Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information

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On the influence of the coherence length on the ionic conductivity in mechanochemically synthesized sodium-conducting halides, $Na_{3-x}In_{1-x}Zr_xCl_6$

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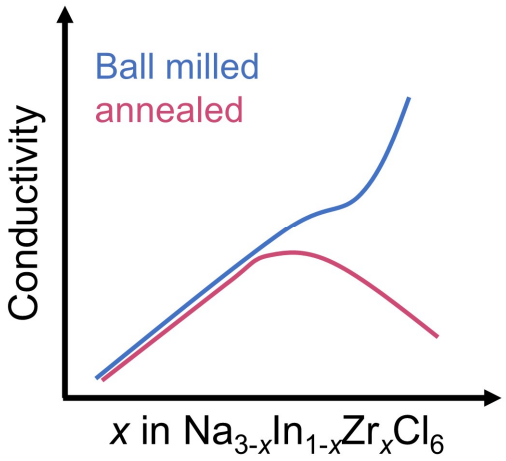

Fig. S1. *Schematic of the differing trends of ionic conductivity against Zr content between ball milled and subsequently annealed* $Na_{3-x}In_{1-x}Zr_xCl_6$.

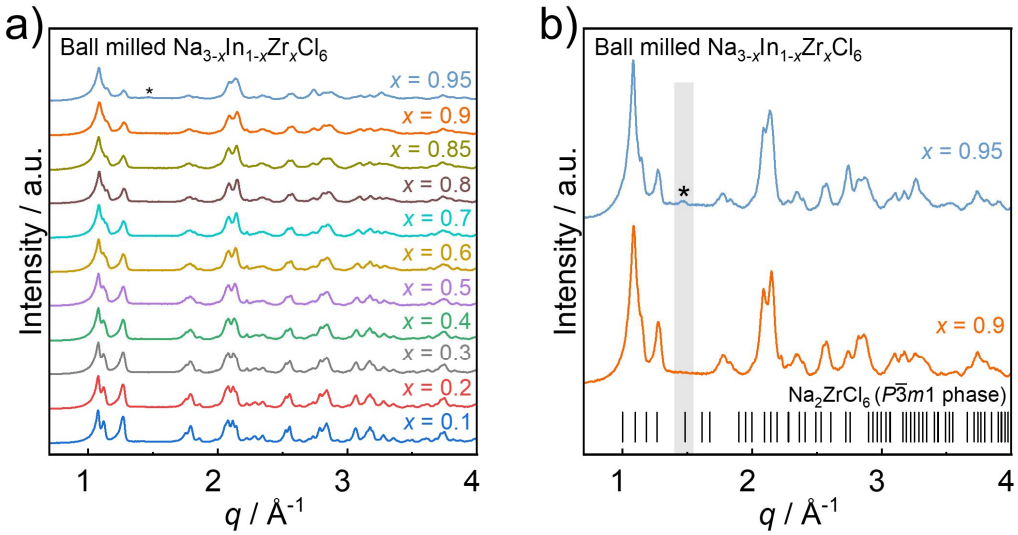

Fig. S2. a) *X-ray diffraction patterns under Ag* $K\alpha_1$ *radiation of the ball milled* $Na_{3-x}In_{1-x}Zr_xCl_6$ *series.* ***b)*** *Comparison of X-ray diffraction patterns of* $Na_{2.05}In_{0.05}Zr_{0.95}Cl_6$ *and* $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$ *with reflections of the trigonal phase of* Na_2ZrCl_6 *(space group* $P\bar{3}m1$*). The dominant additional side-phase reflection (~1.47* $Å^{-1}$*) is marked with an asterisk (*).*

