



Fig. S2a Crystal structure of  $\text{CaIrO}_3$ -type  $\text{ABX}_3$  post-perovskite phase. Spheres show atoms: red, A (8-coordinated cation); blue, B (6-coordinated cation); yellow, X1 (corner-shared anion); green, X2 (edge-shared anion). Dotted lines show seven different neighboring X-X pairs. The  $\text{BX}_6$  octahedron has four different neighboring X-X pairs (sky blue, X2-X2<sub>oh</sub>; green, X2-X2<sub>o</sub>; yellow, X1-X2<sub>oh</sub>; pink, X1-X2<sub>o</sub>. Here o and h denote octahedron and hendecahedron, respectively). The  $\text{AX}_8$  hendecahedron has five different neighboring X-X atoms (sky blue, X2-X2<sub>oh</sub>; yellow, X1-X2<sub>oh</sub>; dark blue, X2-X2<sub>h1</sub>; red, X2-X2<sub>h2</sub>; black, X1-X2<sub>h</sub>).