

Supporting Information

Hollow nanocrystals of silicoaluminophosphate molecular sieve synthesized by an aminothermal co-templating strategy

Dehua Wang, Miao Yang, Wenna Zhang, Dong Fan, Peng Tian*, and Zhongmin Liu*

Table S1. Interaction energies for the SDA in different cavities. (The calculation is based on a unit cell, which includes two different *gme* (*gme1* and *gme2*) and two different *aft* cages (*aft1* and *aft2*))

	$E_{\text{interaction energy}}$ (kcal/mol)
One TMA in a <i>gme1</i> cavity and One TMA in a <i>gme2</i> cavity	-30.18
Two TMAs in a <i>gme1</i> cavity and Two TMAs in a <i>gme2</i> cavity	247.37
One TMA in a <i>aft1</i> cavity and One TMA in a <i>aft2</i> cavity	-29.18
One TEA in a <i>aft1</i> cavity and One TEA in a <i>aft2</i> cavity	-53.18
Two TEAs in a <i>aft1</i> cavity and Two TEAs in a <i>aft2</i> cavity	-103.2
Three TEAs in a <i>aft1</i> cavity and Three TEAs in a <i>aft2</i> cavity	2424.11

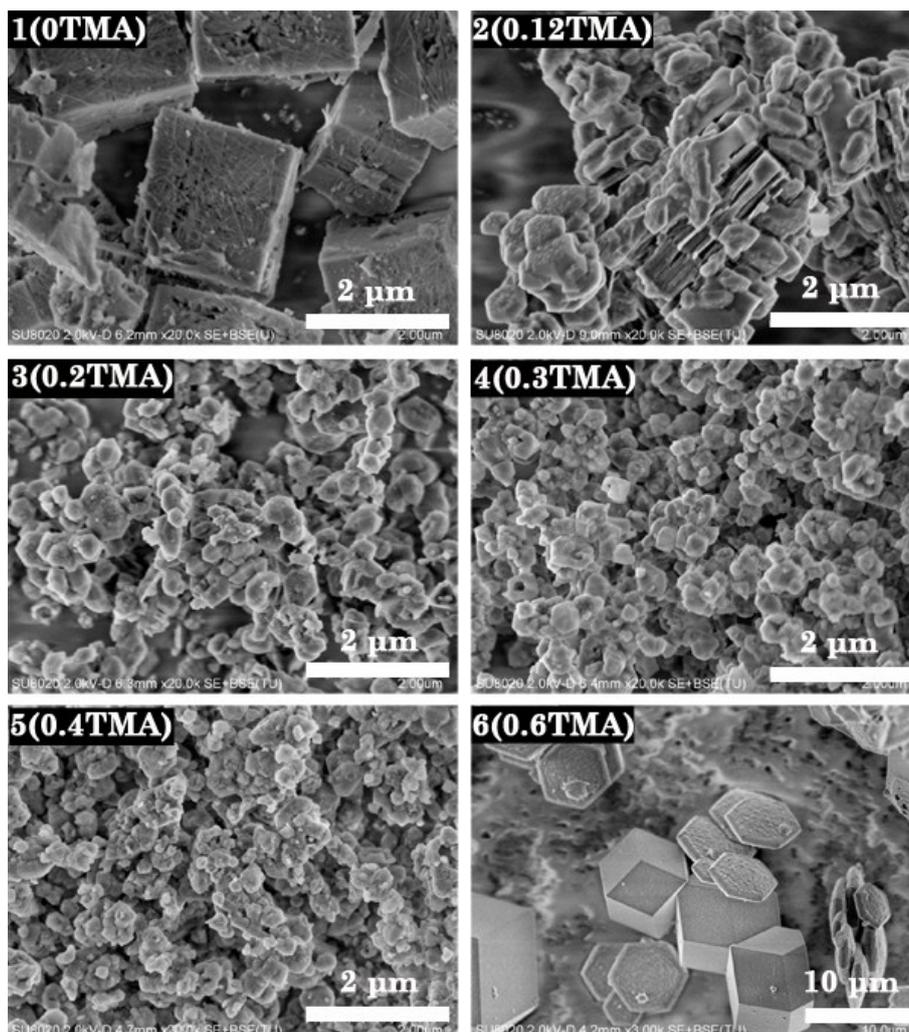
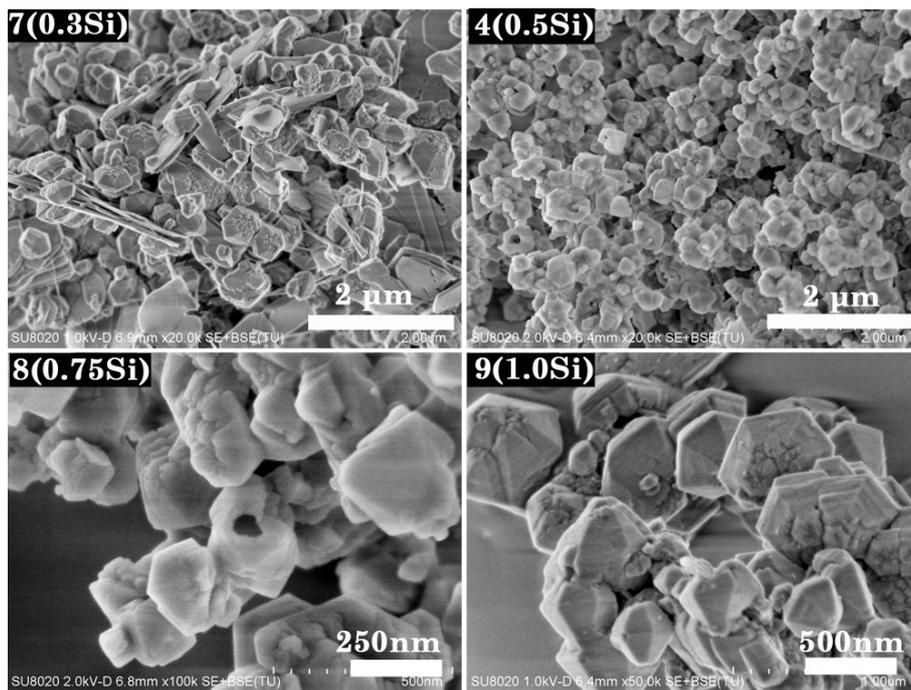
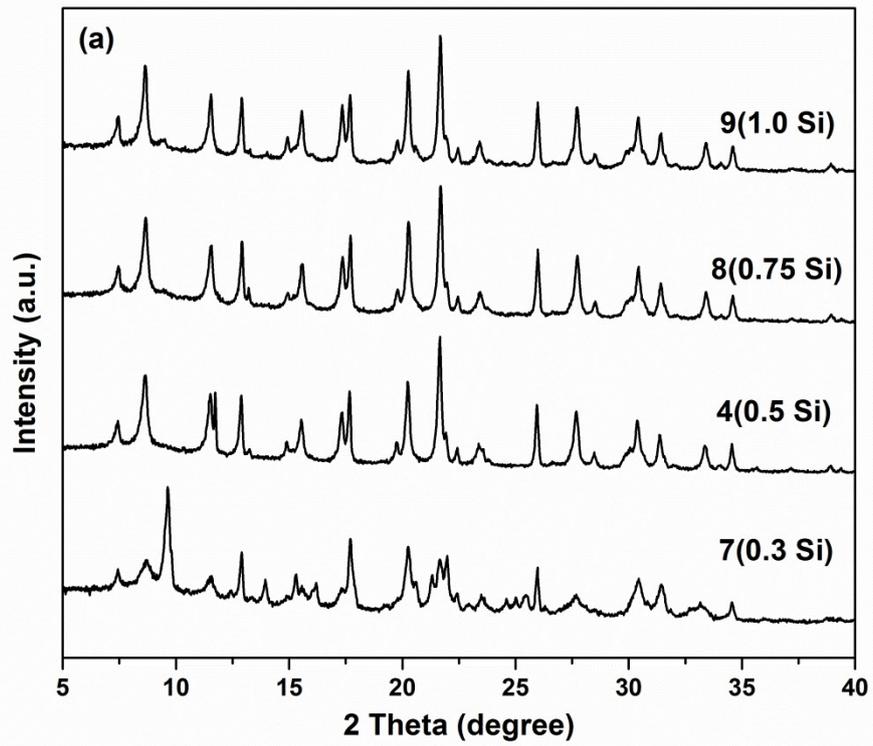


Fig. S1 SEM images of the calcined samples 1 (0TMA), 2 (0.12TMA), 3 (0.2TMA), 4 (0.3TMA), 5 (0.4TMA) and 6 (0.6TMA).