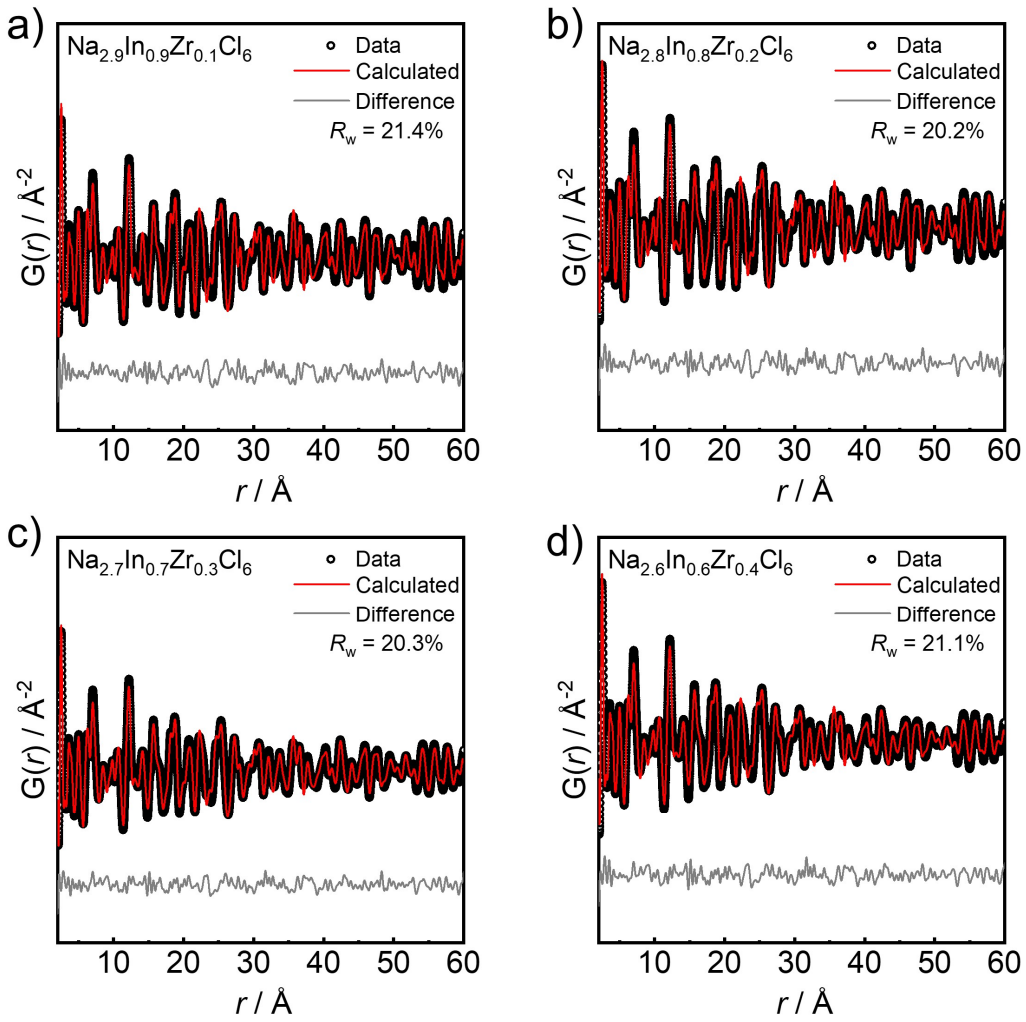

Fig. S3. *Summary of pair distribution function fitting results of ball milled* ***a)*** $Na_{2.9}In_{0.9}Zr_{0.1}Cl_6$, ***b)*** $Na_{2.8}In_{0.8}Zr_{0.2}Cl_6$, ***c)*** $Na_{2.7}In_{0.7}Zr_{0.3}Cl_6$, ***d)*** $Na_{2.6}In_{0.6}Zr_{0.4}Cl_6$.

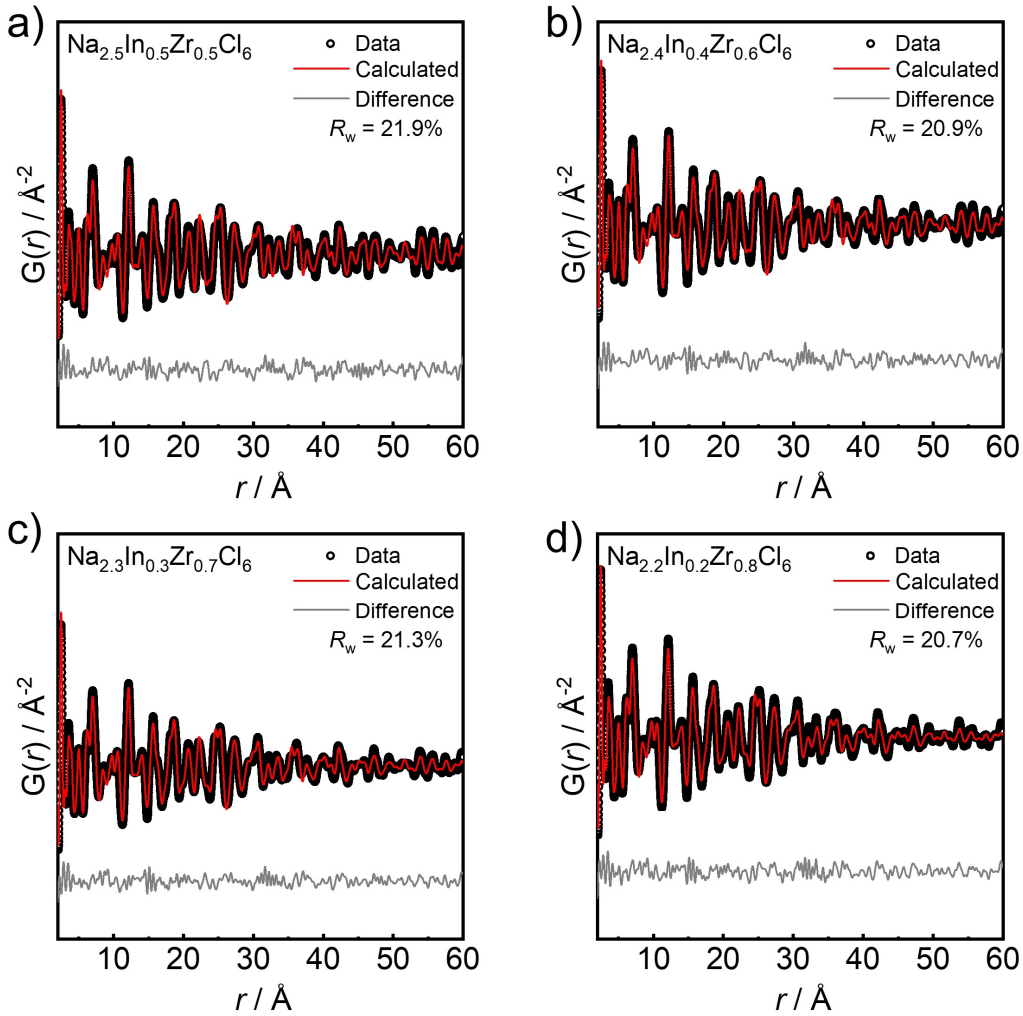

Fig. S4. *Summary of pair distribution function fitting results of ball milled* ***a)*** $Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$, ***b)*** $Na_{2.4}In_{0.4}Zr_{0.6}Cl_6$, ***c)*** $Na_{2.3}In_{0.3}Zr_{0.7}Cl_6$, ***d)*** $Na_{2.2}Zr_{0.2}In_{0.8}Cl_6$.

