SUPPORTING INFORMATION

A retrosynthetic co-templating method for the preparation of silicoaluminophosphate molecular sieves

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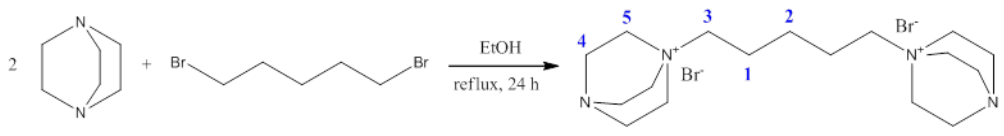
Organic Synthesis of Structure-directing Agents

1,5-(1,4-diazabicyclo[2.2.2]octane)pentyl dibromide (diDABCO-C5)



13.0 g (0.06 mol) of 1,5-dibromopentane was dissolved in 50 mL ethanol and added droop-wise to a solution under stirring at 50 °C of 33.6 g (0.30 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving yellow oil. Subsequently cold

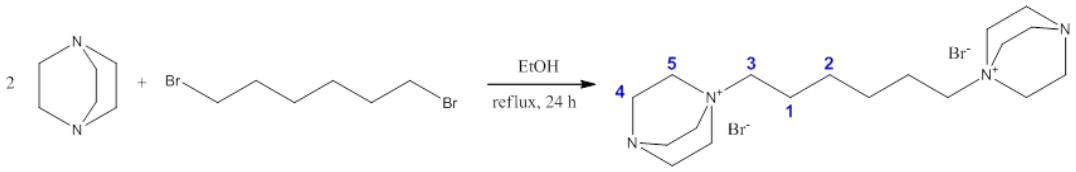
diethyl ether was added to the oil to favour the precipitation of a white solid. That was washed with cold acetone and acetonitrile and dried at 50 °C overnight. The reaction yields 20.27 g (yield 79%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.31 (sept, 2H, 2), 1.75 (sept, 4H, 1), 3.09 (t, 12H, 4), 3.19 (t, 4H, 3), 3.31 (t, 12H, 5).

^{13}C NMR (100 MHz, D_2O, ppm) δ = 21.31 (s, 1), 23.02 (s, 2), 44.52 (s, 4), 52.49 (s, 5), 64.35 (s, 3).

CHN analysis experimental (calculated): C 44.85 (44.95), H 7.42 (7.54), N 12.26 (12.33).

1,6-(1,4-diazabicyclo[2.2.2]octane)hexyl dibromide (diDABCO-C6)



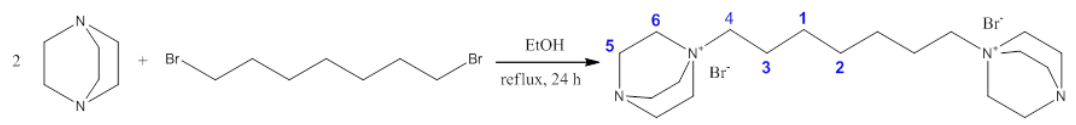
13.0 g (0.05 mol) of 1,6-dibromohexane was dissolved in 50 mL ethanol and added droop-wise to a solution under stirring at 50 °C of 32.0 g (0.29 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving a white solid. That was washed with cold diethyl ether, acetonitrile and acetone and dried at 50 °C overnight. The reaction yields 24.60 g (yield 98%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.30 (m, 4H, 2), 1.66 (m, 4H, 1), 3.06 (t, 12H, 4), 3.14 (t, 4H, 3), 3.28 (t, 12H, 5).

^{13}C NMR (100 MHz, D2O, ppm) δ = 21.43 (s, 1), 25.52 (s, 2), 44.51 (s, 4), 52.42 (s, 5), 64.65 (s, 3).

CHN analysis experimental (calculated): C 46.01 (46.16), H 7.67 (7.75), N 11.91 (11.96).

1,7-(1,4-diazabicyclo[2.2.2]octane)heptyl dibromide (diDABCO-C7)



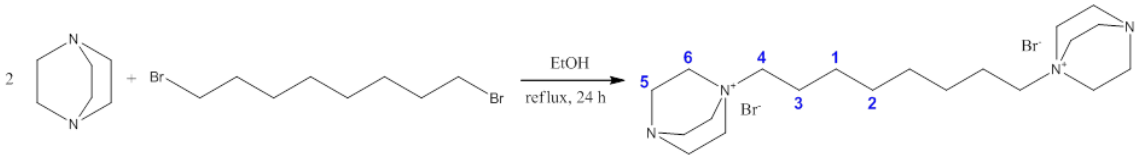
10.0 g (0.04 mol) of 1,7-dibromoheptane was dissolved in 50 mL ethanol and added droop-wise to a solution under stirring at 50 °C of 23.0 g (0.21 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving yellow oil. Subsequently cold diethyl ether was added to the oil to favour the precipitation of a white solid. That was washed with cold acetone and acetonitrile and dried at 50 °C overnight. The reaction yields 17.89 g (yield 96%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.29 (m, 6H, 1, 2), 1.66 (m, 4H, 3), 3.08 (t, 12H, 5), 3.15 (t, 4H, 4), 3.29 (t, 12H, 6).

^{13}C NMR (100 MHz, D2O, ppm) δ = 21.42 (s, 1), 25.68 (s, 2), 28.04 (s, 3), 44.54 (s, 5), 52.42 (s, 6), 64.85 (s, 4).

CHN analysis experimental (calculated): C 47.25 (47.31), H 7.82 (7.94), N 11.54 (11.62).

1,8-(1,4-diazabicyclo[2.2.2]octane)octyl dibromide (diDABCO-C8)



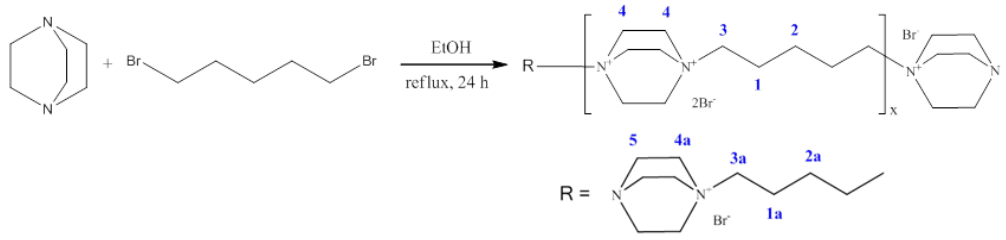
13.0 g (0.05 mol) of 1,8-dibromooctane was dissolved in 50 mL ethanol and added droop-wise to a solution under stirring at 50 °C of 28.4 g (0.25 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving yellow oil. Subsequently cold diethyl ether was added to the oil to favour the precipitation of a white solid. That was washed with cold acetone and acetonitrile and dried at 50 °C overnight. The reaction yields 21.69 g (yield 91%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.26 (m, 8H, 1, 2), 1.65 (m, 4H, 3), 3.08 (t, 12H, 5), 3.15 (t, 4H, 4), 3.29 (t, 12H, 6).

^{13}C NMR (100 MHz, D_2O, ppm) δ = 21.48 (s, 1), 25.77 (s, 2), 28.23 (s, 3), 44.55 (s, 5), 52.41 (s, 6), 64.95 (s, 4).

CHN analysis experimental (calculated): C 48.25 (48.39), H 8.19 (8.12), N 11.21 (11.29).

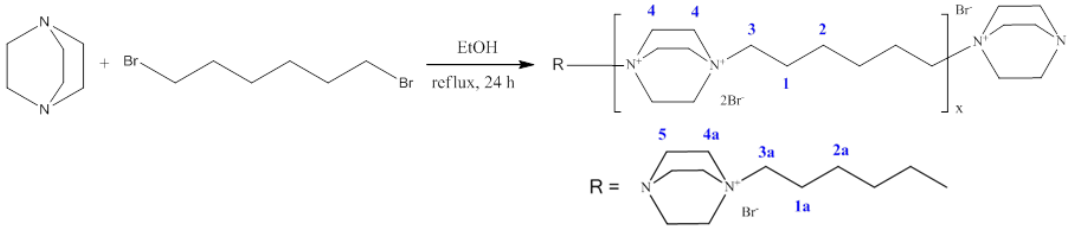
olig-(1,4-diazabicyclo[2.2.2]octane)-pentyl dibromide ([DABCO-C5]$_3$)



21.0 g (0.09 mol) of 1,5-dibromopentane was dissolved in 50 mL ethanol and added to a solution under stirring at 50 °C of 12.3 g (0.11 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving a white solid. That was washed with cold diethyl ether, acetonitrile and acetone and dried at 50 °C overnight. The reaction yields 25.30 g (yield 76%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.39 (m, 4H, 2, 2a), 1.86 (m, 8H, 1, 1a), 3.17 (t, 12H, 5), 3.38 (t, 8H, 3, 3a), 3.54 (t, 12H, 4a), 3.94 (t, 12H, 4).
^{13}C NMR (100 MHz, D_2O, ppm) δ = 21.32 (s, 1a), 21.63 (s, 1), 22.37 (s, 2), 22.66 (s, 2a), 44.49 (s, 5), 51.58 (s, 4), 52.33 (s, 4a), 64.34 (s, 3a), 64.88 (s, 3).
CHN analysis experimental (calculated): C 39.61 (38.6), H 6.72 (6.4), N 9.28 (8.2).

olig-(1,4-diazabicyclo[2.2.2]octane)-hexyl dibromide ([DABCO-C6]$_3$)



20.1 g (0.08 mol) of 1,5-dibromopentane was dissolved in 50 mL ethanol and added to a solution under stirring at 50 °C of 11.0 g (0.10 mol) of 1,4-diazabicyclo[2.2.2]octane (DABCO) dissolved in 100 mL ethanol. The mixture was refluxed for 24 hours. Once cold, the excess of ethanol was removed on a rotary evaporator leaving a white solid. That was washed with cold diethyl ether,

acetonitrile and acetone and dried at 50 °C overnight. The reaction yields 26.94 g (yield 89%) of product which was analysed by NMR and elemental analysis.

^{1}H NMR (400 MHz, D_2O, ppm) δ = 1.39 (m, 8H, 2, 2a), 1.79 (m, 8H, 1, 1a), 3.15 (t, 12H, 5), 3.37 (t, 8H, 3, 3a), 3.52 (t, 12H, 4a), 3.94 (t, 12H, 4).

^{13}C NMR (100 MHz, D_2O, ppm) δ = 21.47 (s, 1a), 21.79 (s, 1), 25.13 (s, 2), 25.46 (s, 2a), 44.54 (s, 5), 51.55 (s, 4), 52.35 (s, 4a), 64.72 (s, 3a), 65.28 (s, 3).

CHN analysis experimental (calculated): C 41.50 (40.47), H 6.99 (6.79), N 8.89 (7.87).

N.B. The number of repeating units for both oligomers was calculated using the ratio between the integration of the peak associated to the di-cationic DABCO (4, 3.94 ppm) and the terminal DABCO (5, 3.17 ppm).