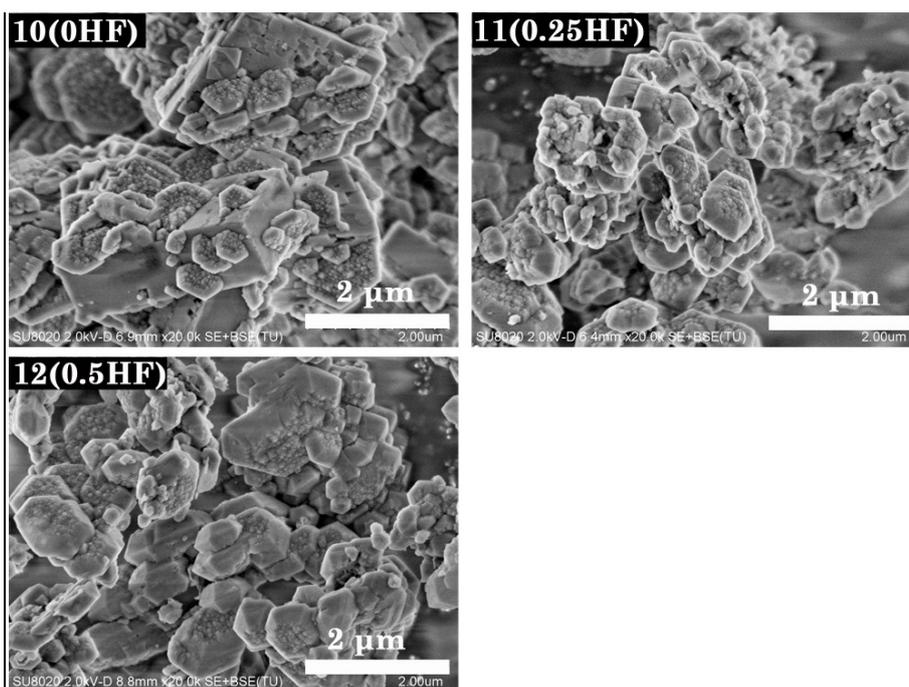
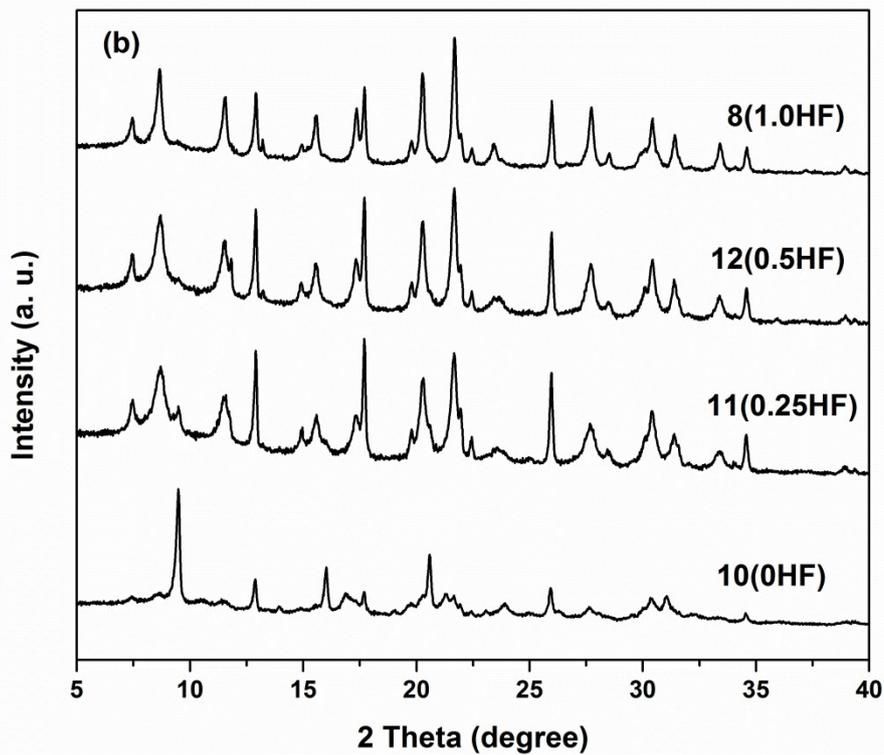


Fig. S2 XRD patterns of the as-synthesized samples 7 (0.3Si), 4 (0.5Si), 8 (0.75Si), 9 (1.0Si), 10 (0HF), 11 (0.25HF) and 12 (0.5HF) and their corresponding SEM images of the calcined form.