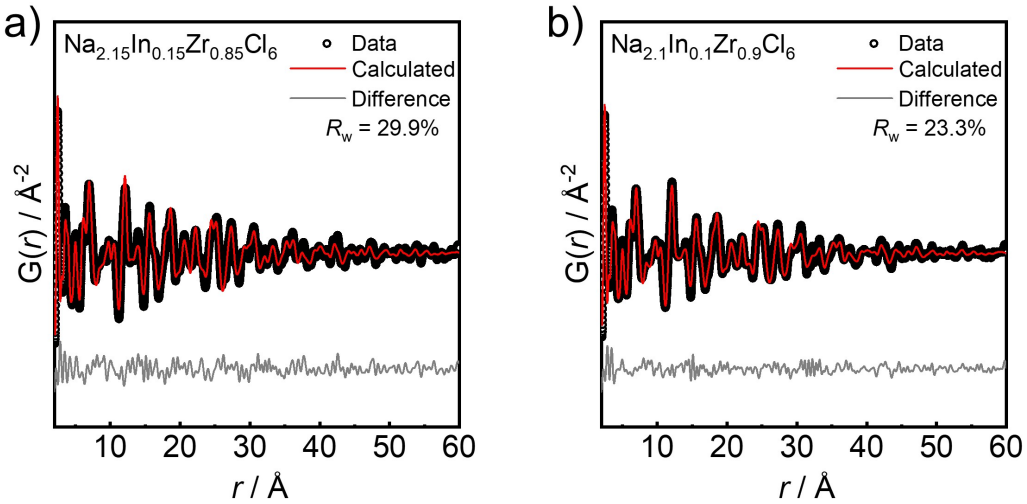

Fig. S5. *Summary of pair distribution function fitting results of ball milled* ***a)*** $Na_{2.15}In_{0.15}Zr_{0.85}Cl_6$,

b) *$Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$.*

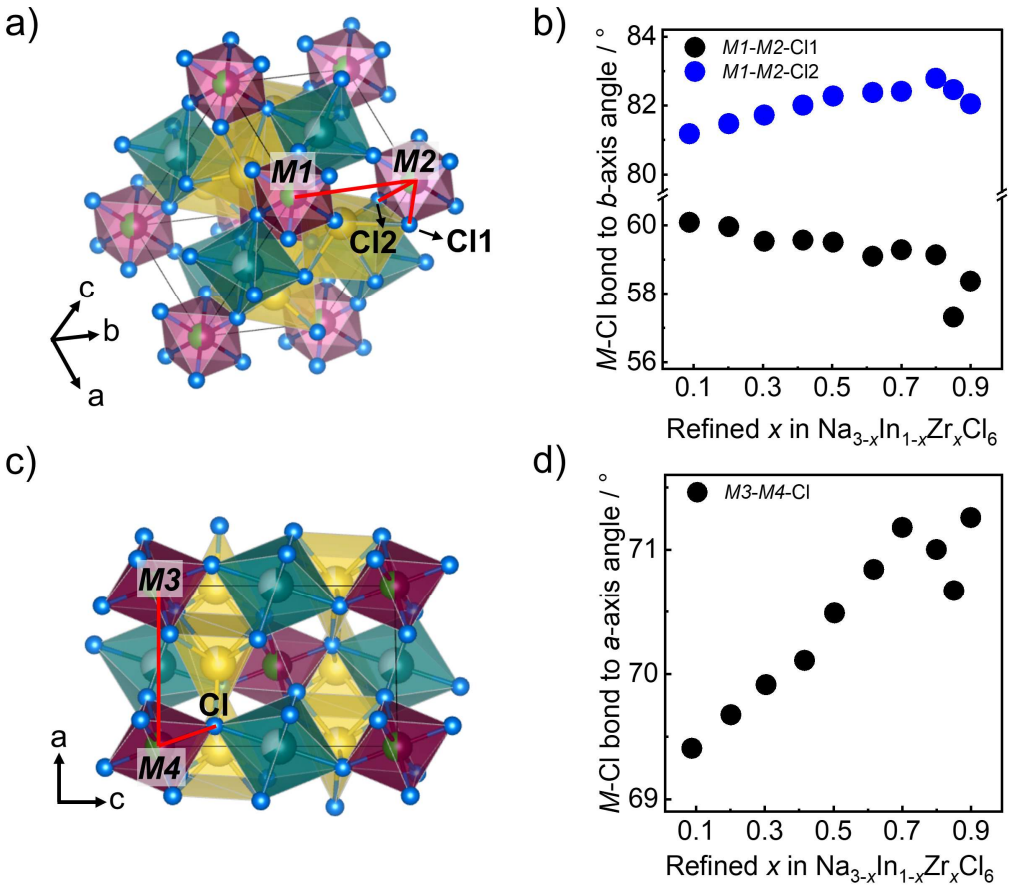

Fig. S6. a) *Schematic of the angles between b axis (parallel to M1-M2 direction) and M-Cl bond (M, M1, M2 =* In; Zr*). **b)** Angles between the b axis and M-Cl bond as a function of refined Zr content. **c)** Schematic of the angles between a axis (parallel to M3-M4 direction) and M-Cl bond (M, M3, M4 =* In; Zr*). **d)** Angles between a axis and M-Cl bond as a function of refined Zr content.*