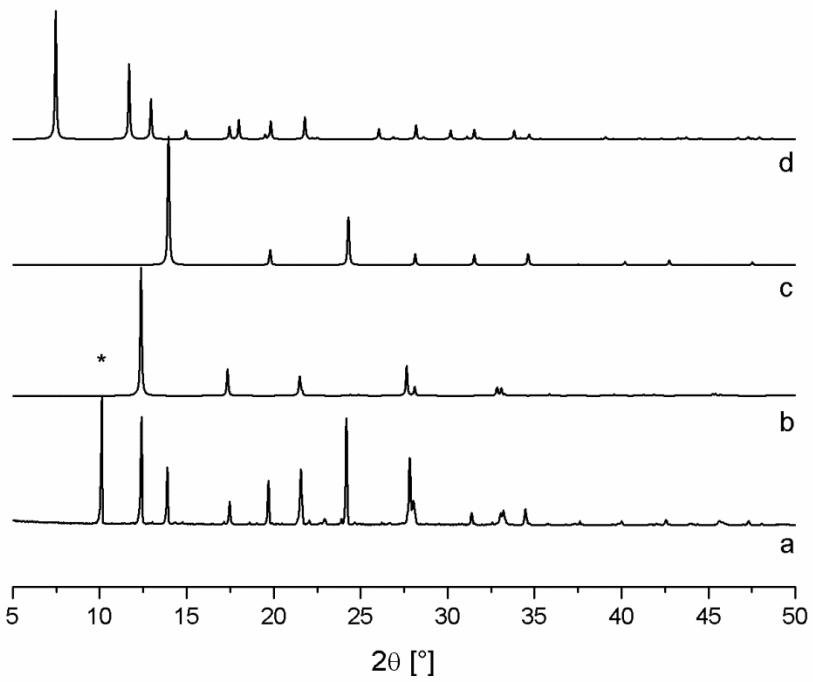


Figure S1. PXRD pattern collected on as-prepared SAPO samples synthesised employing only TrMA as SDA (a). Simulated patterns of MAPO-43 (GIS) (b), SAPO-20 (SOD) (c) and $|Ca_4(H_2O)_{26.4}|$ $[Si_{16}Al_8O_{48}]$ (GME) (d) have been plotted as comparison. The peak marked with the asterisk comes from an unidentified aluminophosphate phase.

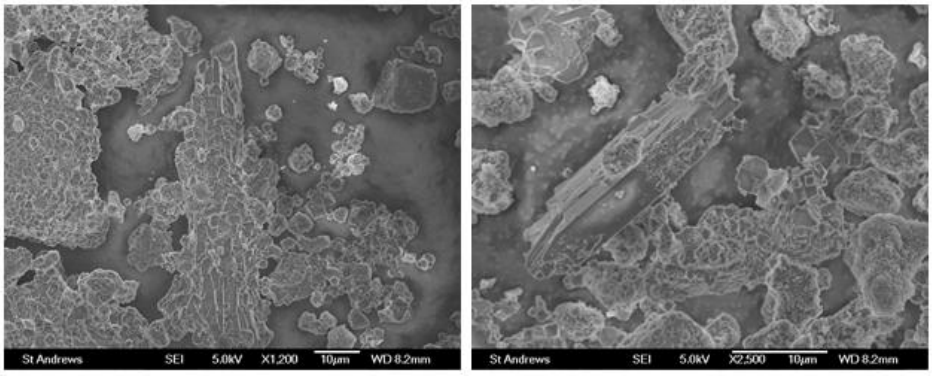


Figure S2. SEM images (two views) of as-prepared SAPO samples synthesised employing TrMA as SDA.

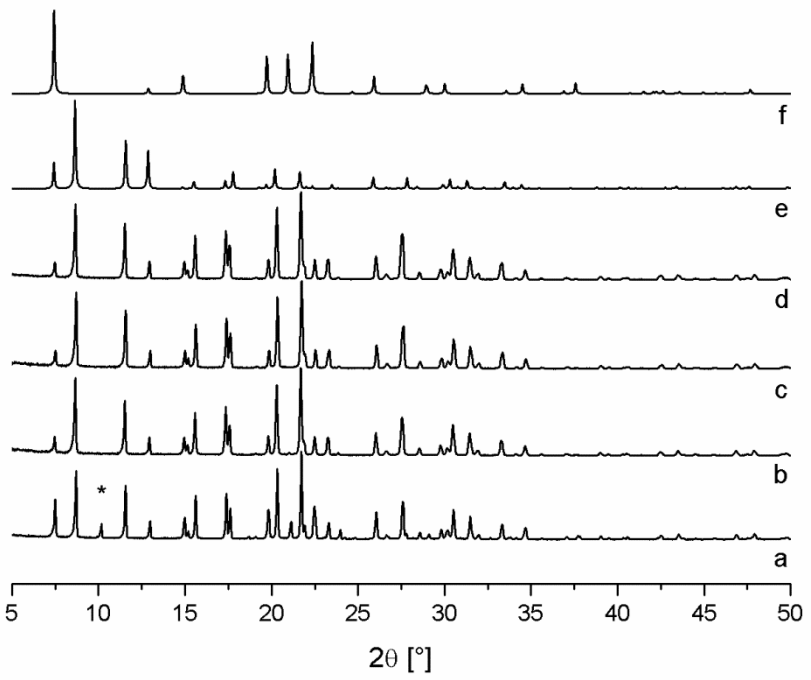


Figure S3. PXRD patterns of the syntheses of SAPO-56 performed at 190 °C using diDABCO-C4 and TrMA as co-SDAs and by varying the Si/Al ratio of the starting gels (composition 1.0 $Al(OH)_3$: 1-x H_3PO_4 : x SiO_2 : 0.1 diDABCO-C4 : 0.21 TrMA : 0.23 TBAOH : 40 H_2O; x = 0.20 (a), 0.23 (b), 0.26 (c) and 0.29 (d)). Simulated patterns of SAPO-56 (AFX) (e) and AlPO-5 (AFI) (f) have been plotted for comparison. The peak marked with the * belong to an unidentified aluminophosphate phase.

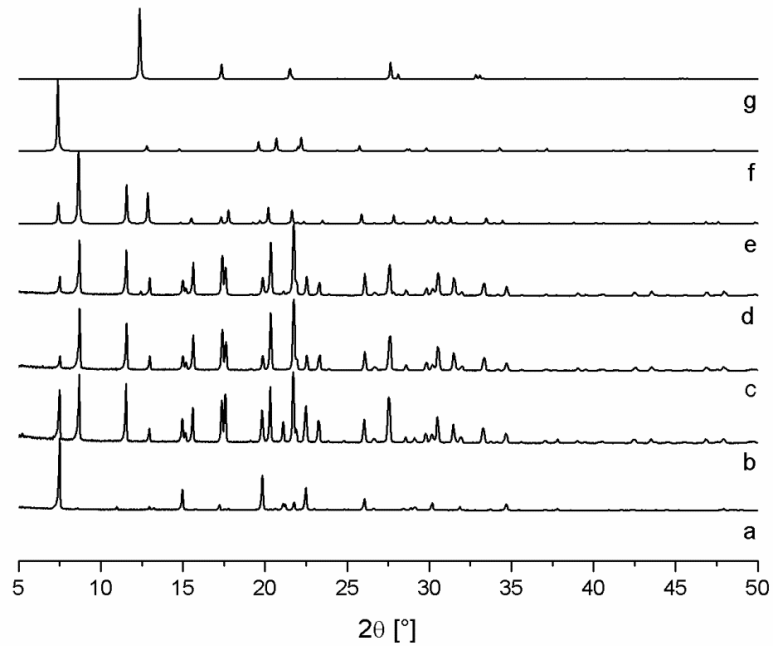


Figure S4. PXRD patterns of samples synthesised at 190 °C by varying the content of TrMA within the starting gel, composition 1.0 $Al(OH)_3$: 0.71 H_3PO_4 : 0.29 SiO_2 : 0.1 diDABCO-C4 : x TrMA : y TBAOH : 40 H_2O; x = 0.0, y = 0.38 (a), x = 0.10, y = 0.28 (b), x = 0.21, y = 0.23 (c) and x = 0.32, y = 0.21 (d). Simulated patterns of SAPO-56 (AFX) (e), AlPO-5 (AFI) (f) and MAPO-43 (GIS) (g) plotted for comparison.

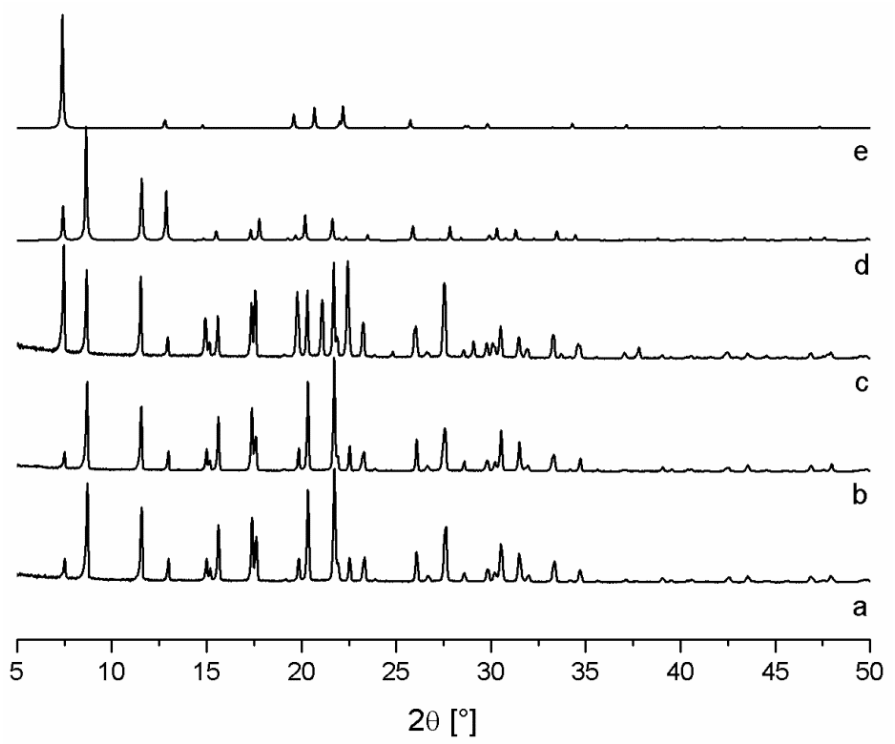


Figure S5. PXRD patterns of the SAPO-56 synthesised at 190 °C using TBAOH (a), TPAOH (b) and TPeAOH (c) as co-bases. Simulated patterns of SAPO-56 (AFX) (d) and AlPO-5 (AFI) (e) as comparison.

