Supplementary information:

Role of the doping level on localized proton motions in acceptor-doped barium zirconate proton conductors

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Supplementary figures and tables

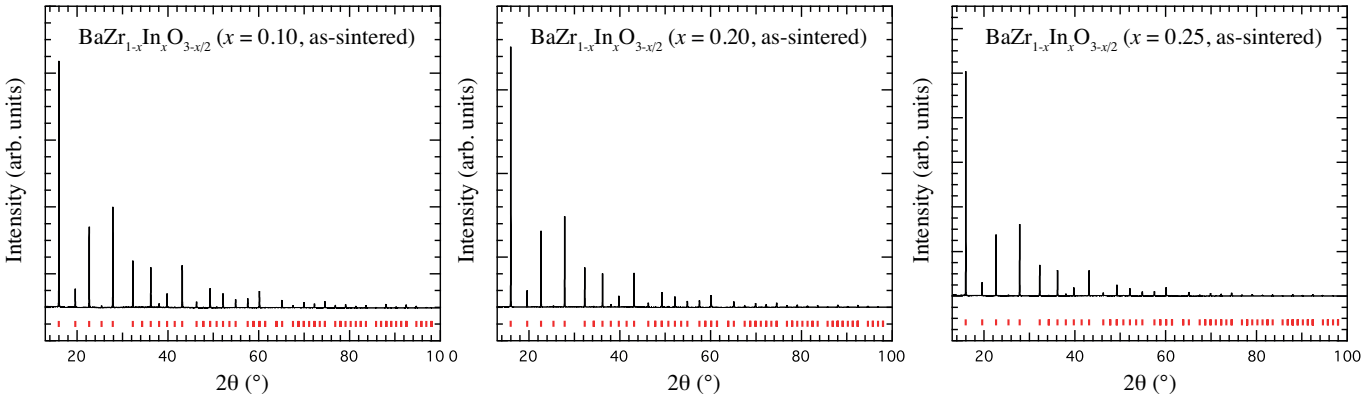

Figure S1 Room temperature high-resolution powder XRD patterns for as-sintered $BaZ_{1-x}In_xO_{3-x/2}$ powders. The red-colored tick marks indicate the positions of Bragg reflections as predicted by a structural model based on $Pm\bar{3}m$ symmetry.

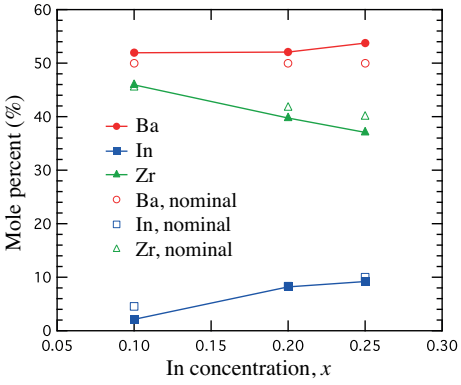

Figure S2 Chemical composition determined by SEM-EDX analysis on $BaZ_{1-x}In_xO_{3-x/2}$ pellets sintered at 1300 °C. Open symbols show expected values based on sample stoichiometry defined in synthesis.

Table S1 Crystallographic data for the as-sintered $BaZ_{1-x}In_xO_{3-x/2}$ powders obtained from the Rietveld fit of room temperature high-resolution powder XRD data shown in Figure S1. The site occupancy factor (SOF) for Ba was constrained to 1 in the structural refinements. The SOFs of Zr and In indicate In dopant levels of 11, 19, and 23%, *i.e.* comparable to the target compositions of 10In/BZO, 20In/BZO, and 25In/BZO, respectively. The SOF of O is close to 1, indicating that the samples had picked up moisture (hydrated) from the atmosphere. Differences in the degree of hydration may explain the slight variation in SOF for O for 20In/BZO and 25In/BZO. B_{iso} stands for isotropic thermal parameter.

$BaZ_{1-x}In_xO_{3-x/2}$	$x = 0.10$	$x = 0.20$	$x = 0.25$
Space group	$Pm\bar{3}m$	$Pm\bar{3}m$	$Pm\bar{3}m$
Lattice parameter (Å)	4.2046(1)	4.2067(1)	4.2067(1)
SOF for Ba (1/2, 1/2, 1/2)	1	1	1
SOF for Zr (0, 0, 0)	0.888(4)	0.806(2)	0.769(4)
SOF for In (0, 0, 0)	0.112(4)	0.194(2)	0.231(2)
SOF for O (1/2, 0, 0)	0.999(3)	0.972(2)	0.979(2)
B_{iso} for Ba (Å^2)	0.651(2)	0.675(2)	0.734(3)
B_{iso} for Zr (Å^2)	0.353(3)	0.386(2)	0.455(3)
B_{iso} for In (Å^2)	0.353(3)	0.386(2)	0.455(3)
B_{iso} for O (Å^2)	0.86(1)	0.87(1)	1.01(1)
χ^2	2.99	2.37	2.46