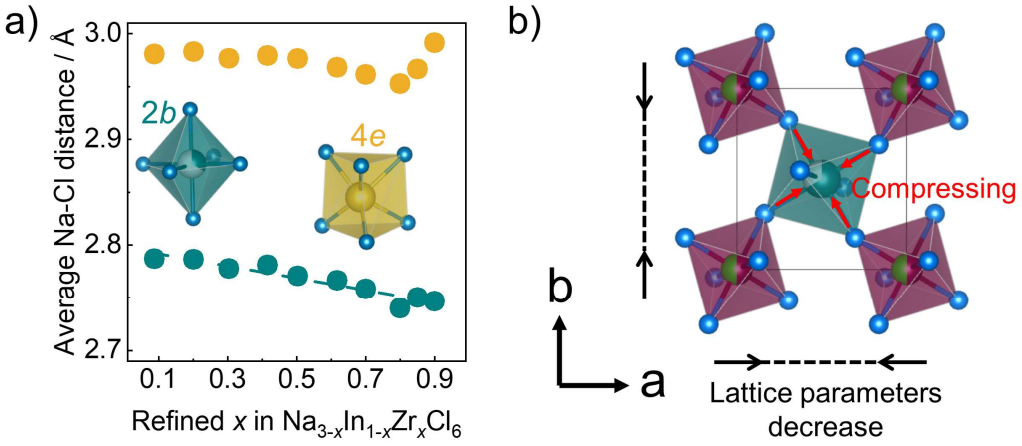

Fig. S7. a) *Average Na-Cl distances of $NaCl_6^{5-}$ octahedra (Na^+ at Wyckoff 2b site) and prism (Na^+ at Wyckoff 4e site). Dashed lines correspond to linear behavior as guides-to-the-eye. **b)** Schematics of $NaCl_6^{5-}$ octahedra compressing upon decreased lattice parameters.*

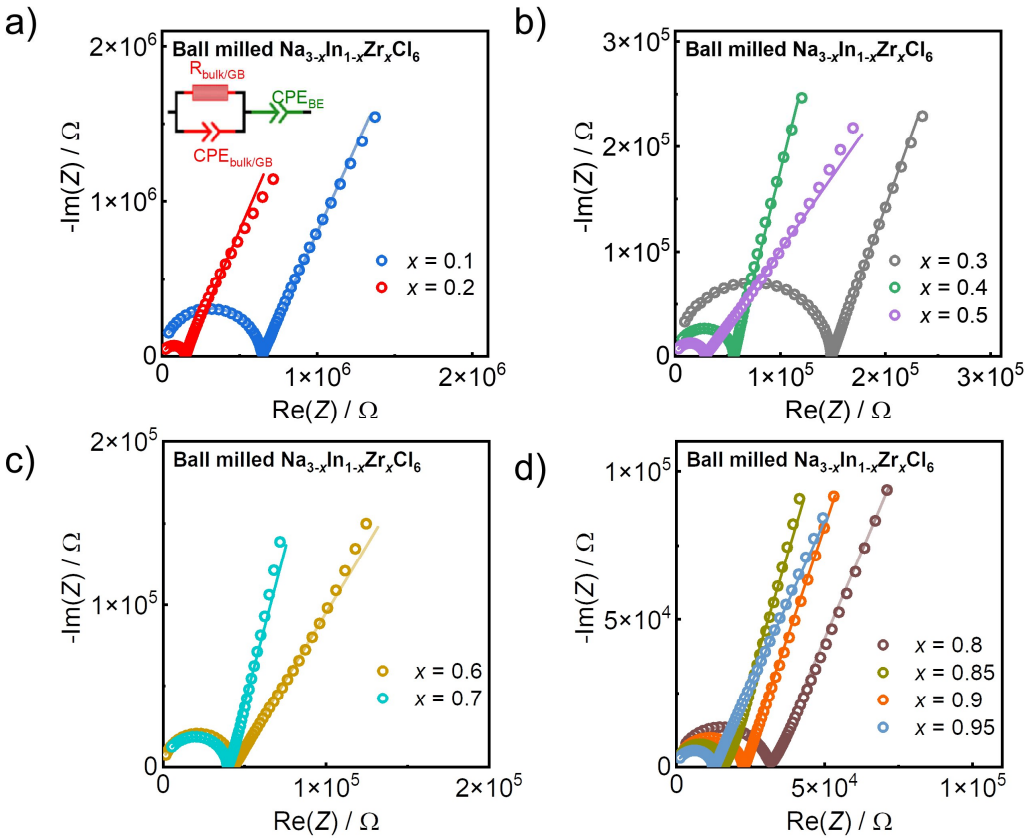

Fig. S8. a) *Nyquist plots of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ (x = 0.1; 0.2). Inset: equivalent circuit model used for fitting the measured impedance spectra.* ***b)*** *Nyquist plots of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ (x = 0.3; 0.4; 0.5).* ***c)*** *Nyquist plots of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ (x = 0.6; 0.7).* ***d)*** *Nyquist plots of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ (x = 0.8; 0.85; 0.9; 0.95). These impedances were measured at room temperature (25 °C).*

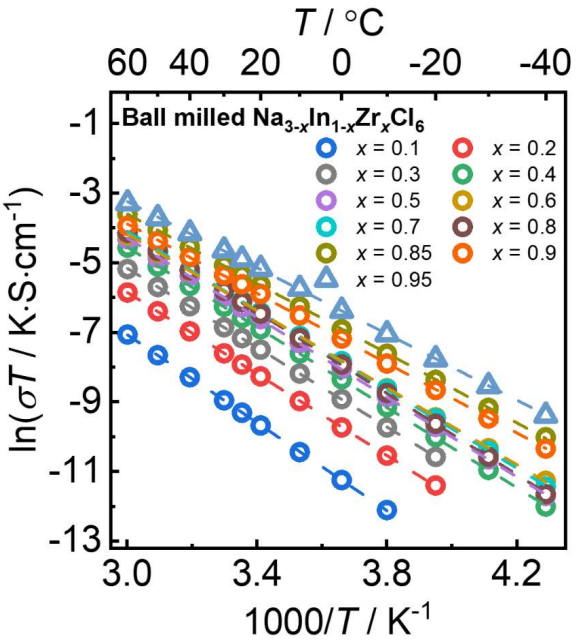

Fig. S9. *Arrhenius plots from the temperature dependent impedance of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$ series.*