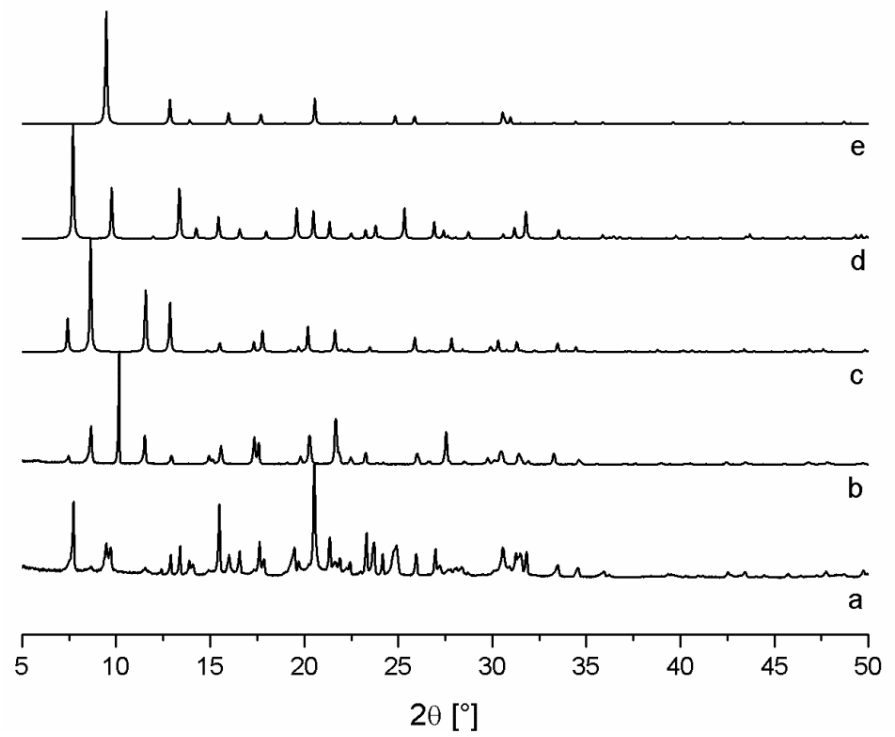


Figure S6. PXRD of samples synthesised at 190 °C using diDABCO-C3 (a) and diDABCO-C5 (b) in gels of composition $Al(OH)_3$: 0.80 H_3PO_4 : 0.20 SiO_2 : 0.1 diDABCO-Cx : 0.21 TrMA : 0.23 TBAOH : 40 H_2O. Simulated patterns of SAPO-56 (AFX) (c), AlPO-17 (ERI) (d) and SAPO-34 (CHA) (e) as comparison.

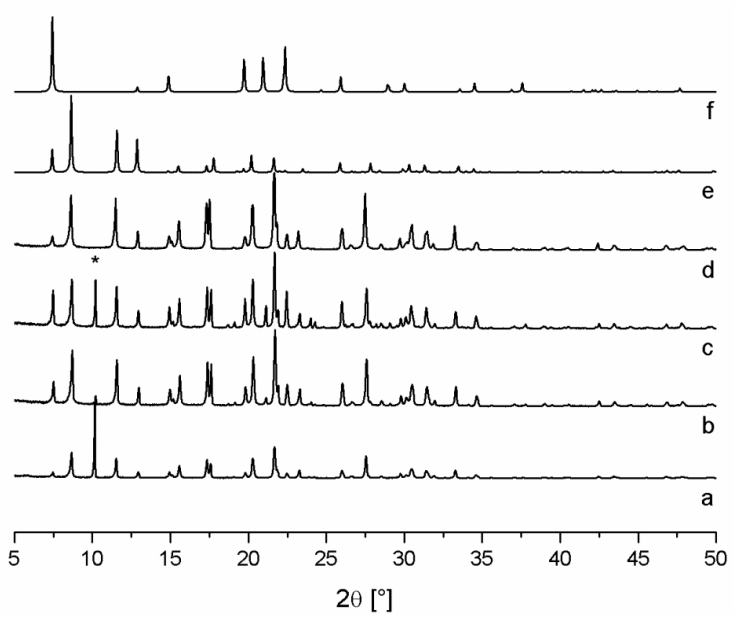


Figure S7. PXRD of SAPO-56 made at 190 °C using diDABCO-C5 and TrMA as SDAs and varying Si/Al of the gels of composition $Al(OH)_3$: 1-x H_3PO_4 : x SiO_2 : 0.1 diDABCO-C5 : 0.21 TrMA : 0.23 TBAOH : 40 H_2O; x = 0.20 (a), 0.23 (b), 0.26 (c) and 0.29 (d). Simulated patterns of SAPO-56 (AFX) (d) and AlPO-5 (AFI) (e) as comparison. Asterisked peak from the unidentified aluminophosphate phase.

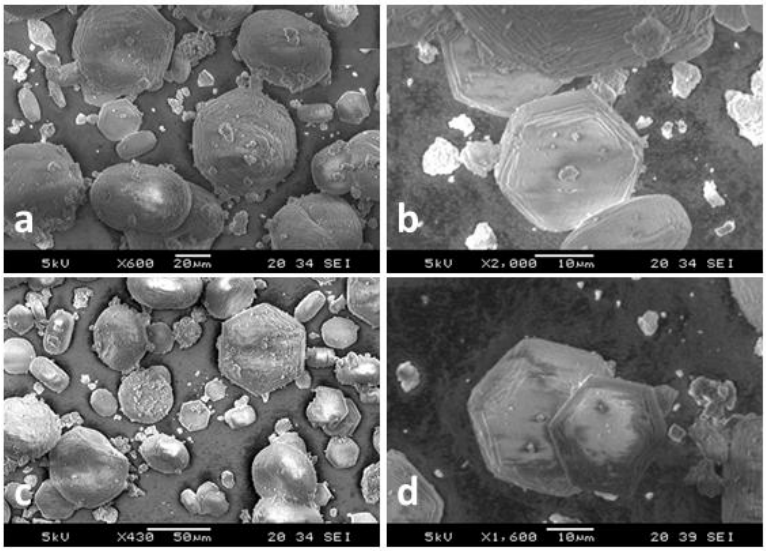


Figure S8. SEM images (two views of each) of SAPO-56 synthesised with TrMA and diDABCO-C4 (a and b) or diDABCO-C5 (c and d) as SDAs.

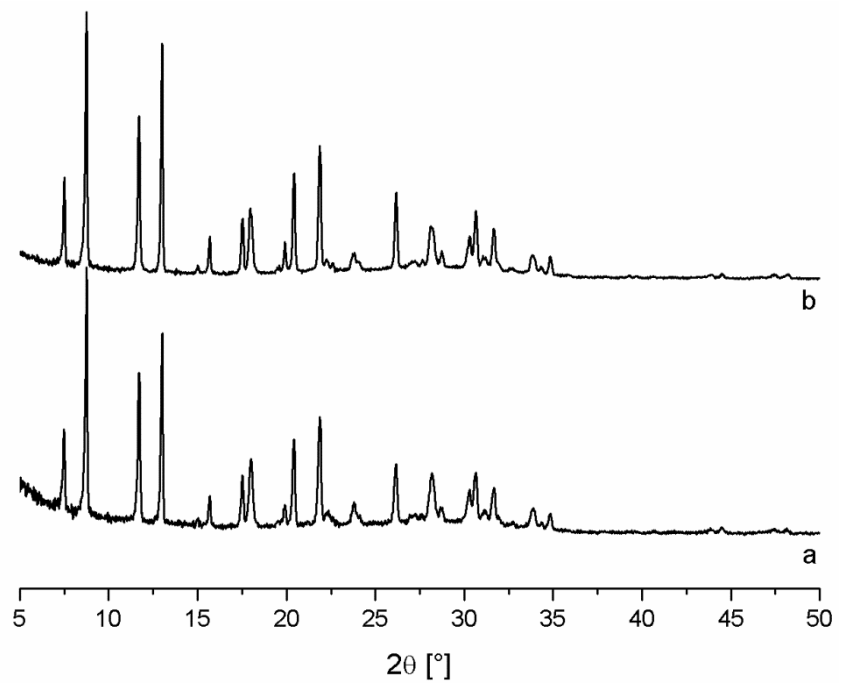


Figure S9. PXRD patterns of calcined SAPO-56 samples prepared with trimethylamine and diDABCO-C4 (a) or diDABCO-C5 (b) as SDAs.

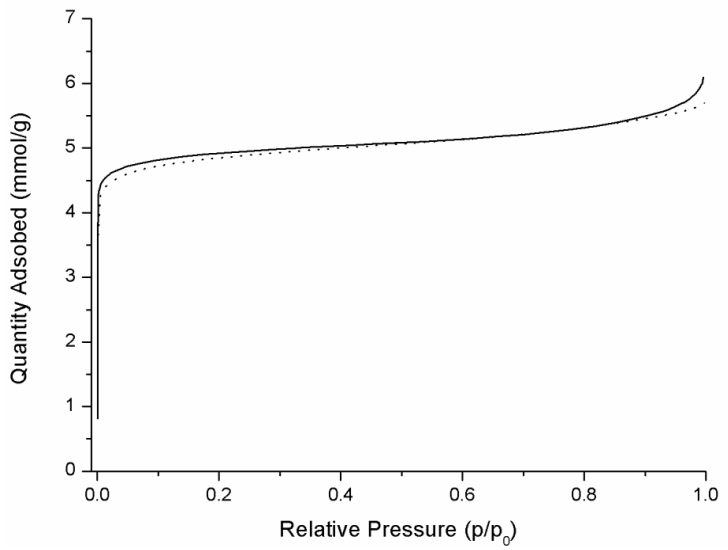


Figure S10. Isotherms for the adsorption of N_2 at -196.15 °C on calcined SAPO-56 samples synthesised using trimethylamine and diDABCO-C4 (solid line) or diDABCO-C5 (dotted line). BET surface areas of 336 and 333 m^2 g^{-1} were calculated for the samples synthesised with diDABCO-C4 and diDABCO-C5, respectively.

