

Supplementary Information for

**Ruddlesden-Popper phases of lithium-hydroxide-halide antiperovskites:
Two dimensional Li-ion conductors**

Anucha Koedtruad,^a Midori Amano Patino,^a Yu-Chun Chuang,^b Wei-tin Chen,^c Daisuke Kan,^a
Yuichi Shimakawa,^{*a}

^a *Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan*

^b *National Synchrotron Radiation Research Center, Hsinchu Science Park, Hsinchu 30076, Taiwan*

^c *Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan*

This supplementary information consists of (1) XRD patterns and refinement results of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 0$), (2) XRD patterns and refinement results of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 0.5$), (3) XRD patterns and refinement results of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 0.5$), (4) XRD patterns of $\text{LiCl}(\text{Li}_{3-p}\text{OH}_p\text{Cl})_n$ ($n = 1$ and $p = 0, 0.5, 1$), (5) Temperature-dependent SXRD patterns of the $n = 2$ RP phase of $\text{LiBr}(\text{Li}_2\text{OHBr})_2$, and (6) DC polarization current of the $n = 2$ RP phase of $\text{LiBr}(\text{Li}_2\text{OHBr})_2$ at 30 °C.

*Corresponding author: shimak@scl.kyoto-u.ac.jp (Y.S.)

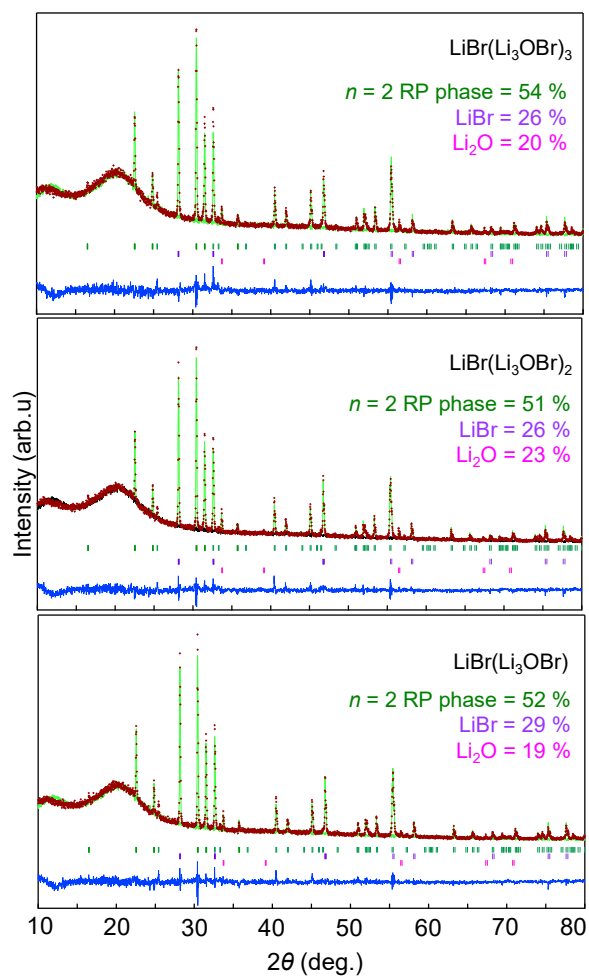


Figure S1a. XRD patterns and refinement results of the samples synthesized with the compositions of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 0$). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green, purple and pink ticks are the allowed Bragg reflection positions for the $n = 2$ RP, LiBr and Li_2O phases, respectively. Fraction of each phase is also presented in the figure.

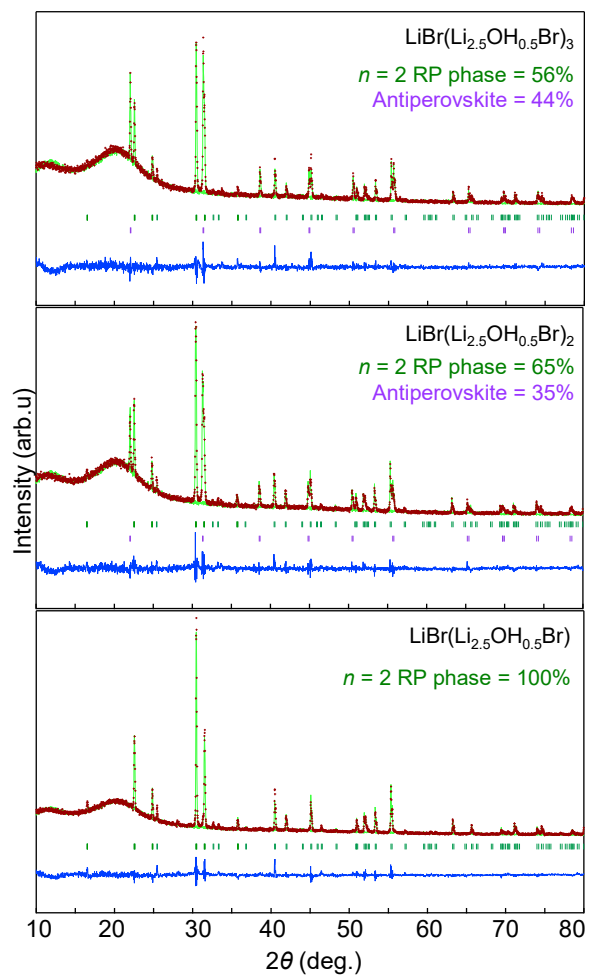


Figure S1b. XRD patterns and refinement results of the samples synthesized with the compositions of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 0.5$). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green and purple ticks are the allowed Bragg reflection positions for the $n = 2$ RP and antiperovskite phases, respectively. Fraction of each phase is also presented in the figure.