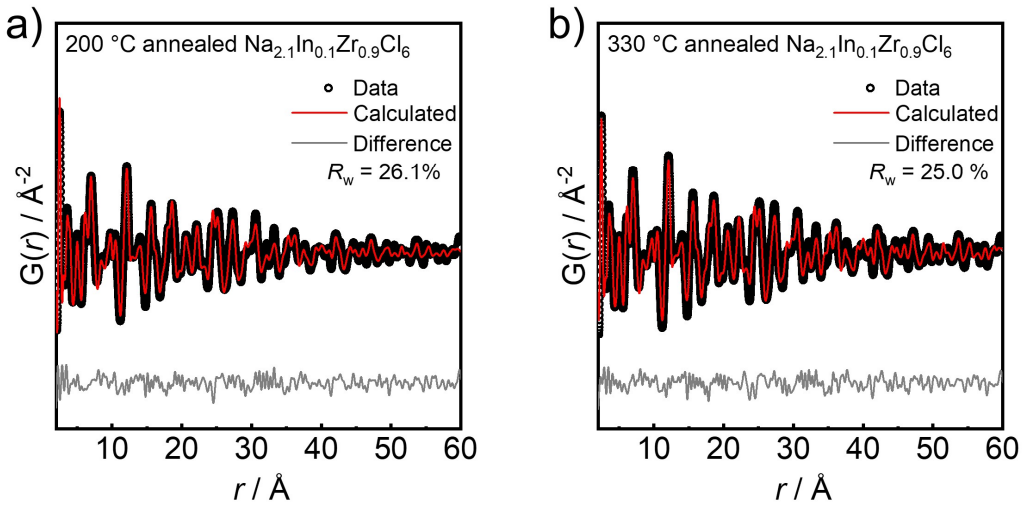

Fig. S10. *Summary of pair distribution function fitting results of $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$ annealed at* ***a)*** *200 °C and* ***b)*** *330 °C for 1 hour.*

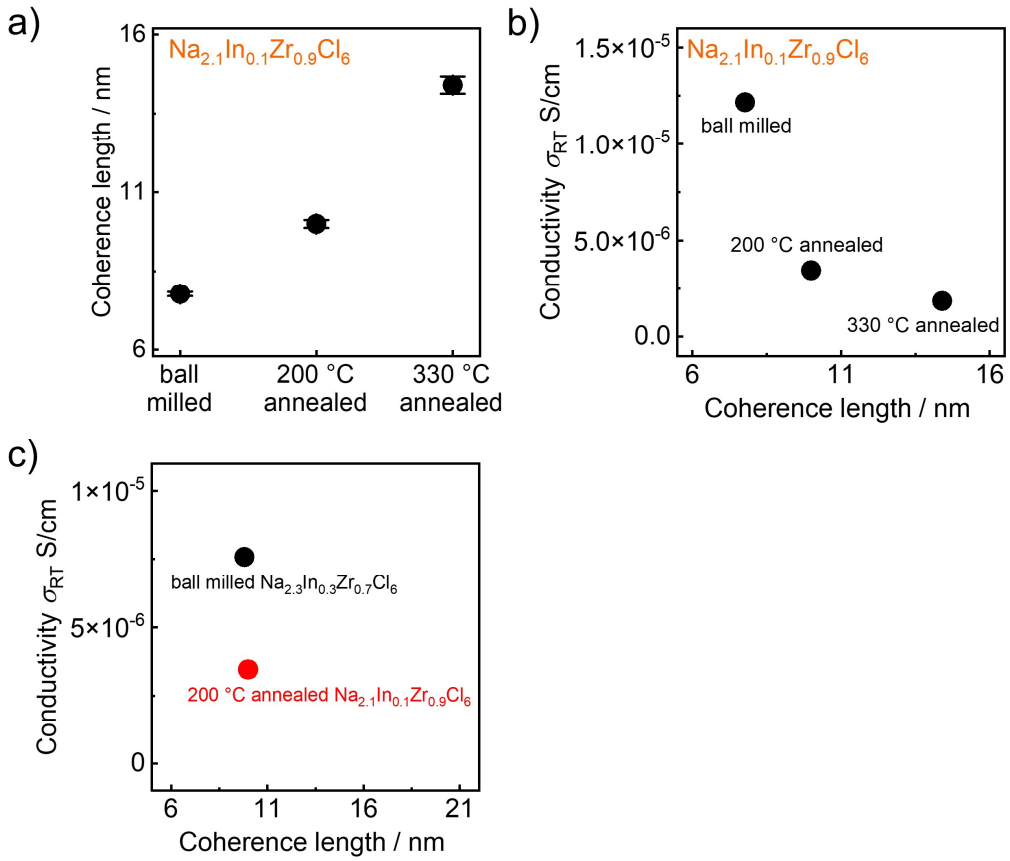

Fig. S11. a) *Coherence lengths of ball milled, 200 °C annealed and 330 °C annealed* $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$*. The uncertainties, where shown, correspond to 1σ.* ***b)*** *Room-temperature ionic conductivities of* $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$ *synthesized by different procedures against coherence length.* ***c)*** *Room-temperature ionic conductivities of 200 °C annealed* $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$ *and ball milled* $Na_{2.3}In_{0.3}Zr_{0.7}Cl_6$ *against coherence length. The ionic conductivities of annealed* $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$ *were extracted from Ref. 31.*