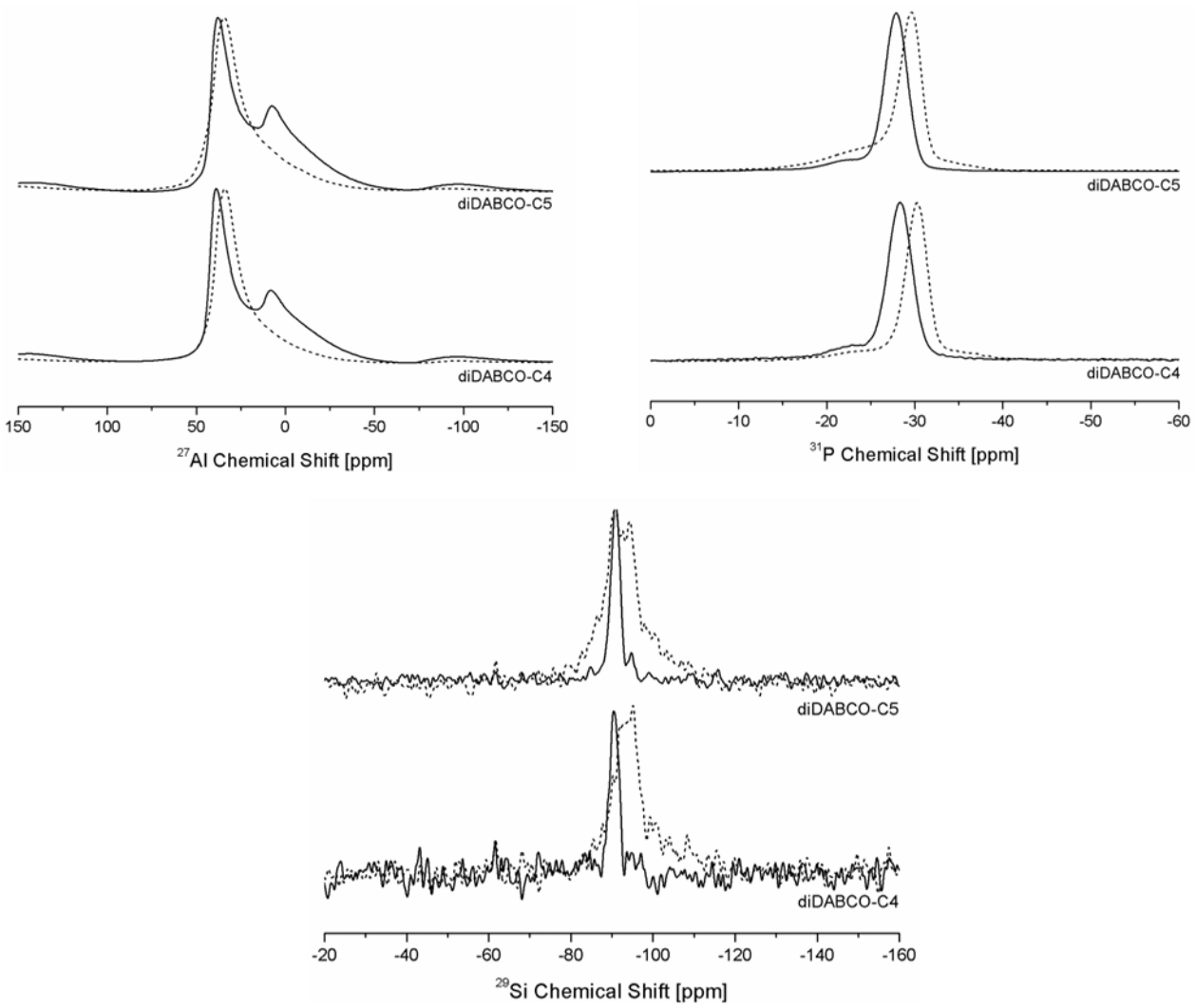


Figure S11. Solid-state MAS NMR spectra for dehydrated as-prepared (solid line) and calcined (dashed line) SAPO-56 samples synthesised using trimethylamine and diDABCO-C4 (a) or diDABCO-C5 (b) as SDAs.

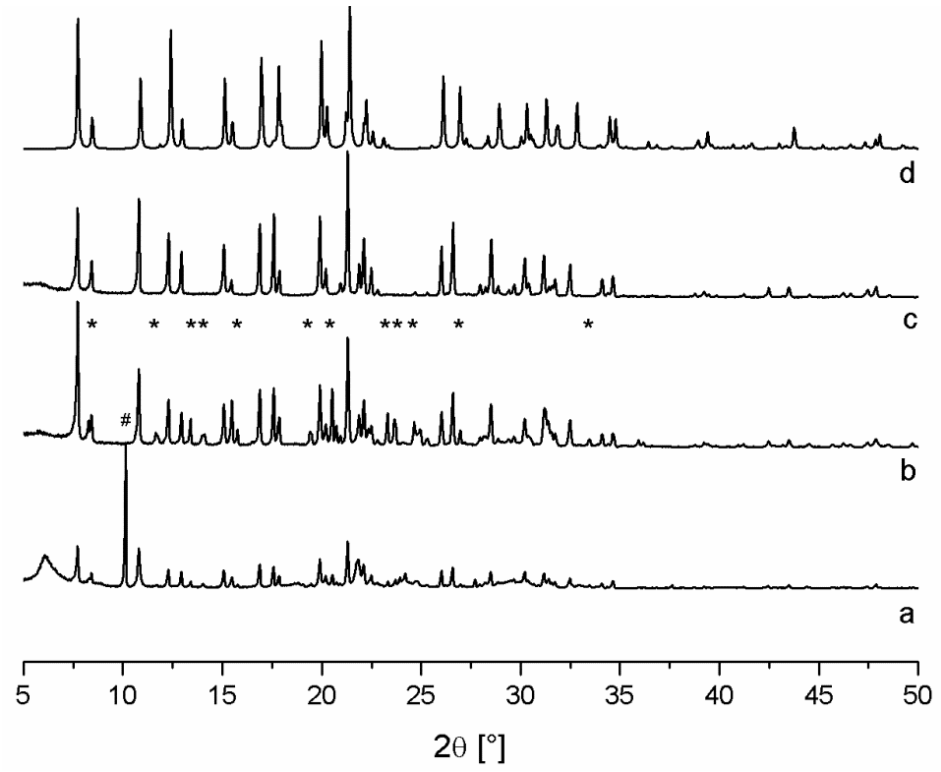


Figure S12. PXRD of SAPO STA-18 synthesised at 190 °C with diDABCO-C6 and TrMA as SDAs and by varying Si/Al ratio of the starting gels having composition $Al(OH)_3$: 1-x H_3PO_4 : x SiO_2 : 0.1 diDABCO-C6 : 0.13 TrMA : 0.28 TBAOH : 40 H_2O; x = 0.1 (a), 0.2 (b) and 0.3 (c). Simulated pattern of SSZ-52 (SFW) as comparison. The peaks marked with an * and # belong to unknown phases.

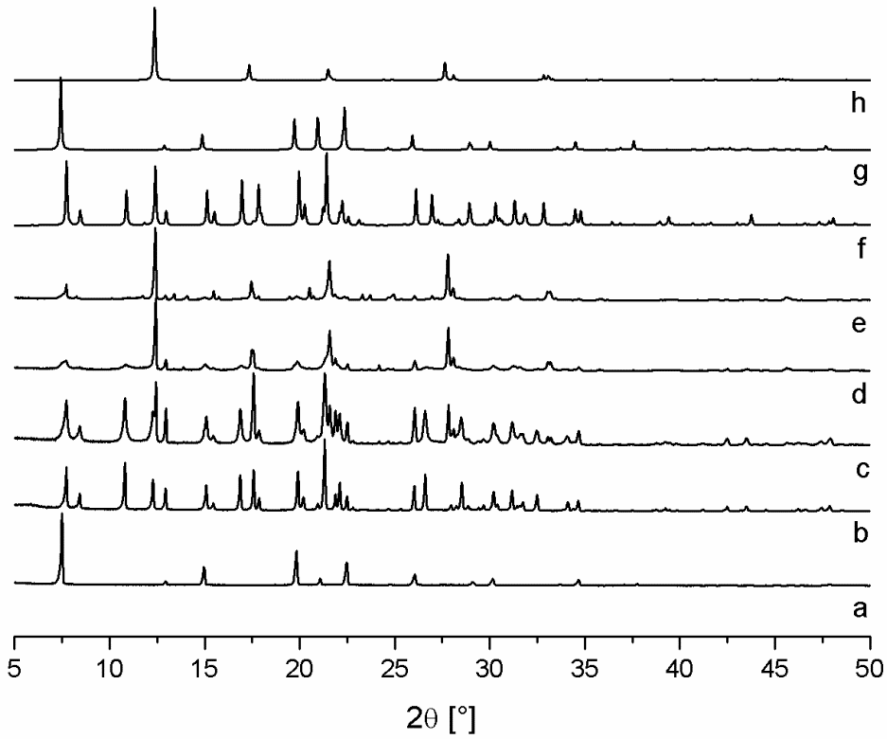


Figure S13. PXRD patterns of samples synthesised at 190 °C by varying the content of TrMA within the starting gel, composition $Al(OH)_3$: 0.7 H_3PO_4 : 0.3 SiO_2 : 0.1 diDABCO-C6 : x TrMA : y TBAOH : 40 H_2O. x = 0.0, y = 0.38 (a), x = 0.13, y = 0.28 (b), x = 0.26, y = 0.20 (c), x = 0.39, y = 0.10 (d) and x = 0.53, y = 0.10 (e). Simulated patterns of SSZ-52 (SFW) (f), AlPO-5 (AFI) (g) and MAPO-43 (GIS) (h) as comparison.

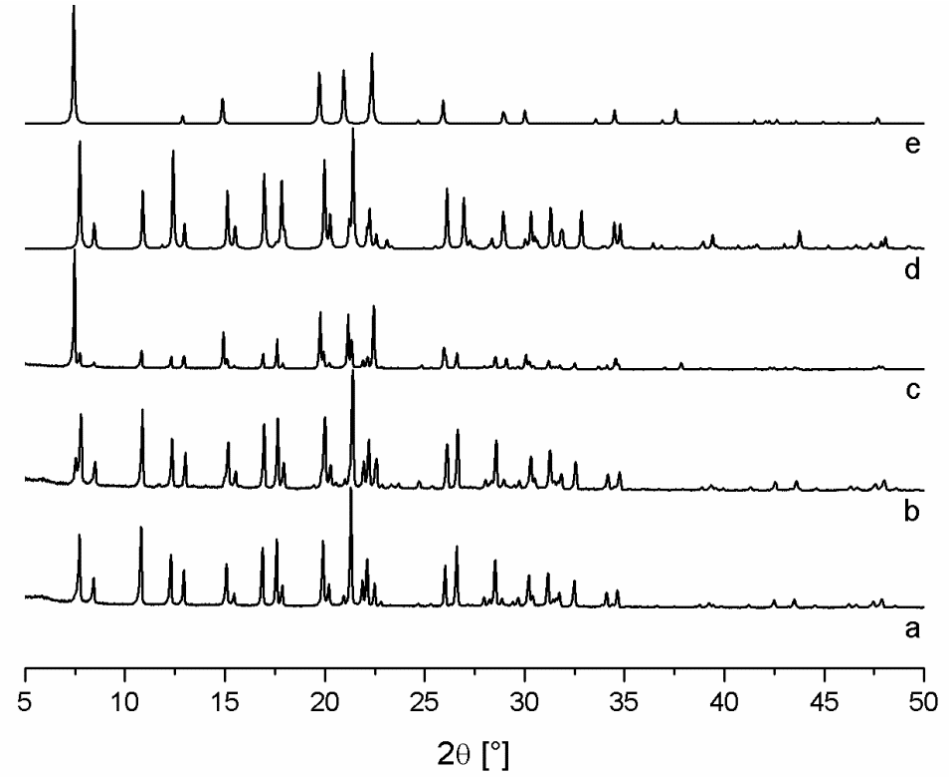


Figure S14. PXRD patterns of the synthesis of SAPO STA-18 performed at 190 °C using TBAOH (a), TPAOH (b) and TPeAOH (c) as co-bases. Simulated patterns of SSZ-52 (SFW) (d) and AlPO-5 (AFI) (e) have been plotted as comparison.

