Supporting information

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

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Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2017
**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.
**Fig. S5** Location of DEA in the framework structure for PST-5. The oxygen atom is omitted for clarity.