmm*; Z = 1,a = 3.9132(1) Å, c =14.757(1) Å, Volume = 225.97(1) Å^3

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