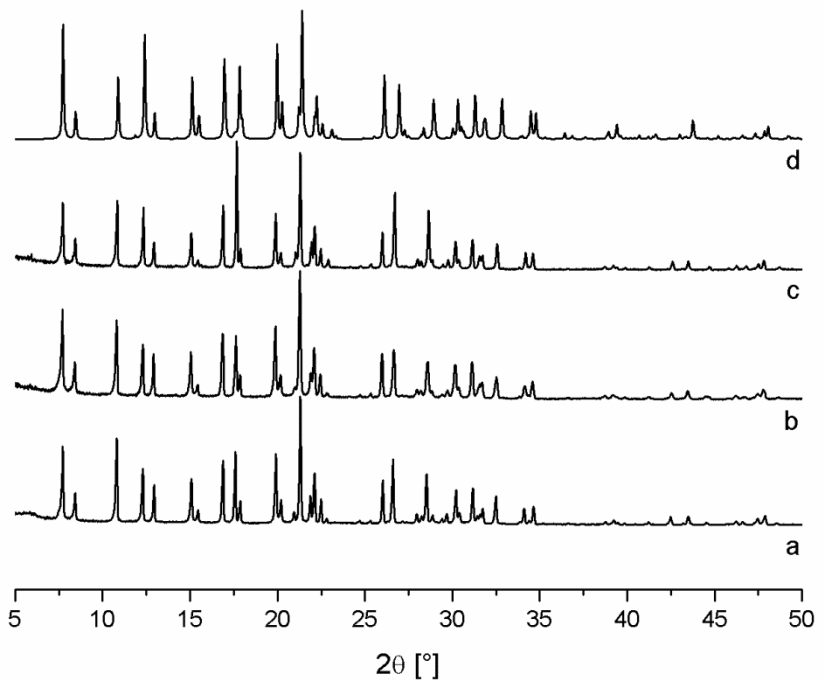


Figure S15. PXRD patterns of samples synthesised at 190 °C using TrMA and diDABCO-C7 (b) or diDABCO-C8 (c) in gels having composition 1.0 $Al(OH)_3$: 0.7 H_3PO_4 : 0.3 SiO_2 : 0.1 diDABCO-Cx : 0.13 TrMA : 0.28 TBAOH : 40 H_2O (0.11 TrMA and 0.30 TBAOH has been used with diDABCO-C8). The PXRD patterns of SAPO STA-18 synthesised with TrMA and diDABCO-C6 (a) and SSZ-52 (SFW) (d) have been plotted for comparison.

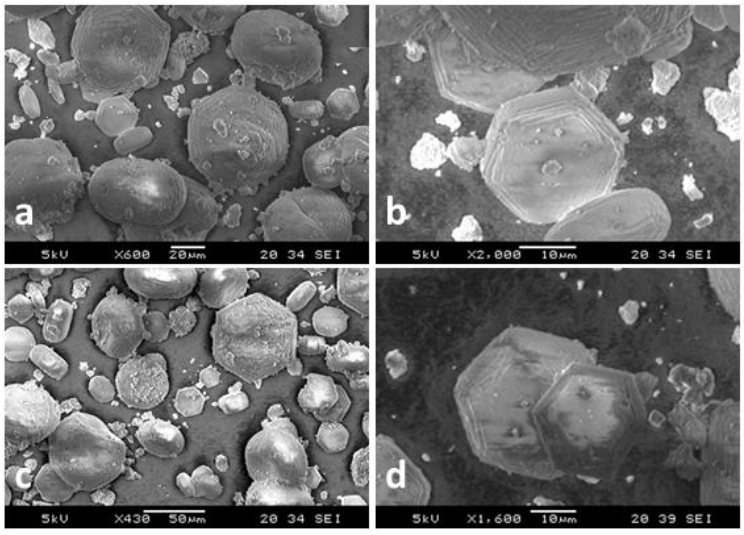


Figure S16. SEM images of SAPO STA-18 synthesised with TrMA and diDABCO-C6 (a), magnification on single crystal (b) or diDABCO-C7 (c) or diDABCO-C8 (d) as SDAs.

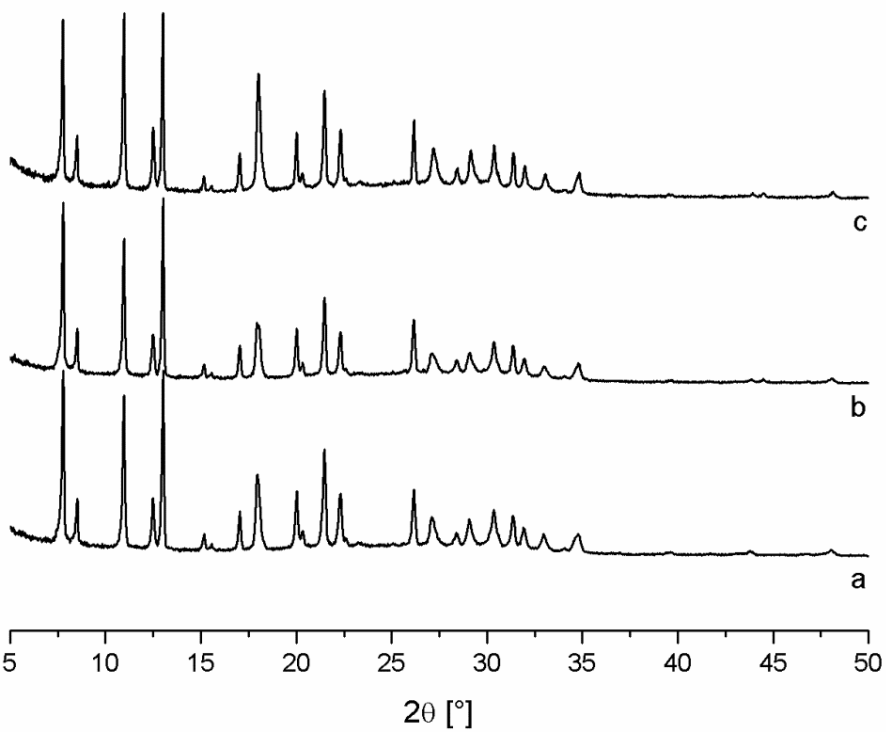


Figure S17. PXRD patterns of calcined SAPO STA-18 samples prepared with trimethylamine and diDABCO-C6 (a) or diDABCO-C7 (b) or diDABCO-C8 (c) as SDAs.

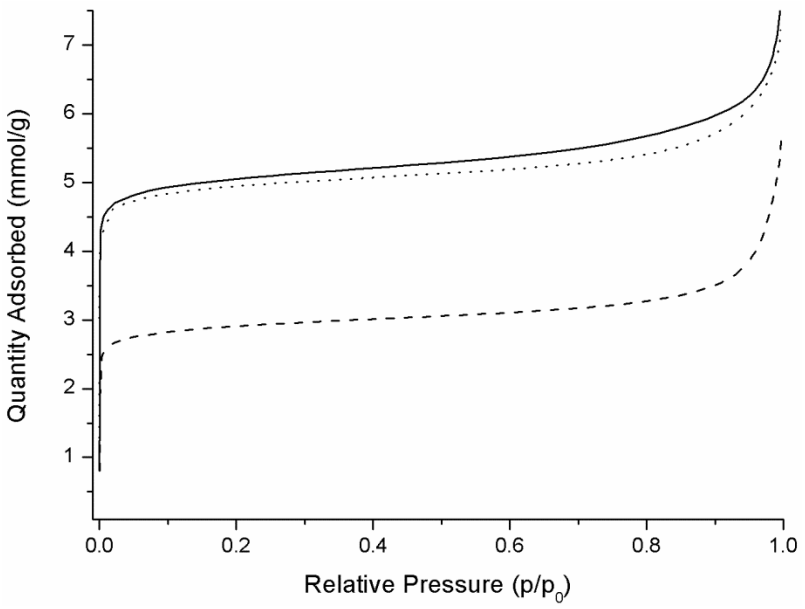


Figure S18. Isotherms for the adsorption of N_2 at -196.15 °C on calcined SAPO STA-18 samples synthesised using TrMA and diDABCO-C6 (solid line) or diDABCO-C7 (dotted line) or diDABCO-C8 (dashed line) as SDAs. The calculated BET surface areas are 347, 336 and 169 m^2 g^{-1} for the materials prepared with diDABCO-C6, diDABCO-C7 and diDABCO-C8, respectively.

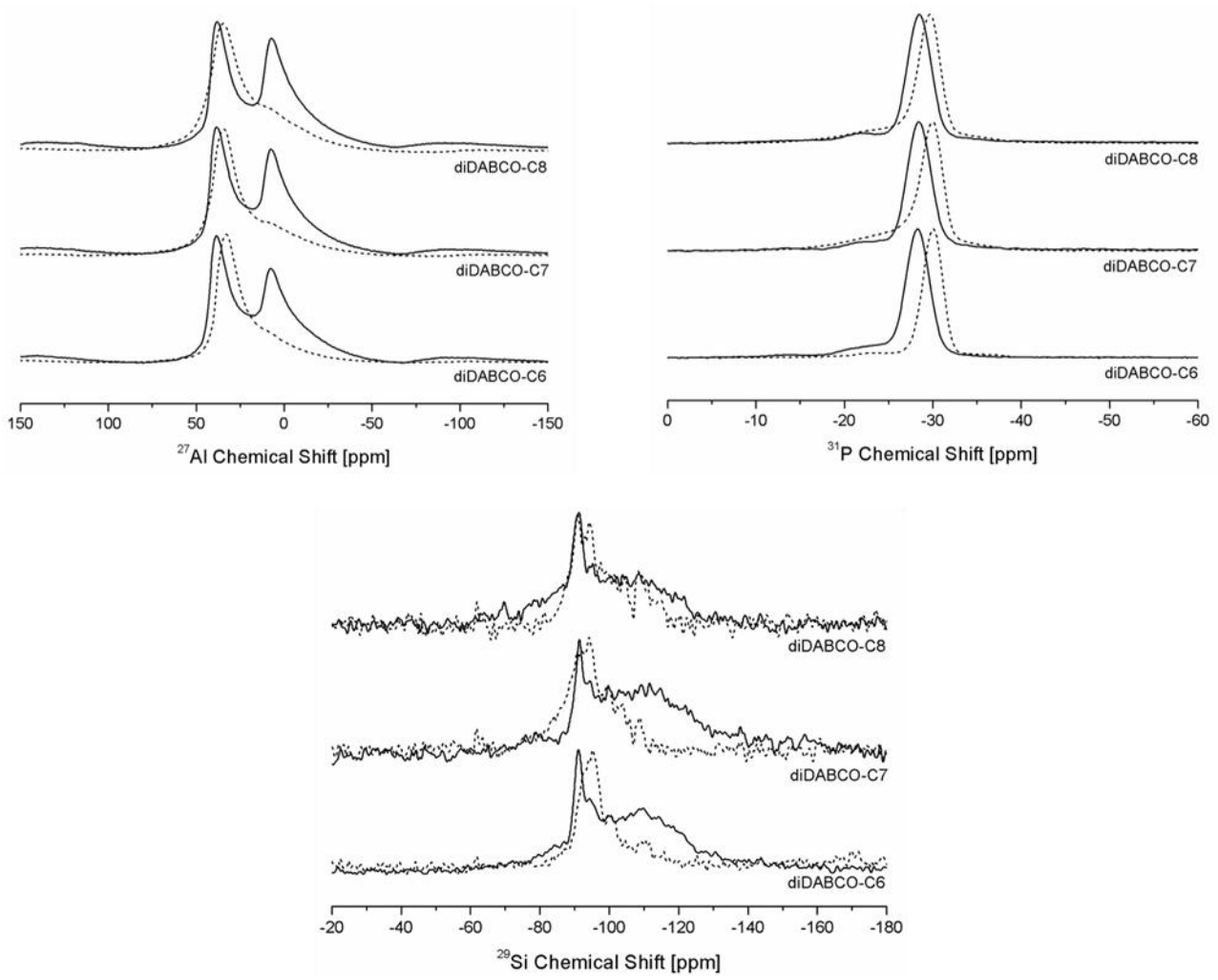


Figure S19. Solid-state MAS NMR spectra for dehydrated as-prepared (solid line) and calcined (dashed line) SAPO STA-18 samples synthesised using trimethylamine and (a) diDABCO-C6, (b) diDABCO-C7 (b) or (c) diDABCO-C8. The ^{27}Al MAS NMR spectra of as-prepared samples show two resonances: one between 6.4–7.8 ppm assigned to five-fold Al and one at 38.1 ppm assigned to tetrahedrally-coordinated Al atoms. Due to the disappearance of the five-fold peak after calcination, the additional coordination is likely to be from charge-balancing hydroxyl groups. The strong signal at -28.5 ppm in the ^{31}P MAS NMR spectra of as-prepared samples is consistent with $P(OAl)_4$ groups. However, as in the case of SAPO-56, a weak signal around -18.9 ppm is present in all three spectra. The $P(OAl)_4$ resonances are shifted *ca.* 2 ppm upfield upon calcination. All the ^{29}Si MAS NMR spectra have a poor signal to noise ratio. The as-made samples show a main resonance at -91 ppm attributable to $Si(OAl)_4$ and a broad hump centred at -110 ppm associated with the presence of amorphous silica. While the signals at -91 ppm shifted to -94 ppm upon calcination, the broad signal flattens out, in particular in the case of diDABCO-C6 and C7.