Table S1: *Used constraints for pair distribution function fitting of ball milled* $Na_{3-x}In_{1-x}Zr_xCl_6$*.*

$Na_{3-x}In_{1-x}Zr_xCl_6$
Lattice Parameter: $\alpha = \gamma = 90°$
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	Pos1	Pos2	Pos3	$(3-x-Occ_{Na})/2$	Th1
Na2	2*b*	0	0	0.5	Occ_{Na}	Th1
Zr1	2*a*	0	0	0	*x*	Th2
In1	2*a*	0	0	0	1−*x*	Th2
Cl1	4*e*	Pos4	Pos5	Pos6	1	Th3
Cl2	4*e*	Pos7	Pos8	Pos9	1	Th3
Cl3	4*e*	Pos10	Pos11	Pos12	1	Th3

Table S2: *Pair distribution function fitting result of ball milled* $Na_{2.9}In_{0.9}Zr_{0.1}Cl_6$*. Fitting range: 2 - 60 Å.*

$Na_{2.9}In_{0.9}Zr_{0.1}Cl_6$
Lattice Parameter: a = 6.7631(5) Å, b = 7.1722(7) Å, c = 9.9708(10) Å, β = 90.537(13)°
Space group: $P2_1/n$

Atom	Wyckoff	Atomic coordinates	*Occ.*	U_{iso} / Å²

	Position	*x*	*y*	*z*		
Na1	4*e*	0.506(2)	−0.0752(7)	0.2474(11)	0.967(11)	0.062(2)
Na2	2*b*	0	0	0.5	0.98(3)	0.062(2)
Zr1	2*a*	0	0	0	0.09(2)	0.0184(4)
In1	2*a*	0	0	0	0.91(2)	0.0184(4)
Cl1	4*e*	0.1610(8)	0.3082(6)	−0.0765(6)	1	0.0433(7)
Cl2	4*e*	0.1339(6)	0.0537(6)	0.2327(6)	1	0.0433(7)
Cl3	4*e*	−0.3071(6)	0.1724(7)	0.0536(5)	1	0.0433(7)

Table S3: *Pair distribution function fitting result of ball milled $Na_{2.8}In_{0.8}Zr_{0.2}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.8}In_{0.8}Zr_{0.2}Cl_6$
Lattice Parameter: a = 6.7598(5) Å, b = 7.1698(7) Å, c = 9.9693(10) Å, β = 90.631(13)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.507(2)	−0.0767(7)	0.2480(11)	0.947(10)	0.067(2)
Na2	2*b*	0	0	0.5	0.90(3)	0.067(2)
Zr1	2*a*	0	0	0	0.20(2)	0.0201(4)
In1	2*a*	0	0	0	0.80(2)	0.0201(4)
Cl1	4*e*	0.1607(8)	0.3072(6)	−0.0770(6)	1	0.0457(7)
Cl2	4*e*	0.1324(6)	0.0517(6)	0.2324(6)	1	0.0457(7)
Cl3	4*e*	−0.3064(7)	0.1727(7)	0.0523(5)	1	0.0457(7)

Table S4: *Pair distribution function fitting result of ball milled $Na_{2.7}In_{0.7}Zr_{0.3}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.7}In_{0.7}Zr_{0.3}Cl_6$
Lattice Parameter: a = 6.7563(6) Å, b = 7.1656(8) Å, c = 9.9670(11) Å, β = 90.750(14)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.507(2)	−0.0783(8)	0.2487(11)	0.960(11)	0.079(3)
Na2	2*b*	0	0	0.5	0.78(3)	0.079(3)
Zr1	2*a*	0	0	0	0.30(2)	0.0226(3)
In1	2*a*	0	0	0	0.70(2)	0.0226(3)
Cl1	4*e*	0.1612(8)	0.3092(6)	−0.0781(6)	1	0.0472(4)
Cl2	4*e*	0.1328(7)	0.0507(6)	0.2350(5)	1	0.0472(4)
Cl3	4*e*	−0.3023(3)	0.1736(4)	0.0523(4)	1	0.0472(4)

Table S5: *Pair distribution function fitting result of ball milled $Na_{2.6}In_{0.6}Zr_{0.4}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.6}In_{0.6}Zr_{0.4}Cl_6$
Lattice Parameter: a = 6.7529(7) Å, b = 7.1611(9) Å, c = 9.9609(13) Å, β = 90.88(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.508(2)	−0.0774(8)	0.2437(13)	0.927(11)	0.083(3)
Na2	2*b*	0	0	0.5	0.73(3)	0.083(3)
Zr1	2*a*	0	0	0	0.42(2)	0.0254(6)
In1	2*a*	0	0	0	0.58(2)	0.0254(6)
Cl1	4*e*	0.1619(9)	0.3064(6)	−0.0797(6)	1	0.0517(8)
Cl2	4*e*	0.1306(7)	0.0483(7)	0.2323(6)	1	0.0517(8)
Cl3	4*e*	−0.3044(7)	0.1743(4)	0.0510(5)	1	0.0517(8)

Table S6: *Pair distribution function fitting result of ball milled $Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$