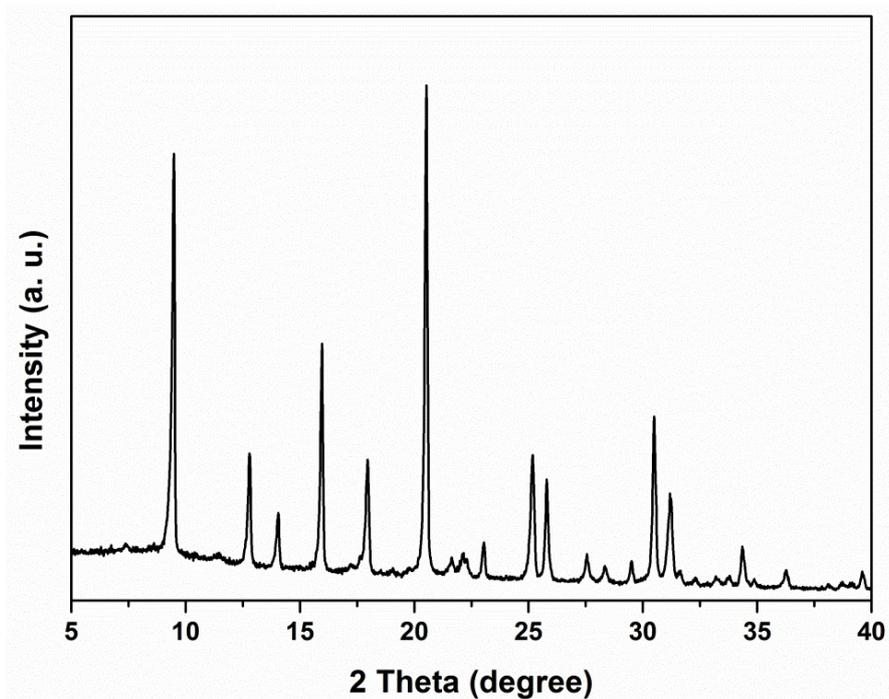


Fig. S3 The XRD pattern of the as-synthesized sample by the route of hydrothermal synthesis (Condition: the gel molar composition of 7TEA/1Al₂O₃/1P₂O₅/0.75SiO₂/0.3TMA/1.0HF/50H₂O at 200 °C for 36 h).