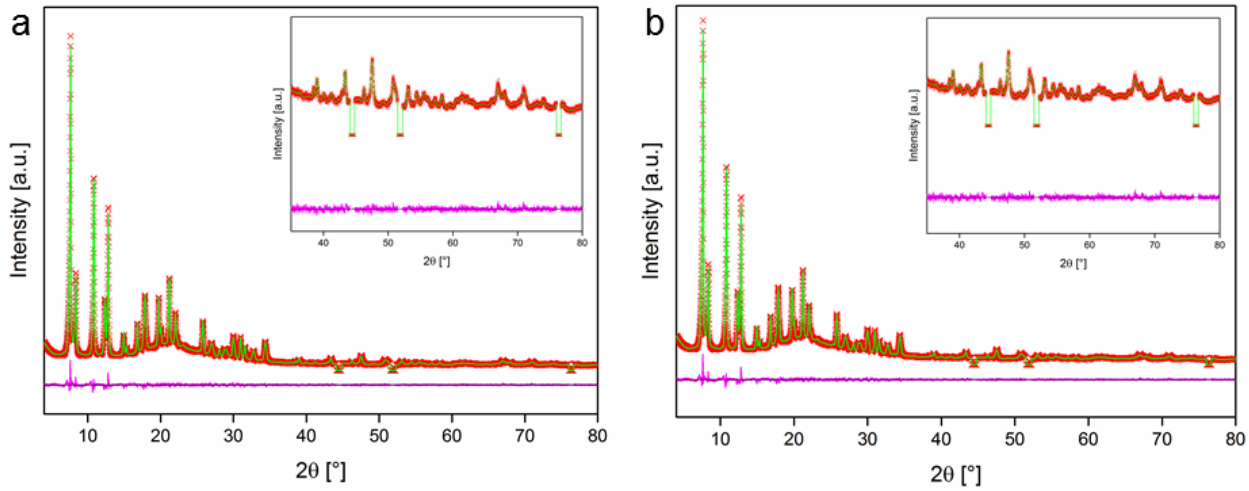


Figure S20. Rietveld plot for calcined dehydrated SAPO STA-18 synthesised using trimethylamine and diDABCO-C7 (a) or diDABCO-C8 (b) as SDAs. Observed data (red crosses), calculated fit (green line), and difference plot (purple line).

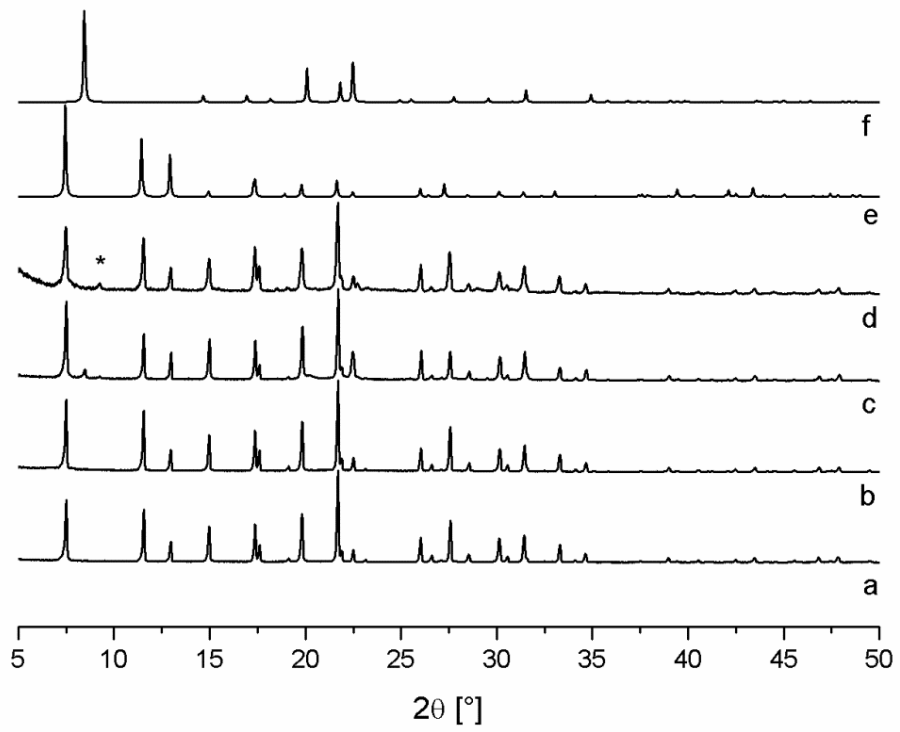


Figure S21. PXRD patterns of the respective syntheses of SAPO STA-19 performed at 160 °C using TrMA and $[DABCO\text{-}C5]_3$ (a) or $[DABCO\text{-}C6]_3$ (b) or $[DABCO\text{-}C6]_5$ (c) or $[DABCO\text{-}C6]_7$ (d) as SDAs using the starting gels having composition 1.0 $Al(OH)_3$: 0.7 H_3PO_4 : 0.3 SiO_2 : 0.15 $[DABCO\text{-}C5(6)]_n$: 0.21 TrMA : 0.24 TBAOH : 40 H_2O. Simulated patterns of $|Ca_4(H_2O)_{26.4}|$ $[Si_{16}Al_8O_{48}]$ (GME) (e) and SAPO-31 (ATO) (f) have been plotted as comparison. The peaks marked with an * belongs to unknown phase.

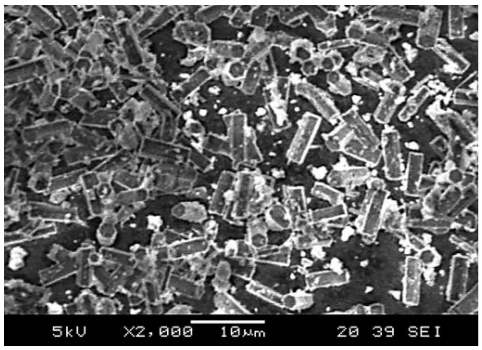


Figure S22. SEM image of SAPO STA-19 synthesised with TrMA and $[DABCO\text{-}C5]_3$ as SDAs

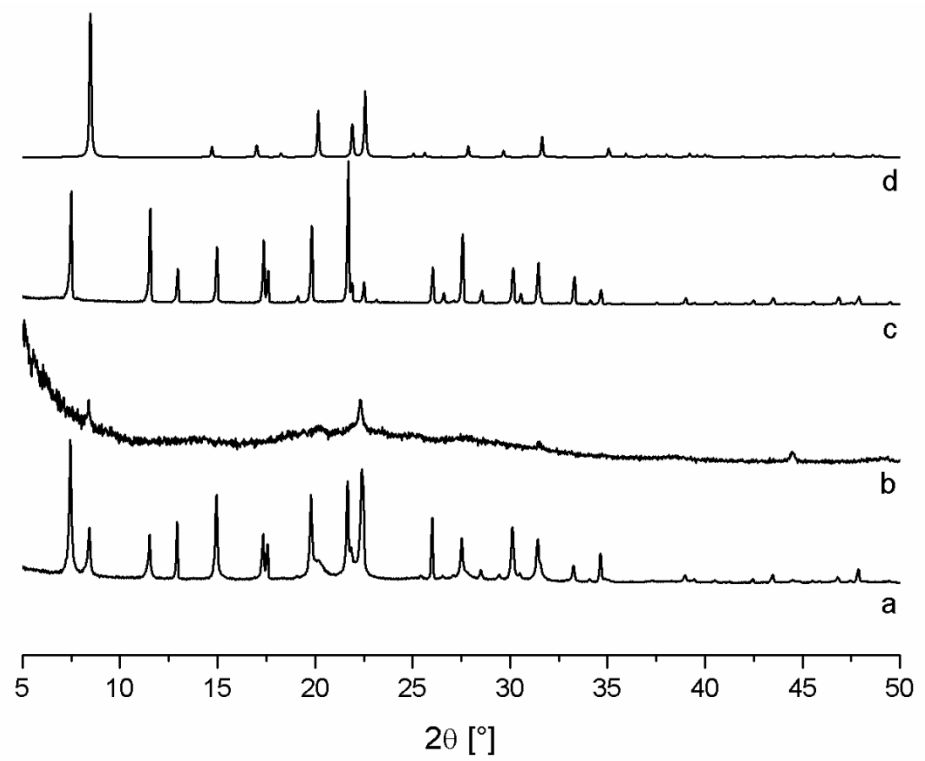


Figure S23. PXRD patterns of the respective synthesis of SAPO STA-19 performed at 160 °C in the absence of TrMA (a) or AFX seeds (b). The experimental pattern of pure SAPO STA-19 prepared with TrMA and $[DABCO\text{-}C6]_3$ and the simulated pattern of SAPO-31 (ATO) have been plotted as comparison.

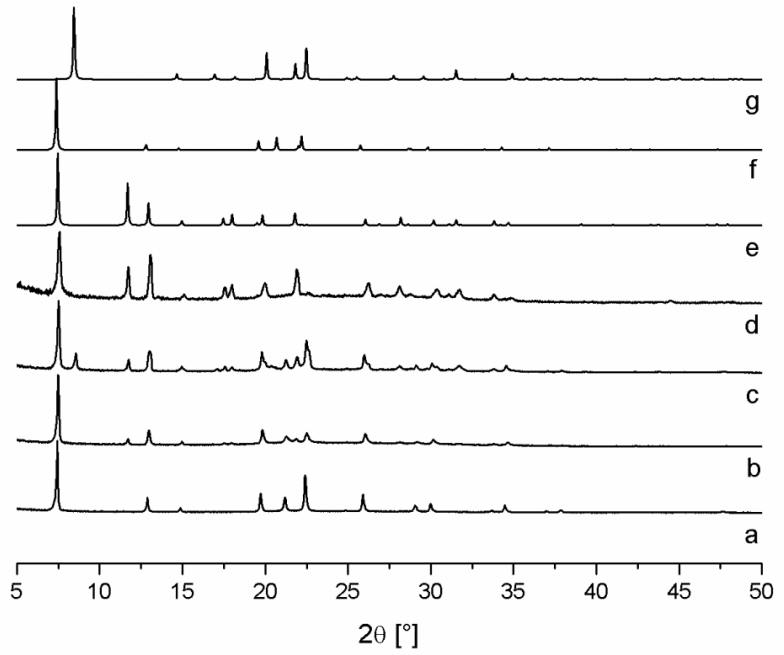


Figure S24. PXRD patterns of calcined SAPO STA-19 samples prepared at 160 °C with trimethylamine and $[DABCO\text{-}C5]_3$ (a) or $[DABCO\text{-}C6]_3$ (b) or $[DABCO\text{-}C6]_5$ (c) or $[DABCO\text{-}C6]_7$ (d) as SDAs. Simulated patterns of $|Ca_4(H_2O)_{26.4}|$ $[Si_{16}Al_8O_{48}]$ (GME) (e), AlPO-5 (AFI) (f) and SAPO-31 (ATO) (g) have been plotted for comparison.