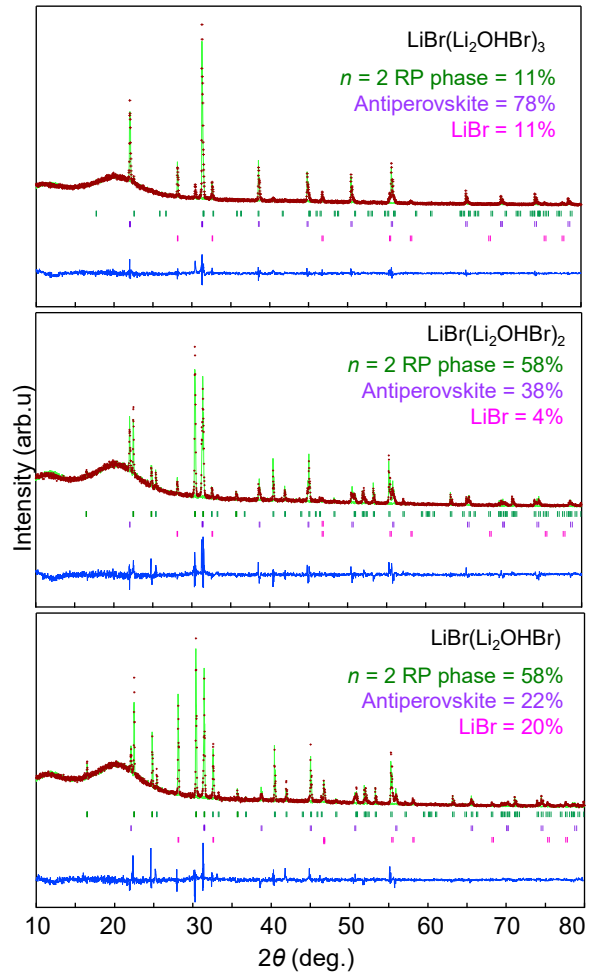


Figure S1c. XRD patterns and refinement results of the samples synthesized with the compositions of $\text{LiBr}(\text{Li}_{3-p}\text{OH}_p\text{Br})_n$ ($n = 1, 2, 3$ and $p = 1$). The red markers and green solid line represent observed and calculated patterns, respectively. The blue line below is the difference between the observed and calculated intensities. The green, purple and pink ticks are the allowed Bragg reflection positions for the $n = 2$ RP, antiperovskite and LiBr phases, respectively. Fraction of each phase is also presented in the figure.

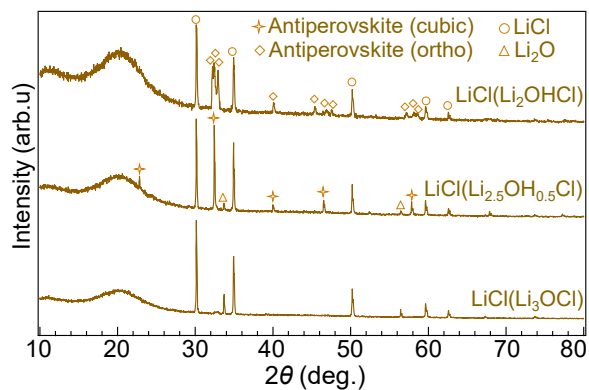


Figure S2. XRD patterns of the samples synthesized with the compositions of $\text{LiCl}(\text{Li}_{3-p}\text{OH}_p\text{Cl})_n$ ($n = 1$ and $p = 0, 0.5, 1$).

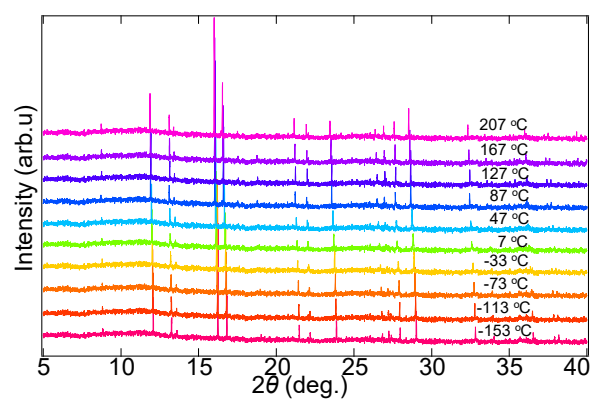


Figure S3. Temperature-dependent SXRD patterns of the $n = 2$ RP phase of $\text{LiBr}(\text{Li}_2\text{OHBr})_2$.

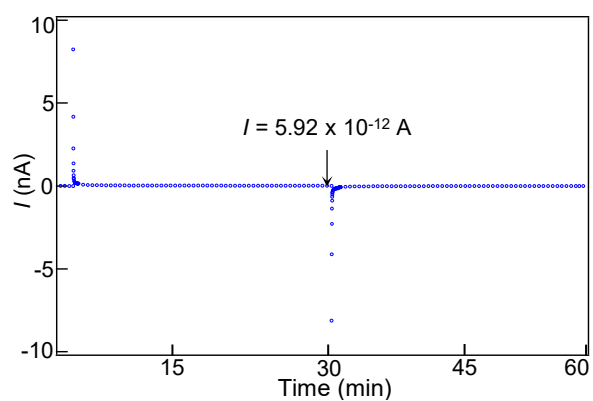


Figure S4. DC polarization current of the $n = 2$ RP phase of $\text{LiBr}(\text{Li}_2\text{OHBr})_2$ at $30\text{ }^\circ\text{C}$. When the applied voltage was set to zero after 30 minutes, the spike inverse current was observed, also confirming the ionic conduction in the sample.