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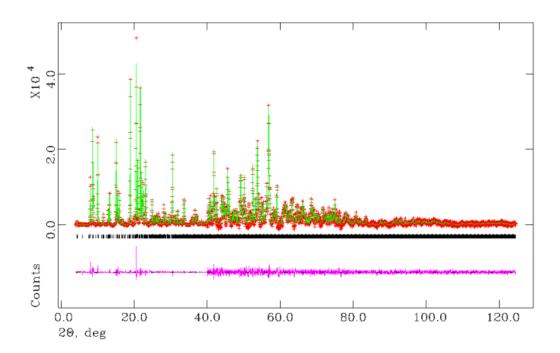
## Supporting information

## Three-dimensional crystal structure of novel aluminophosphate PST-5 solved by powder charge flipping thod

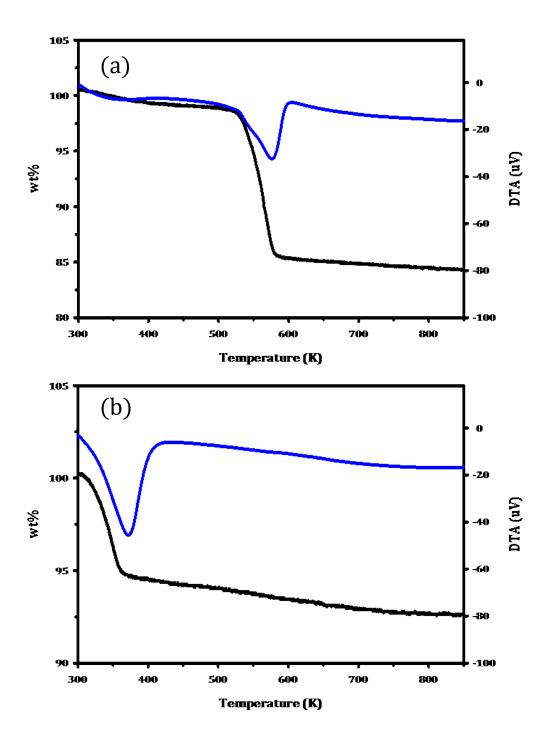
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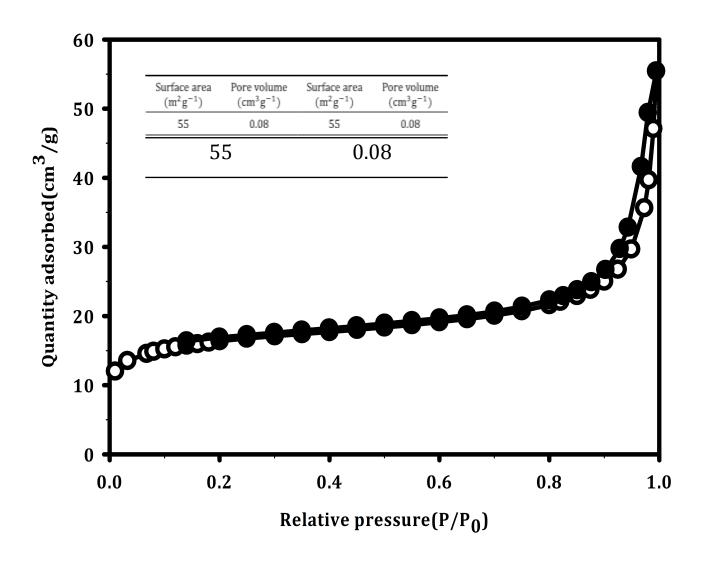
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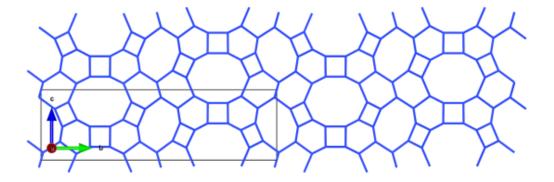
 $\pmb{\text{Fig. S1}}$  Rietveld refinement of XRPD patterns of PST-6 (1day) after the calcination at 823 K flowing oxygen.



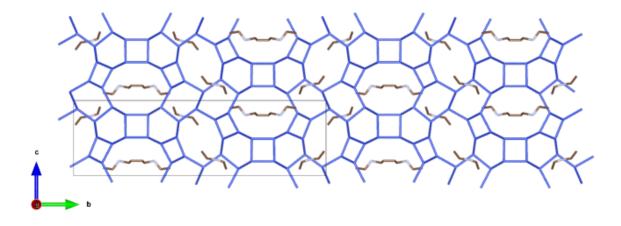
**Fig. S2** TG-DTA of (a) PST-5 and (b) PST-6 after the calcination at 423 K with ozone flowing oxygen. The black and blue lines indicate the weight decrease and the DTA against the temperature.



**Fig. S3** Nitrogen adsorption-desorption isotherm at 77 K on PST-6 after the calcination at 423 K with ozone flowing oxygen. The open and close symbol represents the adsorption and desorption isotherm, respectively.



**Fig. S4** Best possible framework structure for PST-5 obtained from *Focus* program suites.



 $\textbf{Fig. S5} \ Location \ of \ DEA \ in \ the \ framework \ structure \ for \ PST-5. \ The \ oxygen \ atom \ is \ omitted \ for \ clarity.$