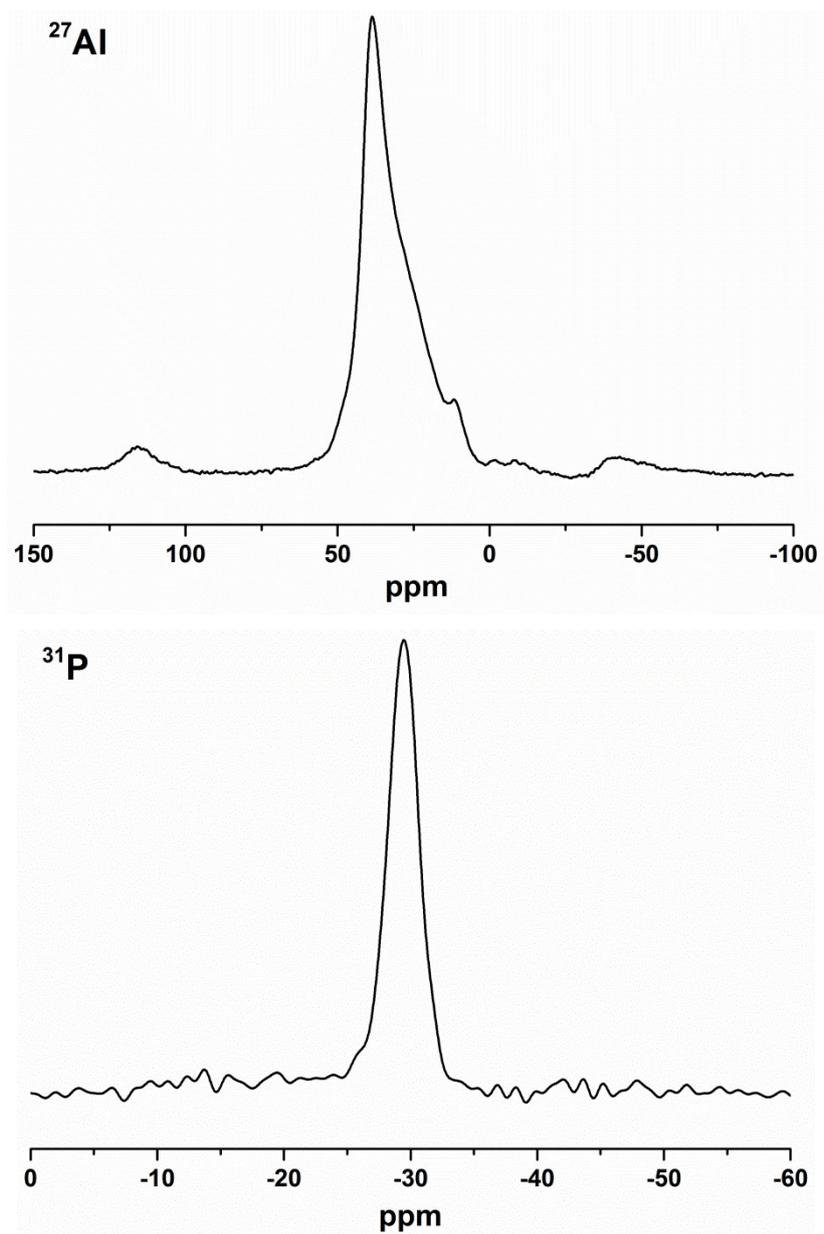


Fig. S4 ^{27}Al and ^{31}P MAS NMR of the as-synthesized SAPO-56 (sample 8).

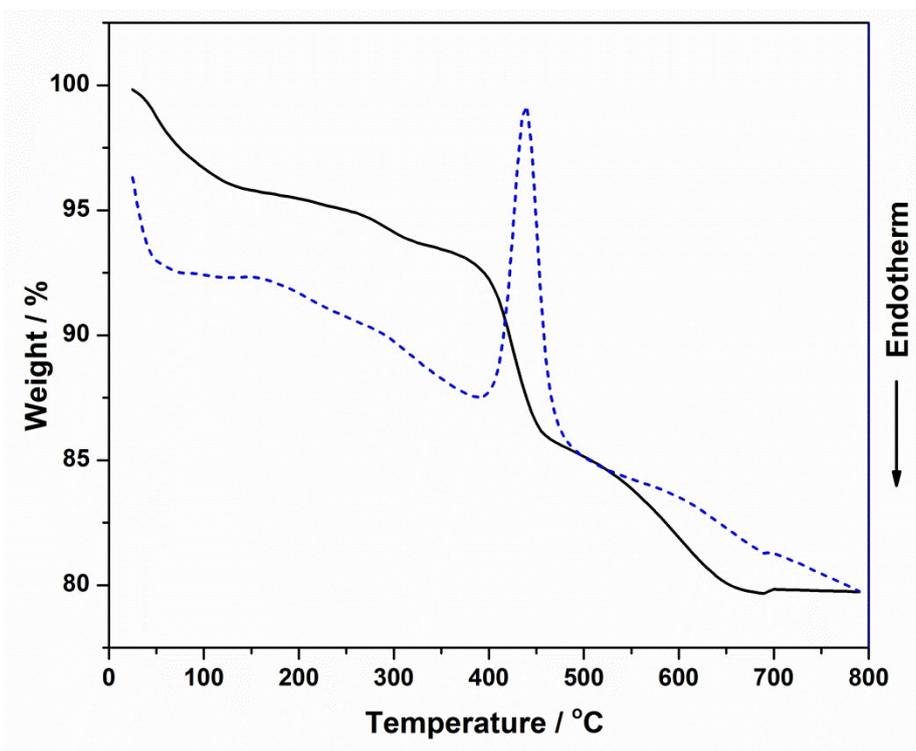


Fig. S5 TG (solid)-DSC (dotted) curves of the sample 8.

