

Supporting Information of Proton conductivity in mixed cation phosphate, $\text{KMg}_{1-x}\text{H}_{2x}(\text{PO}_3)\cdot y\text{H}_2\text{O}$, with a layered structure at low-intermediate temperatures

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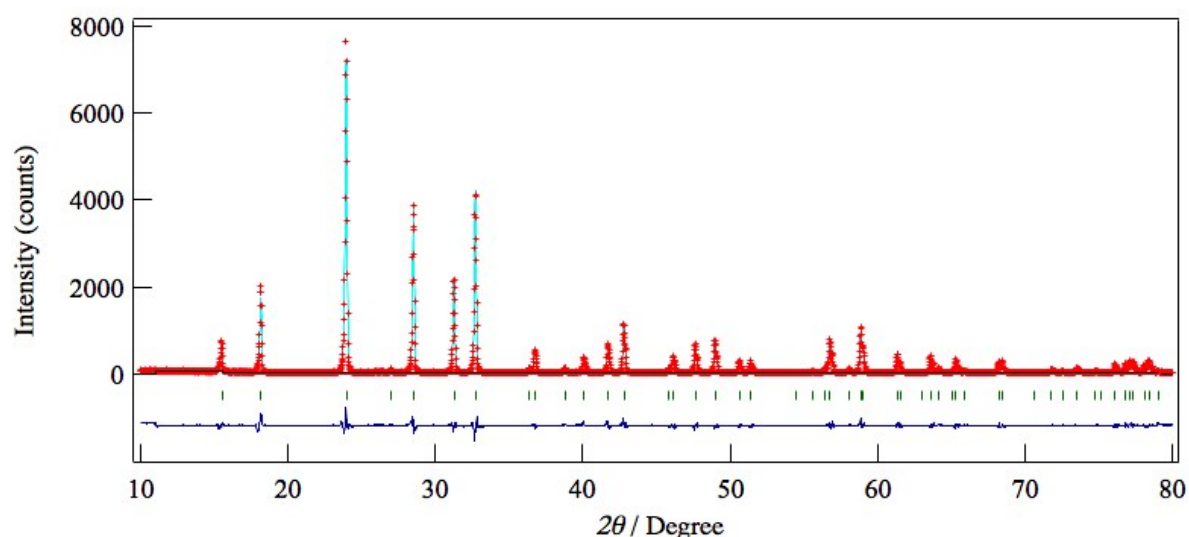


Fig. S1 The final X-ray Rietveld refinement patterns for $\text{KMg}_{1-x}\text{H}_{2x}(\text{PO}_3)\cdot y\text{H}_2\text{O}$ ($x = 0$).

Table S1 The refined structural parameters for the sample with $x = 0$.

Atom	Site	<i>g</i>	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> / Å ²
K	2e	1.0	2/3	1/3	0	0.5
Mg	2c	1.0	1/3	2/3	0	0.5
P	6k	1.0	0.2235(3)	-0.0605(3)	1/4	0.5
O(1)	6k	1.0	0.2408(7)	0.1885(5)	1/4	1.0
O(2)	12l	1.0	0.3271(4)	-0.0772(3)	0.1196(2)	1.0

Space group: *P*-6*c*2, *a* = 6.6057(2) Å, 9.7709(10) Å, *R*_{wp} (%) = 14.65,
*R*_p (%) = 10.14, *R*_e (%) = 9.35, *R*_B (%) = 3.75, *R*_F (%) = 3.35, *S* = 1.57.

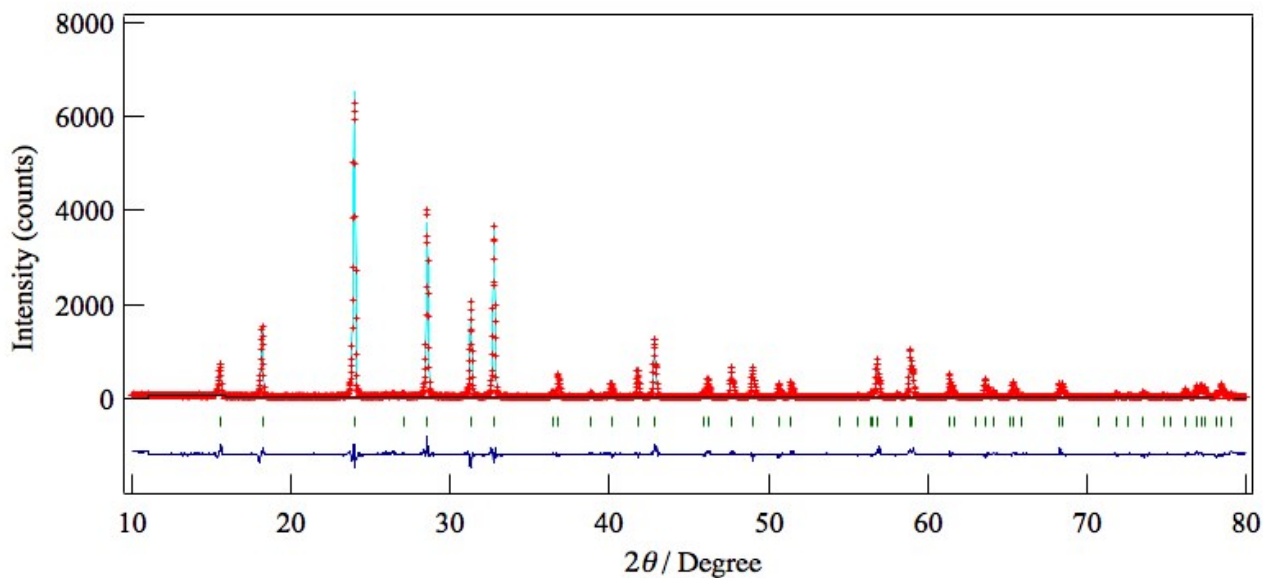


Fig. S2 The final X-ray Rietveld refinement patterns for $\text{KMg}_{1-x}\text{H}_{2x}(\text{PO}_3) \cdot y\text{H}_2\text{O}$ ($x = 0.10$).

