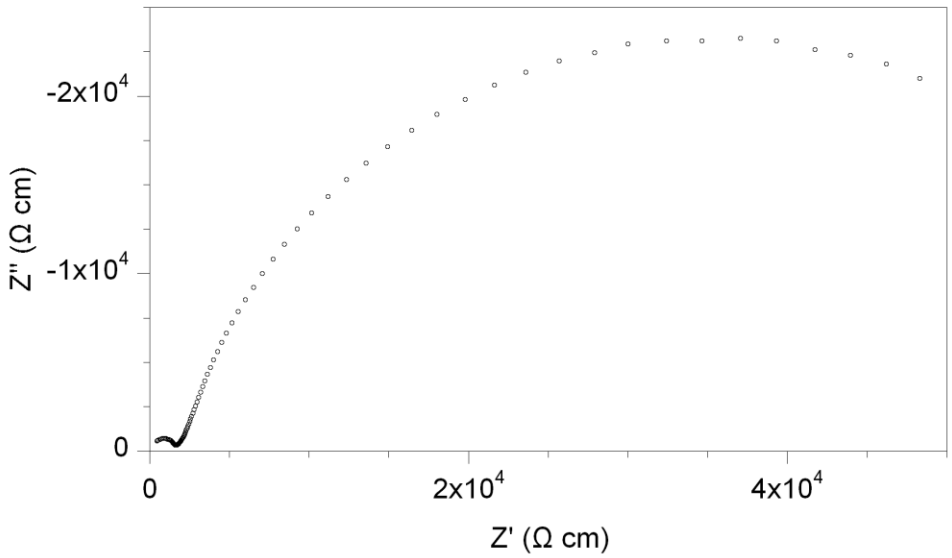
Synthesis and characterization of proton conducting oxyanion doped $Ba_2Sc_2O_5$

Supplementary data

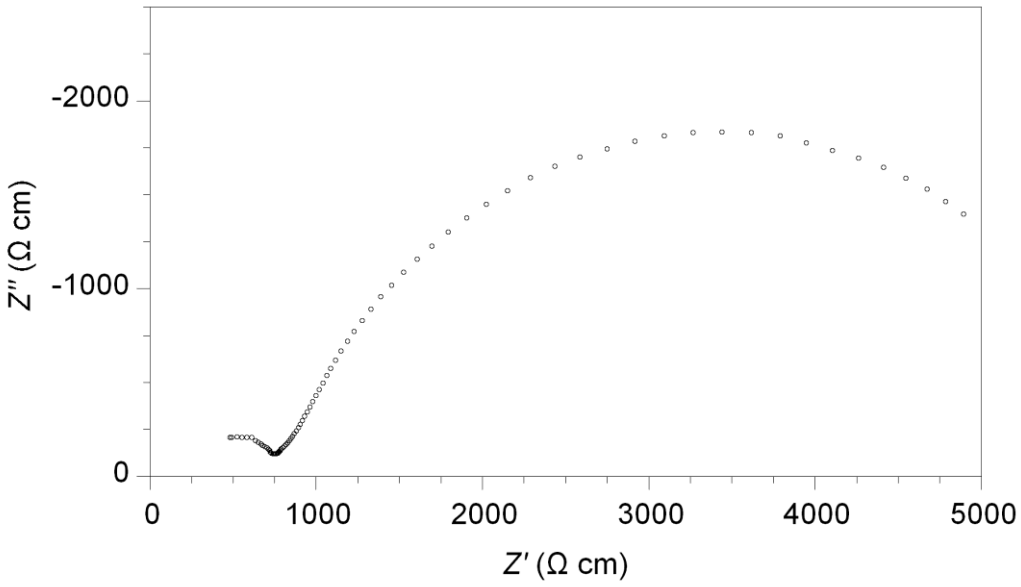
Impedance Data

Fig 1. Impedance spectra for $Ba_2Sc_{1.6}P_{0.4}O_{5.4}$ in dry N_2 at (a) 300 °C, (b) 380 °C showing typical bulk and grain boundary semicircles

(a)



(b)



Structure refinements using X-ray diffraction data

Fig. 2 Observed (cross), calculated (line), reflection positions and difference plots (observed − calculated) of $Ba_2Sc_{1.6}P_{0.4}O_{5.4}$ from the Rietveld refinement for room temperature X-ray diffraction data.