Lattice Parameter: a = 6.7463(7) Å, b = 7.1544(11) Å, c = 9.952(2) Å, β = 91.05(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.511(2)	−0.0792(8)	0.2516(13)	0.924(11)	0.091(4)
Na2	2*b*	0	0	0.5	0.65(3)	0.091(4)
Zr1	2*a*	0	0	0	0.50(2)	0.0287(6)
In1	2*a*	0	0	0	0.50(2)	0.0287(6)
Cl1	4*e*	0.1649(9)	0.3080(7)	−0.0793(7)	1	0.0572(9)
Cl2	4*e*	0.1287(8)	0.0464(7)	0.2319(6)	1	0.0572(9)
Cl3	4*e*	−0.3035(7)	0.1741(8)	0.0500(5)	1	0.0572(9)

Table S7: *Pair distribution function fitting result of ball milled $Na_{2.4}In_{0.4}Zr_{0.6}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.4}In_{0.4}Zr_{0.6}Cl_6$
Lattice Parameter: a = 6.7395(8) Å, b = 7.1475(11) Å, c = 9.937(2) Å, β = 91.24(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.515(2)	−0.0797(9)	0.2439(12)	0.932(11)	0.092(4)
Na2	2*b*	0	0	0.5	0.52(3)	0.092(4)
Zr1	2*a*	0	0	0	0.62(2)	0.0287(6)
In1	2*a*	0	0	0	0.38(2)	0.0287(6)
Cl1	4*e*	0.1648(8)	0.3043(6)	−0.0799(6)	1	0.0573(9)
Cl2	4*e*	0.1279(8)	0.0459(7)	0.2329(6)	1	0.0573(9)
Cl3	4*e*	−0.3018(7)	0.1765(8)	0.0514(5)	1	0.0573(9)

Table S8: *Pair distribution function fitting result of ball milled $Na_{2.3}In_{0.3}Zr_{0.7}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.3}In_{0.3}Zr_{0.7}Cl_6$
Lattice Parameter: a = 6.7308(9) Å, b = 7.1387(11) Å, c = 9.918(2) Å, β = 91.51(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.517(2)	−0.0813(9)	0.2461(12)	0.932(11)	0.094(4)
Na2	2*b*	0	0	0.5	0.44(3)	0.094(4)
Zr1	2*a*	0	0	0	0.70(2)	0.02862(13)
In1	2*a*	0	0	0	0.30(2)	0.02862(13)
Cl1	4*e*	0.1671(9)	0.3023(7)	−0.0784(6)	1	0.05863(14)
Cl2	4*e*	0.1286(9)	0.0461(7)	0.2357(4)	1	0.05863(14)
Cl3	4*e*	−0.2996(3)	0.1742(4)	0.0517(4)	1	0.05863(14)

Table S9: *Pair distribution function fitting result of ball milled $Na_{2.2}In_{0.2}Zr_{0.8}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.2}In_{0.2}Zr_{0.8}Cl_6$
Lattice Parameter: a = 6.7182(10) Å, b = 7.1300(12) Å, c = 9.894(2) Å, β = 91.781(15)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.520(2)	−0.0863(9)	0.2487(12)	0.978(13)	0.099(4)
Na2	2*b*	0	0	0.5	0.24(3)	0.099(4)
Zr1	2*a*	0	0	0	0.80(2)	0.0282(3)
In1	2*a*	0	0	0	0.20(2)	0.0282(3)
Cl1	4*e*	0.1733(9)	0.3012(7)	−0.0759(7)	1	0.0587(3)
Cl2	4*e*	0.1319(10)	0.0440(7)	0.2367(5)	1	0.0587(3)
Cl3	4*e*	−0.2985(1)	0.1749(3)	0.0522(4)	1	0.0587(3)

Table S10: *Pair distribution function fitting result of ball milled $Na_{2.15}In_{0.15}Zr_{0.85}Cl_6$. Fitting*

range: 2 - 60 Å.

$Na_{2.15}In_{0.15}Zr_{0.85}Cl_6$
Lattice Parameter: a = 6.710(2) Å, b = 7.121(2) Å, c = 9.883(3) Å, β = 91.91(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.513(3)	−0.0814(13)	0.247(2)	0.95(2)	0.100(6)
Na2	2*b*	0	0	0.5	0.25(2)	0.100(6)
Zr1	2*a*	0	0	0	0.85(3)	0.0288(7)
In1	2*a*	0	0	0	0.15(3)	0.0288(7)
Cl1	4*e*	0.1576(12)	0.2993(10)	−0.0797(10)	1	0.0599(9)
Cl2	4*e*	0.1306(10)	0.0446(10)	0.2290(3)	1	0.0599(9)
Cl3	4*e*	−0.3061(9)	0.1918(12)	0.0497(8)	1	0.0599(9)

Table S11: *Pair distribution function fitting result of ball milled $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$
Lattice Parameter: a = 6.7067(14) Å, b = 7.116(2) Å, c = 9.873(2) Å, β = 92.05(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.498(2)	−0.0690(13)	0.2142(13)	0.96(2)	0.100(5)
Na2	2*b*	0	0	0.5	0.18(4)	0.100(5)
Zr1	2*a*	0	0	0	0.90(3)	0.0300(10)
In1	2*a*	0	0	0	0.10(3)	0.0300(10)
Cl1	4*e*	0.1664(10)	0.2967(8)	−0.0761(8)	1	0.0636(11)
Cl2	4*e*	0.1290(9)	0.0474(9)	0.2315(4)	1	0.0636(11)
Cl3	4*e*	−0.3030(8)	0.1834(11)	0.0539(6)	1	0.0636(11)

Table S12: *Pair distribution function fitting result of ball milled $Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$. Fitting range: 2 - 20 Å.*

$Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$
Lattice Parameter: a = 6.746(3) Å, b = 7.150(3) Å, c = 9.952(6) Å, β = 91.17(7)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.515(2)	−0.0817(10)	0.259(2)	1.00(2)	0.075(5)
Na2	2*b*	0	0	0.5	0.48(5)	0.075(5)
Zr1	2*a*	0	0	0	0.52(3)	0.027(2)
In1	2*a*	0	0	0	0.48(3)	0.027(2)
Cl1	4*e*	0.1642(14)	0.3157(12)	−0.0845(11)	1	0.055(2)
Cl2	4*e*	0.126(2)	0.0429(13)	0.2333(7)	1	0.055(2)
Cl3	4*e*	−0.3019(4)	0.177(2)	0.052(2)	1	0.055(2)

Table S13: *Pair distribution function fitting result of ball milled $Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$. Fitting range: 2 - 40 Å.*

$Na_{2.5}In_{0.5}Zr_{0.5}Cl_6$
Lattice Parameter: a = 6.7472(11) Å, b = 7.156(2) Å, c = 9.952(2) Å, β = 91.18(2)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.514(2)	−0.0840(9)	0.2584(12)	0.946(13)	0.074(4)
Na2	2*b*	0	0	0.5	0.58(4)	0.074(4)
Zr1	2*a*	0	0	0	0.52(3)	0.0262(6)
In1	2*a*	0	0	0	0.48(3)	0.0262(6)
Cl1	4*e*	0.1678(10)	0.3107(8)	−0.0838(8)	1	0.0543(9)
Cl2	4*e*	0.1287(9)	0.0417(8)	0.2321(6)	1	0.0543(9)
Cl3	4*e*	−0.3039(6)	0.1745(9)	0.0500(6)	1	0.0543(9)

Table S14. *Fitted parameters of room-temperature impedance spectra of ball milled $Na_{3-x}In_{1-x}Zr_xCl_6$, where x represents nominal Zr content; $R_{bulk/GB}$ and $CPE_{bulk/GB}$ represent the resistance and CPE capacitance of $Na_{3-x}In_{1-x}Zr_xCl_6$ pellets respectively; $\alpha_{bulk/GB}$ is the ideal indicator of $CPE_{bulk/GB}$; CPE_{BE} represent the CPE capacitance of blocking electrode; α_{BE} is the ideal indicator of CPE_{BE}.*

x in $Na_{3-x}In_{1-x}Zr_xCl_6$	$R_{bulk/GB}$	$CPE_{bulk/GB}$	$\alpha_{bulk/GB}$	CPE_{BE}	α_{BE}
0.1	6.37×10^5	7.56×10^{-11}	0.98	7.37×10^{-7}	0.73
0.2	1.46×10^5	4.33×10^{-11}	0.97	4.43×10^{-7}	0.74
0.3	1.48×10^5	3.75×10^{-11}	0.97	5.90×10^{-6}	0.78
0.4	5.56×10^4	5.00×10^{-11}	0.98	2.07×10^{-6}	0.84
0.5	2.81×10^4	8.04×10^{-11}	0.94	2.42×10^{-6}	0.61
0.6	4.32×10^4	5.79×10^{-11}	0.97	2.59×10^{-6}	0.66
0.7	3.97×10^4	4.06×10^{-11}	0.96	2.52×10^{-6}	0.84
0.8	3.18×10^4	2.17×10^{-10}	0.88	1.38×10^{-6}	0.75
0.85	1.61×10^4	1.11×10^{-10}	0.97	5.51×10^{-6}	0.82
0.9	2.27×10^4	9.56×10^{-11}	0.91	2.10×10^{-6}	0.79
0.95	1.25×10^4	8.88×10^{-11}	0.93	4.73×10^{-6}	0.73

Table S15: *Pair distribution function fitting result of 200 °C annealed $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$
Lattice Parameter: a = 6.7117(11) Å, b = 7.1204(12) Å, c = 9.880(2) Å, β = 91.907(14)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.505(2)	−0.0757(12)	0.2256(15)	0.949(15)	0.100(5)
Na2	2*b*	0	0	0.5	0.19(4)	0.100(5)
Zr1	2*a*	0	0	0	0.91(3)	0.0216(8)
In1	2*a*	0	0	0	0.09(3)	0.0216(8)
Cl1	4*e*	0.1693(10)	0.2984(8)	−0.0782(8)	1	0.0216(8)
Cl2	4*e*	0.1285(9)	0.0470(9)	0.2315(4)	1	0.0566(10)
Cl3	4*e*	−0.3044(8)	0.1858(10)	0.0525(6)	1	0.0566(10)

Table S16: *Pair distribution function fitting result of 330 °C annealed $Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$. Fitting range: 2 - 60 Å.*

$Na_{2.1}In_{0.1}Zr_{0.9}Cl_6$
Lattice Parameter: a = 6.7058(9) Å, b = 7.1113(9) Å, c = 9.8744(12) Å, β = 91.908(10)°
Space group: $P2_1/n$

Atom	Wyckoff Position	Atomic coordinates			*Occ.*	U_{iso} / Å²
		x	*y*	*z*		
Na1	4*e*	0.511(2)	−0.0853(10)	0.2451(13)	0.955(14)	0.090(4)
Na2	2*b*	0	0	0.5	0.20(4)	0.090(4)
Zr1	2*a*	0	0	0	0.89(3)	0.0205(7)
In1	2*a*	0	0	0	0.11(3)	0.0205(7)
Cl1	4*e*	0.1692(8)	0.2990(6)	−0.0722(6)	1	0.0452(8)
Cl2	4*e*	0.1266(8)	0.0424(7)	0.2289(3)	1	0.0452(8)
Cl3	4*e*	−0.3098(7)	0.1821(8)	0.0532(5)	1	0.0452(8)

The uncertainties shown in the tables correspond to 1σ.