Table S2 The refined structural parameters for the sample with $x = 0.10$

Atom	Site	g	x	y	z	$B / \text{\AA}^2$
K	2e	1.0	2/3	1/3	0	0.5
Mg	2c	0.9	1/3	2/3	0	0.5
P	6k	1.0	0.2266(3)	-0.064(3)	1/4	0.5
O(1)	6k	1.0	0.2415(7)	0.1795(5)	1/4	1.0
O(2)	12l	1.0	0.3244(4)	-0.0814(4)	0.1160(2)	1.0

Space group: $P-6c2$, $a = 6.6005(2) \text{ \AA}$, $9.7665(4) \text{ \AA}$, $R_{\text{wp}} (\%) = 16.08$,
 $R_p (\%) = 11.50$, $R_e (\%) = 9.65$, $R_B (\%) = 7.41$, $R_F (\%) = 5.71$, $S = 1.66$.

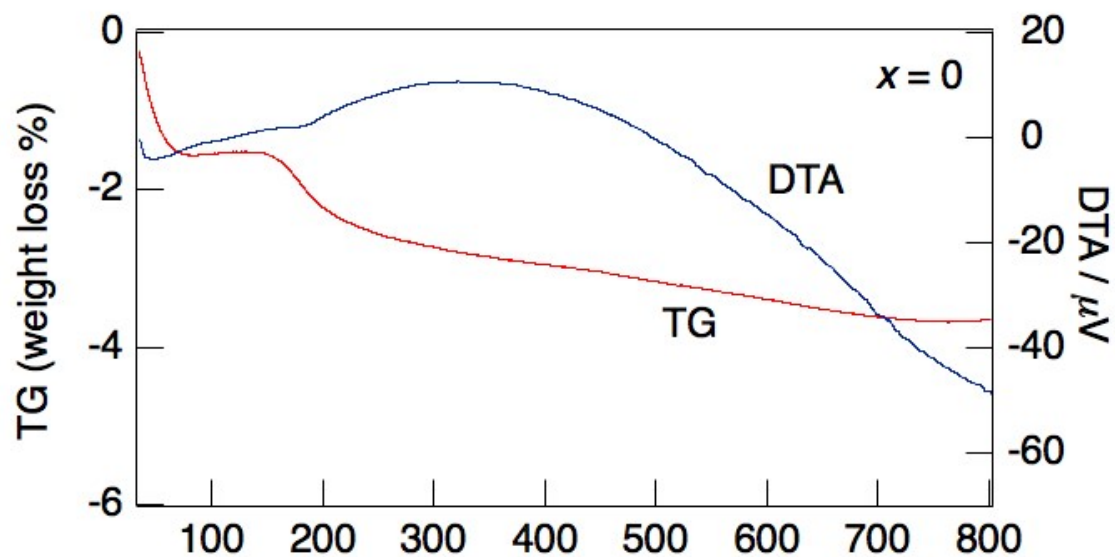


Fig. 3S TG/DTA curves for the sample with $x = 0$ between 30°C and 800°C measured in a N_2 gas flow.

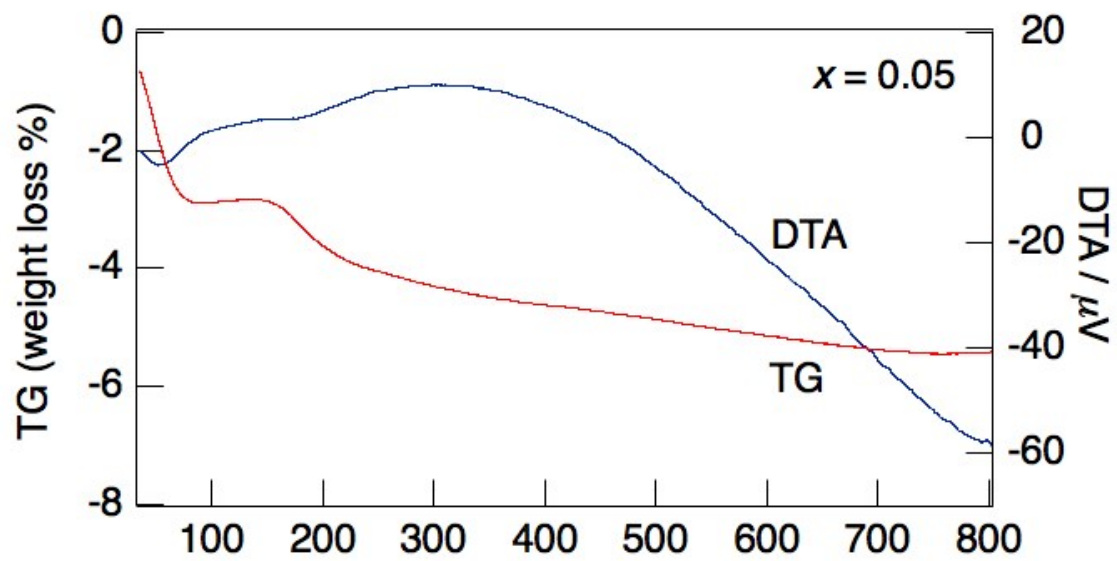


Fig. 4S TG/DTA curves for the sample with $x = 0.05$ between 30°C and 800°C measured in a N_2 gas flow.