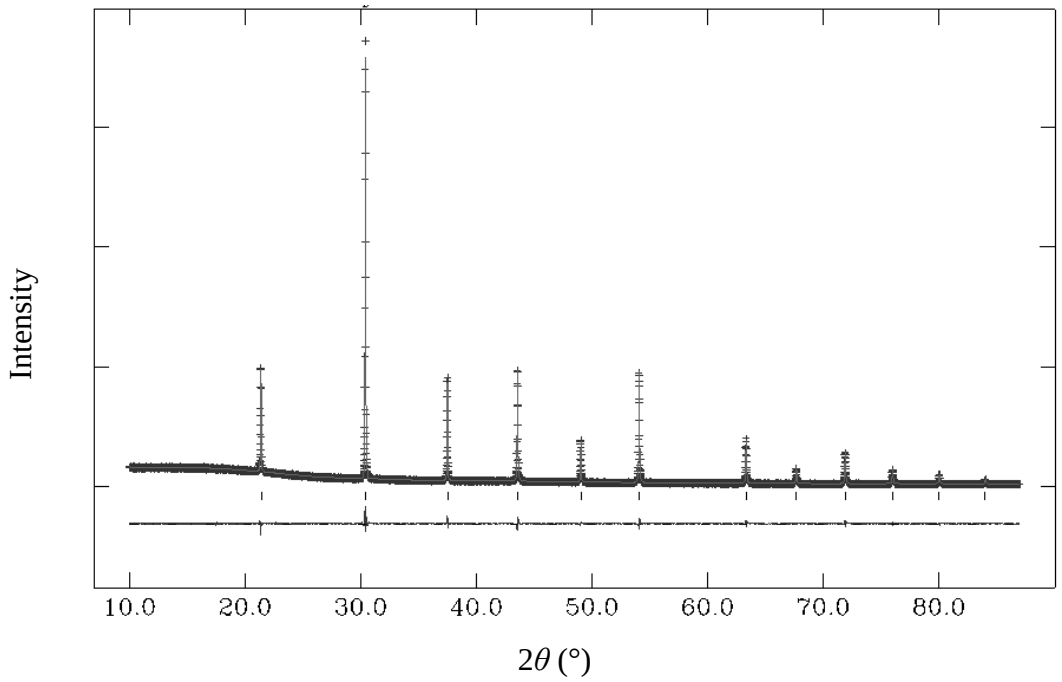


Table 1 Refined crystal structure of $Ba_2Sc_{1.6}P_{0.4}O_{5.4}$ using cubic *Pm3m* (221) space group using room temperature X-ray diffraction data.

		a (Å)		R_{wp}	R_p	χ^2
		4.1504 (1)		5.15	3.70	1.83
		x	*y*	*z*	Fractional occupancy	U_{iso} (Å^2 x 100)
Ba	1(b)	½	½	½	1.00	2.22 (2)
Sc	1(a)	0	0	0	0.794 (8)	2.67 (6)
P	1(a)	0	0	0	0.206 (8)	2.67 (6)
O	3(d)	0	0	½	0.896 (5)	3.6 (1)

Fig. 3 Observed (cross), calculated (line), reflection positions and difference plots (observed − calculated) of $Ba_2Sc_{1.5}P_{0.5}O_{5.5}$ from the Rietveld refinement for room temperature X-ray diffraction data.