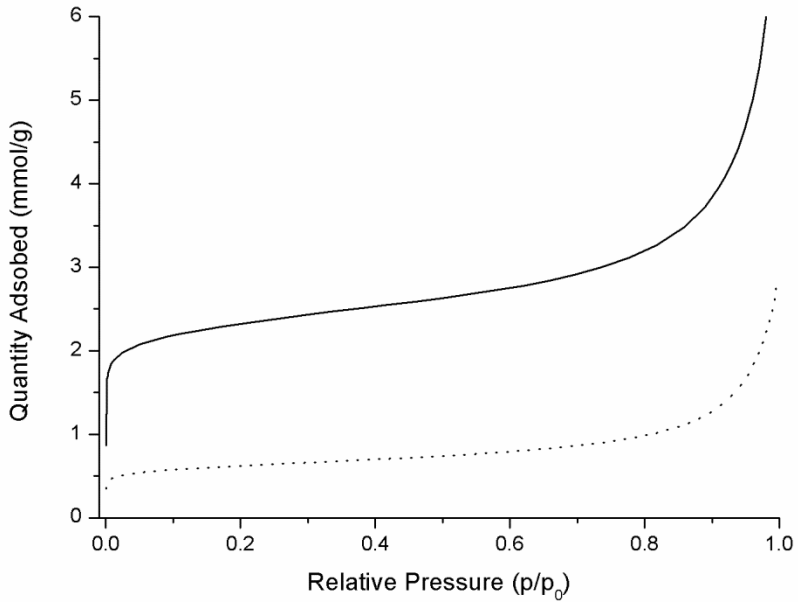


Figure S25. Isotherms for the adsorption of N_2 at -196.15 °C on calcined SAPO STA-19 samples synthesised using TrMA and $[DABCO\text{-}C6]_3$ (dotted line) or $[DABCO\text{-}C6]_7$ (solid line) as SDAs.

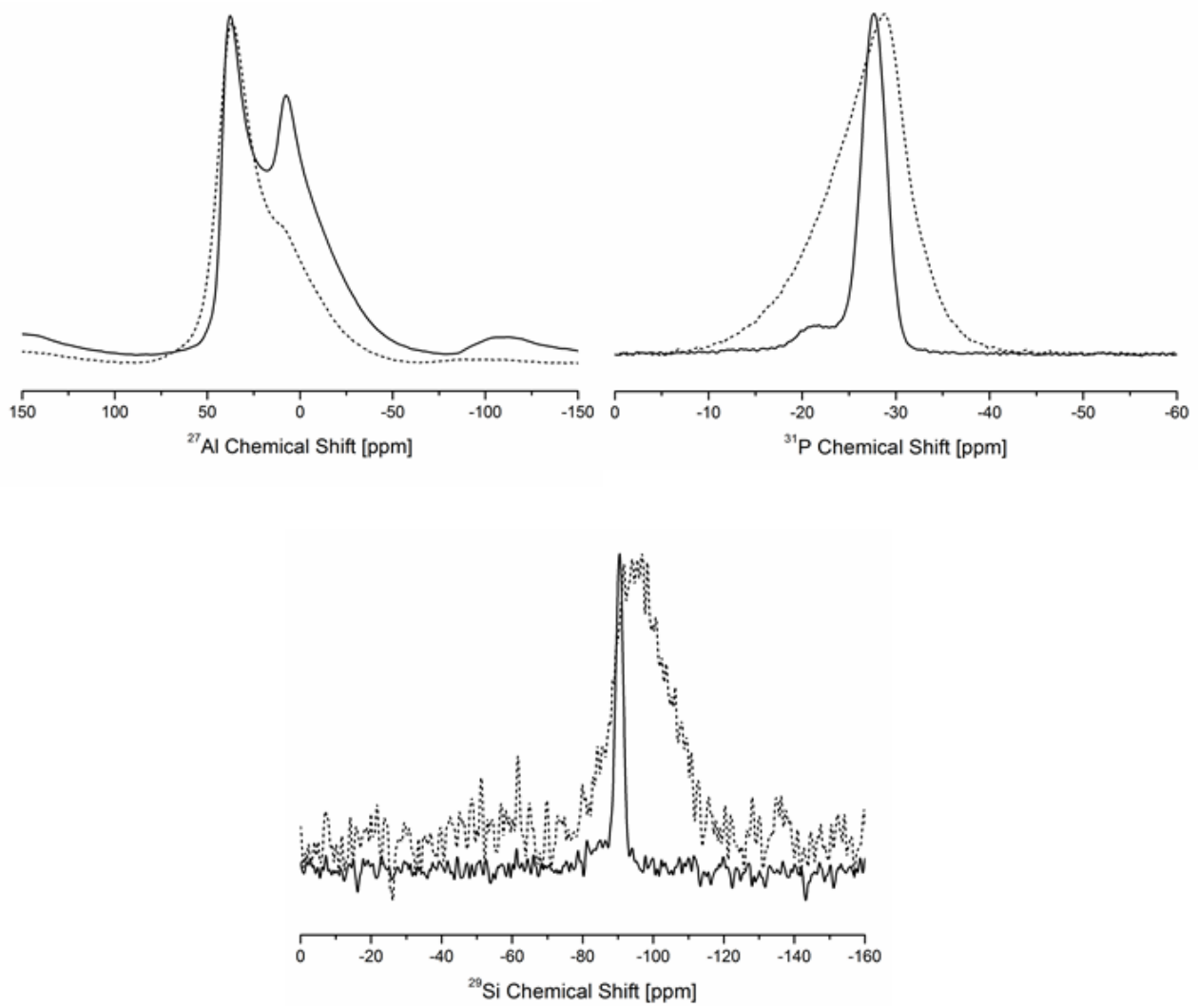


Figure S26. Solid-state MAS NMR spectra for dehydrated as-prepared (solid line) and calcined (dashed line) SAPO STA-19 samples synthesised using trimethylamine and [DABCO-C6]. The ^{27}Al MAS MAS NMR spectrum of an as-prepared sample indicates tetrahedral (37.4 ppm) and five-fold (7.2 ppm) Al atoms. The spectrum of the calcined material only shows the resonance of tetrahedral Al (36.5 ppm). The ^{31}P MAS NMR spectrum of the as-made sample contains the characteristic resonance of tetrahedral $P(OAl)_4$ at -27.8 ppm. After calcination only one broad resonance at -28.8 ppm was observed. The sharp signal at -90.5 ppm in the ^{29}Si MAS NMR spectrum of the as-prepared sample can be associated with $Si(OAl)_4$. A broad resonance centered at -96.9 ppm was detected in the calcined sample.

Table S1. Atomic coordinates and thermal parameters for as-prepared and dehydrated SAPO-56 synthesised using trimethylamine and diDABCO-C4 as SDAs.

atom	*x*	*y*	*z*	occupancy	*U*iso	multiplicity
Al1	0.9990(5)	0.7645(5)	0.5745(4)	1	0.0144(4)	12
Al2	0.6683(5)	0.5718(5)	0.67624(35)	1	0.0144(4)	12
P1	-0.00015(34)	0.22635(34)	0.07835(34)	0.75	0.0144(4)	12
P2	0.33332(34)	0.44032(34)	0.17172(34)	0.75	0.0144(4)	12
Si1	-0.00015(34)	0.22635(34)	0.07835(34)	0.25	0.0144(4)	12
Si2	0.33332(34)	0.44032(34)	0.17172(34)	0.25	0.0144(4)	12
O1	0.0099(11)	0.3230(8)	0.1214(6)	1	0.0253(9)	12
O2	0.9792(11)	0.6553(9)	0.6267(7)	1	0.0253(9)	12
O3	0.0956(4)	0.2014(5)	0.0907(4)	1	0.0253(9)	12
O4	0.2369(4)	0.4661(5)	0.1598(4)	1	0.0253(9)	12
O5	0.8806(5)	0.1300(5)	0.0922(4)	1	0.0253(9)	12
O6	0.3308(6)	0.3924(6)	0.24137(31)	1	0.0253(9)	12
O7	0.4488(5)	0.5433(5)	0.1583(5)	1	0.0253(9)	12
O8	-0.0032(18)	0.2643(11)	0.00799(34)	1	0.0253(9)	12
C1	-0.116	-0.034	0.7444	0.4830(26)	0.005	12
C2	0.4692	0.7032	0.5169	0.3230(6)	0.005	12
C3	0.2868	0.6791	0.4782	0.3230(6)	0.005	12
C4	0.407	0.8361	0.5545	0.3230(6)	0.005	12
C5	0.4085	0.6242	0.5815	0.3230(6)	0.005	12
C6	0.2253	0.5979	0.5416	0.3230(6)	0.005	12
C7	0.3441	0.7572	0.6187	0.3230(6)	0.005	12
C8	0.2409	0.5548	0.6627	0.3230(6)	0.005	12
C9	0.3099	0.5696	0.7282	0.3230(6)	0.005	12
N1	0.0012	0.002	0.7233	0.1610(9)	0.005	12
N2	0.4048	0.7659	0.495	0.3230(6)	0.005	12
N3	0.3039	0.6313	0.6038	0.3230(6)	0.005	12
H1	-0.1444	0.0231	0.7241	0.4830(26)	0.005	12
H2	-0.1228	-0.034	0.8001	0.4830(26)	0.005	12
H3	-0.1762	-0.1202	0.7264	0.4830(26)	0.005	12
H4	0.4722	0.651	0.4748	0.3230(6)	0.005	12
H5	0.5584	0.7632	0.5296	0.3230(6)	0.005	12
H6	0.2822	0.6284	0.4333	0.3230(6)	0.005	12
H7	0.2389	0.7218	0.4645	0.3230(6)	0.005	12
H8	0.3645	0.8842	0.5405	0.3230(6)	0.005	12
H9	0.4937	0.9009	0.5693	0.3230(6)	0.005	12
H10	0.3862	0.5363	0.5693	0.3230(6)	0.005	12
H11	0.4719	0.651	0.6228	0.3230(6)	0.005	12
H12	0.1957	0.5094	0.526	0.3230(6)	0.005	12
H13	0.1473	0.6007	0.5532	0.3230(6)	0.005	12
H14	0.2726	0.7696	0.6333	0.3230(6)	0.005	12

