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Supporting Information

Elucidating the Diffusion Pathway of Protons in Ammonium Polyphosphate: a potential Electrolyte for Intermediate Temperature Fuel Cells

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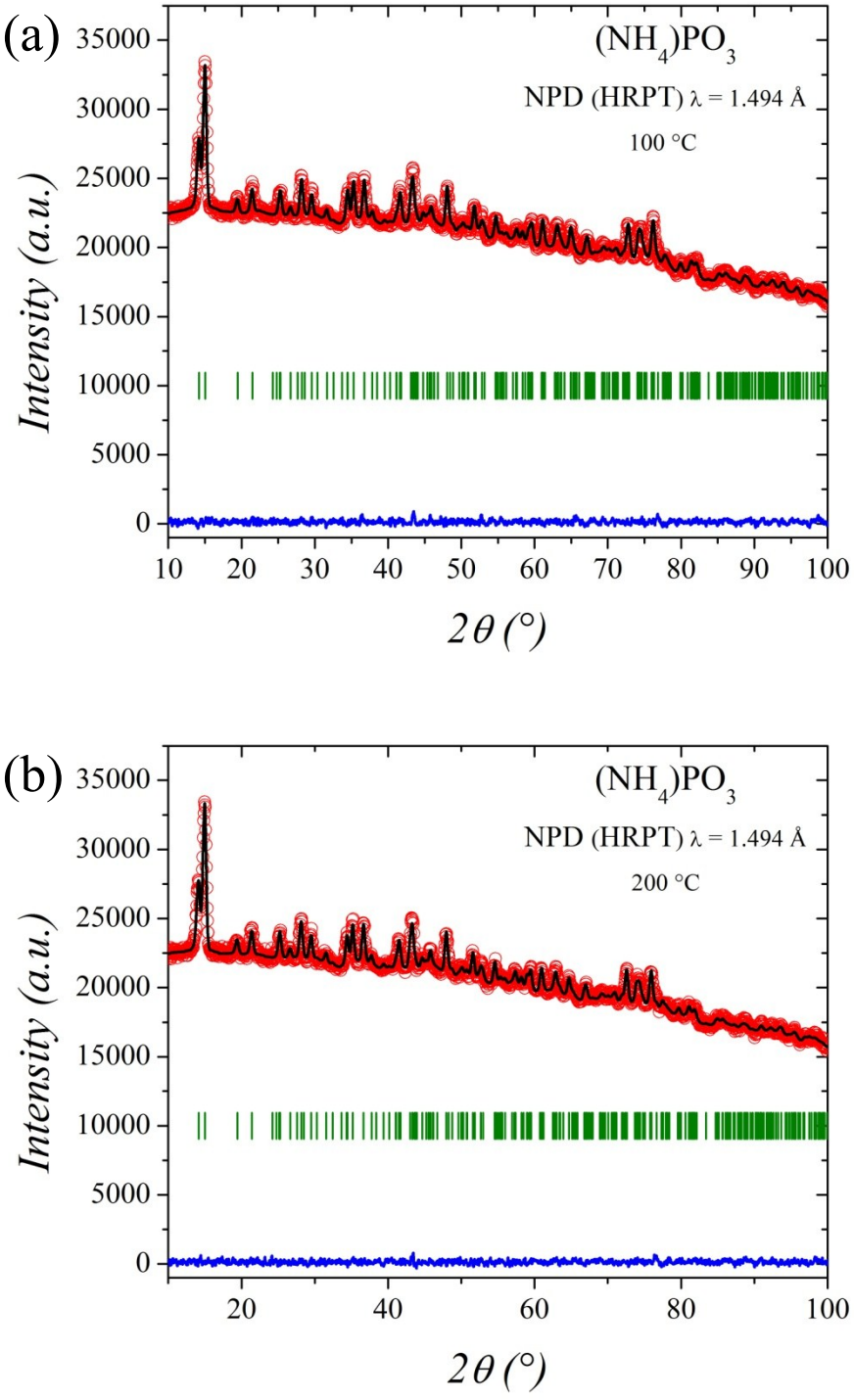

Fig. S1: Observed (circles), calculated (line), and difference (bottom) neutron-diffraction patterns of the NH_4PO_3 at (a) 100 and (b) 200 °C.

Table S1: Crystallographic data for NH_4PO_3 phase from the XRPD refinements at RT. System: orthorhombic, space group: $P2_12_12_1$.

Unit-cell parameters: a=12.049(1) Å, b=6.4709(5) Å, c=4.2486(4) Å and V = 331.26(5) Å^3.					
Atom	x/a	y/b	z/c	B_{iso}	Occ
P	0.1800(3)	0.5659(6)	0.277(1)	3.31(8)	1
O1	0.1801(6)	0.777(1)	0.134(1)	4.0(2)	1
O2	0.0813(6)	0.493(1)	0.437(1)	4.0(2)	1
O3	0.287(7)	0.590(1)	0.515(2)	4.0(2)	1
N	0.0883(5)	0.065(1)	0.614(1)	1.2(2)	1
R_p: 10.2%; R_{wp}: 13.9%; R_{exp}: 7.1%; χ^2: 3.8; R_{Bragg}: 7.3%					

Table S2. Crystallographic data for NH_4PO_3 phase from NPD at a) 100 °C and b) 200°C System: orthorhombic, Space group: $P2_12_12_1$.

a) T= 100 °C. Unit-cell parameters: a=12.094(2) Å, b=6.476(1) Å, c=4.2543(8) Å and V = 333.2(1) Å^3.					
Atom	x/a	y/b	z/c	B_{iso}	Occ
P	0.184(1)	0.568(2)	0.272(3)	2.1(3)	1
O1	0.179(1)	0.791(2)	0.132(3)	1.4(2)	1
O2	0.077(1)	0.484(2)	0.403(3)	1.4(2)	1
O3	0.284(1)	0.589(2)	0.556(3)	1.4(2)	1
N	0.0903(9)	0.055(2)	0.612(3)	3.0(2)	1
H1	0.076(3)	-0.024(6)	0.431(8)	7.7(4)	1
H2	0.155(3)	0.008(5)	0.717(7)	7.7(4)	1
H3	0.024(2)	0.052(7)	0.785(7)	7.7(4)	1
H4	0.103(3)	0.202(6)	0.543(9)	7.7(4)	1
R_p: 0.8%; R_{wp}: 0.9%; R_{exp}: 0.8%; χ^2: 1.6; R_{Bragg}: 6.2%					
b) T = 200 °C. Unit-cell parameters: a=12.143(2) Å, b=6.493(1) Å, c=4.2627(8) Å and V = 336.1(1) Å^3.					
Atom	x/a	y/b	z/c	B_{iso}	Occ
P	0.181(1)	0.567(2)	0.266(3)	2.9(3)	1
O1	0.181(1)	0.789(2)	0.134(3)	2.6(1)	1
O2	0.076(1)	0.485(2)	0.404(3)	2.6(1)	1
O3	0.283(1)	0.589(2)	0.514(2)	2.6(1)	1
N	0.0874(9)	0.053(1)	0.621(2)	10(1)	1
H1	0.072(3)	-0.018(6)	0.447(8)	8.8(9)	1
H2	0.154(3)	-0.001(5)	0.726(7)	8.6(9)	1
H3	0.027(3)	0.043(7)	0.791(8)	8.7(9)	1
H4	0.100(2)	0.206(6)	0.556(9)	8.3(8)	1
R_p: 0.7%; R_{wp}: 0.9%; R_{exp}: 0.8%; χ^2: 1.4; R_{Bragg}: 7.1%					