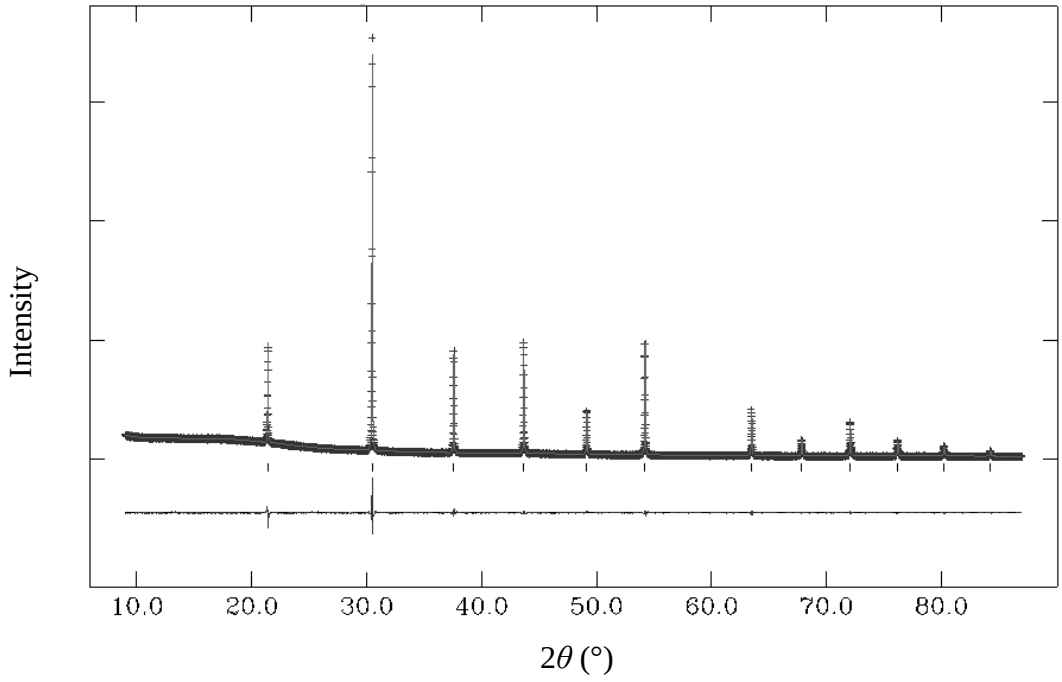


Table 2. Refined crystal structure of $Ba_2Sc_{1.5}P_{0.5}O_{5.5}$ using cubic *Pm3m* (221) space group using room temperature X-ray diffraction data.

		a (Å)			R_{wp}	R_p	χ^2
		4.1404 (1)			4.00	2.71	2.44
		x	*y*	*z*		Fractional occupancy	U_{iso} (Å^2 x 100)
Ba	1(b)	½	½	½		1.000	1.88 (1)
Sc	1(a)	0	0	0		0.748 (7)	2.59 (5)
P	1(a)	0	0	0		0.252 (7)	2.59 (5)
O	3(d)	0	0	½		0.917 (4)	3.9 (1)

Fig. 4 Observed (cross), calculated (line), reflection positions and difference plots (observed − calculated) of $Ba_2Sc_{1.4}Si_{0.6}O_{5.3}$ from the Rietveld refinement for room temperature X-ray diffraction data.

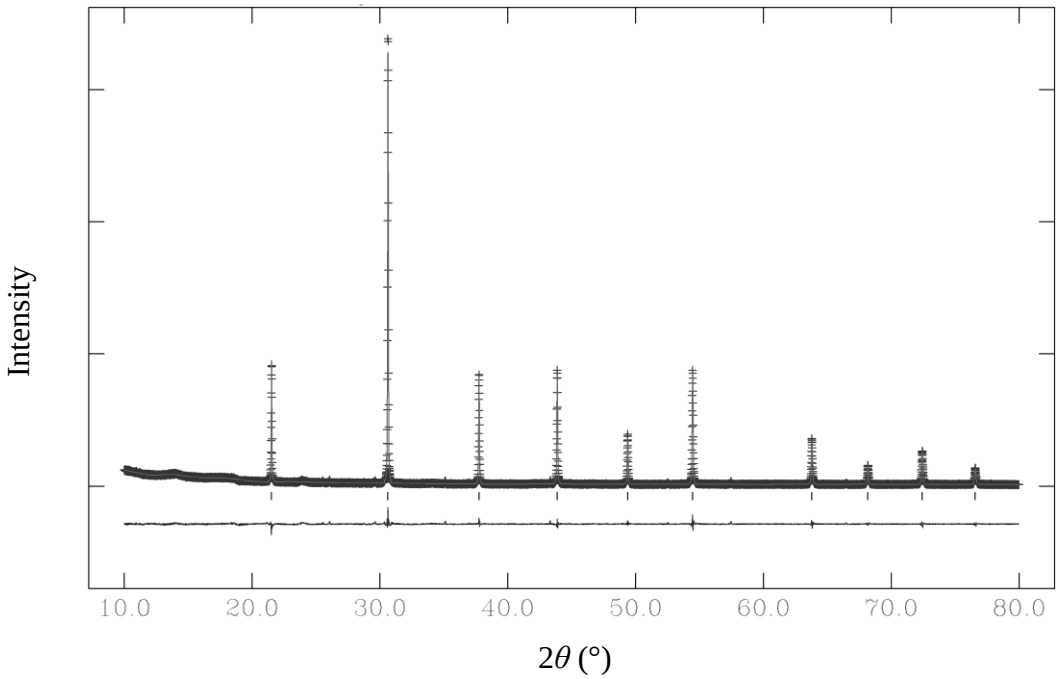


Table 3. Refined crystal structure of $Ba_2Sc_{1.4}Si_{0.6}O_{5.3}$ using cubic *Pm3m* (221) space group using room temperature X-ray diffraction data.

		a (Å)			R_{wp}	R_p	χ^2
		4.1225 (1)			8.72	6.07	2.81
		x	*y*	*z*		Fractional occupancy	U_{iso} (Å^2 x 100)
Ba	1(b)	½	½	½		1.000	1.69 (2)
Sc	1(a)	0	0	0		0.739 (8)	3.12 (7)
Si	1(a)	0	0	0		0.261 (8)	3.12 (7)
O	3(d)	0	0	½		0.874 (5)	3.6 (1)