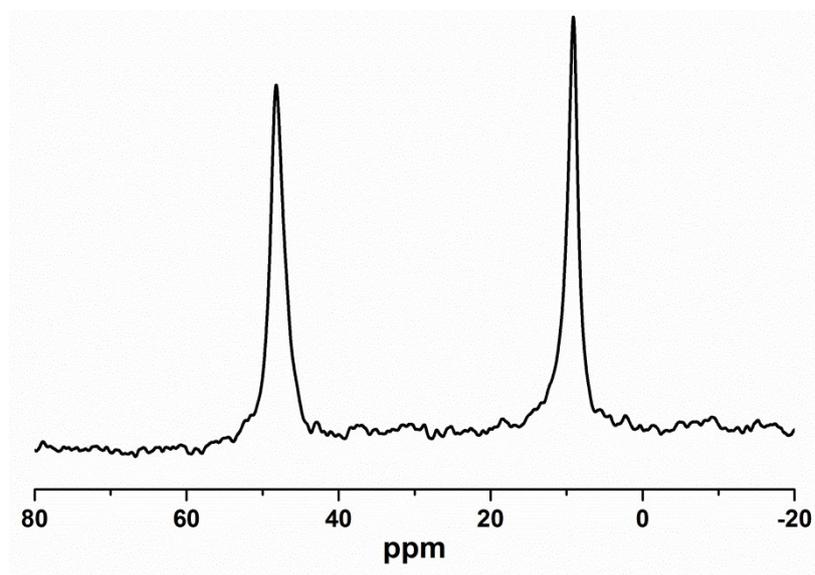


Fig. S6 ¹³C MAS NMR spectrum of the SAPO-34 (sample 2.33h). The two peaks are integrated and their ratio is close to 1/1, suggesting that the inclusion in SAPO-34 is only TEA. The peak centered at 48 and 9.5 ppm can be ascribed to the $-\text{CH}_2-$ and $-\text{CH}_3$ groups of TEA.

The ^{19}F MAS NMR spectra were recorded on a Bruker AVANCE III 400 WB spectrometer equipped with a 2.5 mm standard bore CP MAS probehead whose X channel was tuned to 376.55 MHz for ^{19}F , using a magnetic field of 9.39 T at 297 K. The dried and finely powdered samples were packed in the ZrO_2 rotor closed with Kel-F cap which were spun at 20 kHz rate. A total of 2000 scans were recorded with 3 s recycle delay for each sample. All ^{19}F MAS NMR chemical shifts are referenced to the resonances of trichlorofluoromethane (CFCl_3) standard ($\delta=0.00$).

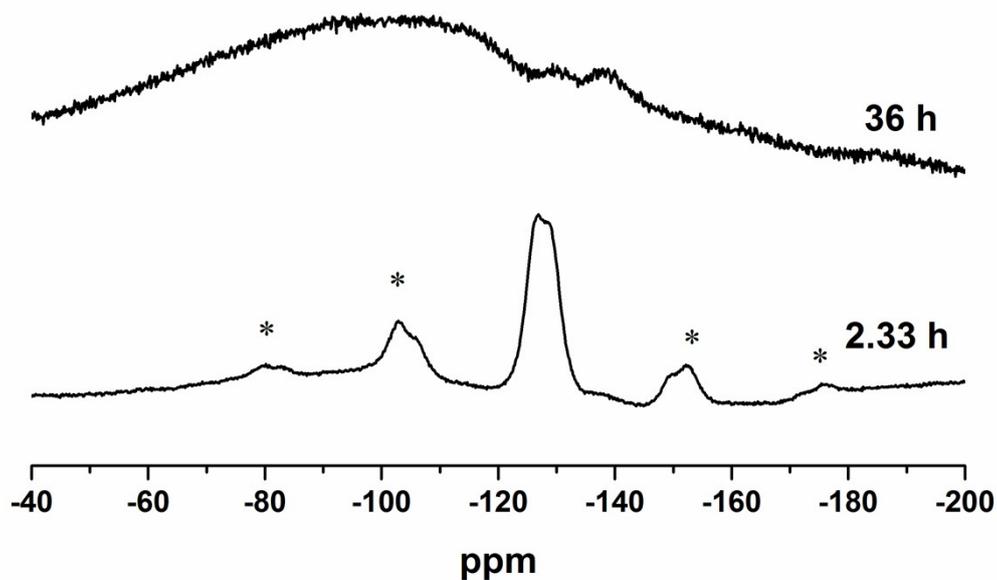


Fig. S7 ^{19}F MAS NMR spectra of the samples crystallizing at 2.33 h (SAPO-34) and 36 h (SAPO-56).