



Fig. S2a Crystal structure of CaIrO_3 -type 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 BX_6 octahedron has four different neighboring X-X pairs (sky blue, X2-X2_oh; green, X2-X2_o; yellow, X1-X2_oh; pink, X1-X2_o. Here o and h denote octahedron and hendecahedron, respectively). The AX_8 hendecahedron has five different neighboring X-X atoms (sky blue, X2-X2_oh; yellow, X1-X2_oh; dark blue, X2-X2_h1; red, X2-X2_h2; black, X1-X2_h).