H15	0.4036	0.7896	0.6621	0.3230(6)	0.005	12
H16	0.2016	0.4648	0.6469	0.3230(6)	0.005	12
H17	0.1676	0.5656	0.6753	0.3230(6)	0.005	12
H18	0.3695	0.5381	0.7193	0.3230(6)	0.005	12
H19	0.3638	0.6597	0.7407	0.3230(6)	0.005	12

Table S2. Selected bond lengths and angles for as-prepared and dehydrated SAPO-56 synthesised using trimethylamine and diDABCO-C4 as SDAs.

bond length / Å		**bond angle / °**	
Al1-O	1.730(4)	O-Al1-O	109.5(7)
Al2-O	1.734(4)	O-Al2-O	109.4(6)
Al-O (Avg.)	1.732(4)	O-T-O (Avg.)	109.4(7)
P1(Si1)-O	1.523(4)	O-P1(Si1)-O	109.4(12)
P2(Si2)-O	1.536(4)	O-P2(Si2)-O	109.4(10)
P(Si)-O (Avg.)	1.529(4)	O-P(Si)-O (Avg.)	109.3(11)
T-O (Avg.)	1.631(4)	O-T-O (Avg.)	109.4(9)

Table S3. Atomic coordinates and thermal parameters for calcined and dehydrated SAPO-56 synthesised using trimethylamine and diDABCO-C4 as SDAs.

atom	***x***	***y***	***z***	**occupancy**	***U*iso**	**multiplicity**
Al1	0.0076(6)	0.2299(5)	0.0753(4)	1	0.0218(7)	12
Al2	0.3266(5)	0.4314(6)	0.1741(4)	1	0.0218(7)	12
P1	0.10608(31)	0.44279(31)	0.16824(31)	0.75	0.0218(7)	12
P2	0.22761(34)	0.22017(34)	0.08322(34)	0.75	0.0218(7)	12
O1	-0.1161(4)	0.1194(5)	0.1015(4)	1	0.0246(15)	12
O2	0.1083(4)	0.1957(6)	0.0959(4)	1	0.0246(15)	12
O3	0.0287(7)	0.3479(6)	0.1207(5)	1	0.0246(15)	12
O4	0.0084(11)	0.2607(8)	-0.00957(31)	1	0.0246(15)	12
O5	0.2249(4)	0.4651(6)	0.1542(5)	1	0.0246(15)	12
O6	0.0944(8)	0.5475(6)	0.1515(5)	1	0.0246(15)	12
O7	0.0786(9)	0.4083(8)	0.24073(26)	1	0.0246(15)	12
O8	0.3023(5)	0.3083(6)	0.1337(4)	1	0.0246(15)	12
Si1	0.10608(31)	0.44279(31)	0.16824(31)	0.25	0.0218(7)	12
Si2	0.22761(34)	0.22017(34)	0.08322(34)	0.25	0.0218(7)	12

Table S4. Selected bond lengths and angles for calcined and dehydrated SAPO-56 synthesised using trimethylamine and diDABCO-C4 as SDAs.

bond length / Å		bond angle / °	
Al1-O	1.728(7)	O-Al1-O	109.5(5)
Al2-O	1.724(7)	O-Al2-O	109.5(5)
Al-O (Avg.)	1.726(7)	O-T-O (Avg.)	109.5(5)
P1(Si1)-O	1.529(6)	O-P1(Si1)-O	109.5(5)
P2(Si2)-O	1.529(6)	O-P2(Si2)-O	109.4(5)
P(Si)-O (Avg.)	1.525(6)	O-P(Si)-O (Avg.)	109.5(5)
T-O (Avg.)	1.626(7)	O-T-O (Avg.)	109.5(5)

Table S5. Crystallographic data for calcined dehydrated SAPO STA-18 synthesised using trimethylamine and diDABCO-C7 or diDABCO-C8 as SDAs

	SAPO STA-18 (diDABCO-C7) calcined, dehydrated	**SAPO STA-18 (diDABCO-C8) calcined, dehydrated**
Chemical composition	$Al_{54}P_{36.6}Si_{17.4}O_{216}$	$Al_{54}P_{24.7}Si_{29.3}O_{216}$
Data collection		
Wavelength / Å	1.54056	1.54056
Diffractometer geometry	Debye-Scherrer	Debye-Scherrer
Sample	Spinning 0.7 mm capillary	Spinning 1.0 mm capillary
Scanned region / 2θ°	3.0–80.0	3.0–80.0
Step size / 2θ°	0.01	0.01
Unit cell		
Chemical formula	$Al_{54}P_{40.5}Si_{13.5}O_{216}$	$Al_{54}P_{40.5}Si_{13.5}O_{216}$
Crystal system	trigonal	trigonal
Space group	*R -3*	*R -3*
a / Å	13.78419(17)	13.79468(13)
b / Å	13.78419(17)	13.79468(13)
c / Å	44.5996(15)	44.6557(9)
Volume / Å^3	7338.79(22)	7359.20(15)
FWHM[a]		
[009] / °	0.383	0.212
[101] / °	0.174	0.141
Rietveld refinement		
Refined region / 2θ°	4.0–80.0	5.0–80.0
Background	44.09–44.80, 51.49–52.24, 76.02–76.60	
R_{wp}	Chebyschev 30 terms	Chebyschev 28 terms
R_p	0.041	0.057
R_F^2	0.032	0.045
X^2	0.040	0.067

[a] (009) peak (or more specifically the (00l) family of peaks) is not affected by possible stacking faults while the (101) peak correspond to maximum peak of calcined SAPO STA-18.

Table S6. Atomic coordinates and thermal parameters for as-prepared and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C6 as SDAs.

atom	*X*	*y*	*z*	occupancy	*U*iso	multiplicity
Al1	0.9917(9)	0.2240(8)	0.25693(31)	1	0.0181(6)	18
Al2	0.2349(7)	-0.0019(8)	0.81222(31)	1	0.0181(6)	18
Al3	0.9935(9)	0.2328(8)	0.03299(33)	1	0.0181(6)	18
P1	0.23021(29)	0.00111(29)	0.74312(29)	0.75	0.0181(6)	18
P2	0.00752(32)	0.23612(32)	0.18912(32)	0.75	0.0181(6)	18
P3	0.22843(28)	0.00853(28)	0.96533(28)	0.75	0.0181(6)	18
Si1	0.23021(29)	0.00111(29)	0.74312(29)	0.25	0.0181(6)	18
Si2	0.00752(32)	0.23612(32)	0.18912(32)	0.25	0.0181(6)	18
Si3	0.22843(28)	0.00853(28)	0.96533(28)	0.25	0.0181(6)	18
O1	0.2619(23)	0.9972(28)	0.77480(27)	1	0.0129(11)	18
O2	0.9998(27)	0.2674(23)	0.22079(28)	1	0.0129(11)	18
O3	0.1228(9)	0.2353(13)	0.2642(4)	1	0.0129(11)	18
O4	0.8955(7)	0.0811(9)	0.26151(34)	1	0.0129(11)	18
O5	0.3188(15)	0.9876(18)	0.7259(5)	1	0.0129(11)	18
O6	0.9702(17)	0.3120(18)	0.2807(5)	1	0.0129(11)	18
O7	0.9034(9)	0.1181(8)	0.18445(33)	1	0.0129(11)	18
O8	0.9955(15)	0.3211(15)	0.1696(7)	1	0.0129(11)	18
O9	0.1066(7)	0.2295(8)	0.17925(31)	1	0.0129(11)	18
O10	1.0014(30)	0.2671(19)	0.99597(29)	1	0.0129(11)	18
O11	0.1186(9)	0.2395(13)	0.0431(4)	1	0.0129(11)	18
O12	0.8837(8)	0.0972(8)	0.03975(35)	1	0.0129(11)	18
C1	-0.2668	-0.7188	0.4436	0.4345(31)	0.005	18
C2	0.333	0.5948	0.0176	0.1618(5)	0.005	18
C3	0.2445	0.7023	0.0355	0.1618(5)	0.005	18
C4	0.4505	0.7971	0.0288	0.1618(5)	0.005	18
C5	0.3465	0.5646	0.0523	0.1618(5)	0.005	18
C6	0.2576	0.6725	0.0703	0.1618(5)	0.005	18
C7	0.4651	0.7675	0.0636	0.1618(5)	0.005	18
C8	0.3745	0.6261	0.1064	0.1618(5)	0.005	18
C9	0.3898	0.7088	0.1322	0.1618(5)	0.005	18
C10	0.3955	0.6607	0.1629	0.1618(5)	0.005	18
C11	0.39739	0.73387	0.18931	0.1618(5)	0.005	18
C12	0.38983	0.67733	0.21972	0.1618(5)	0.005	18
C13	0.37696	0.74291	0.2464	0.1618(5)	0.005	18
C14	0.24573	0.57449	0.27939	0.1618(5)	0.005	18
C15	0.22447	0.52135	0.31322	0.1618(5)	0.005	18
C16	0.45246	0.67028	0.28818	0.1618(5)	0.005	18
C17	0.42962	0.61673	0.32197	0.1618(5)	0.005	18
C18	0.34586	0.76628	0.30115	0.1618(5)	0.005	18
C19	0.32381	0.71227	0.33494	0.1618(5)	0.005	18

C20	-0.2668	-0.7188	0.4244	0.4345(31)	0.005	18
N1	-0.33333	-0.6672	0.434	0.2896(21)	0.005	18
N2	0.3381	0.7083	0.0155	0.1618(5)	0.005	18
N3	0.3617	0.6577	0.0748	0.1618(5)	0.005	18
N4	0.35634	0.68979	0.27718	0.1618(5)	0.005	18
N5	0.31838	0.59828	0.33483	0.1618(5)	0.005	18
H1	-0.1804	-0.6724	0.4347	0.4345(31)	0.005	18
H2	-0.3044	-0.8065	0.4359	0.4345(31)	0.005	18
H3	-0.2614	-0.719	0.4681	0.4345(31)	0.005	18
H4	0.4	0.5943	0.004	0.1618(5)	0.005	18
H5	0.2527	0.5265	0.0087	0.1618(5)	0.005	18
H6	0.1609	0.6382	0.0272	0.1618(5)	0.005	18
H7	0.2451	0.7828	0.0353	0.1618(5)	0.005	18
H8	0.5217	0.8042	0.0155	0.1618(5)	0.005	18
H9	0.4584	0.881	0.0285	0.1618(5)	0.005	18
H10	0.4188	0.5504	0.053	0.1618(5)	0.005	18
H11	0.2716	0.4833	0.0578	0.1618(5)	0.005	18
H12	0.179	0.5957	0.0767	0.1618(5)	0.005	18
H13	0.2624	0.7408	0.0844	0.1618(5)	0.005	18
H14	0.5425	0.7621	0.0648	0.1618(5)	0.005	18
H15	0.4803	0.8403	0.0775	0.1618(5)	0.005	18
H16	0.4466	0.6115	0.1071	0.1618(5)	0.005	18
H17	0.3006	0.5438	0.1118	0.1618(5)	0.005	18
H18	0.4666	0.7905	0.1287	0.1618(5)	0.005	18
H19	0.3192	0.7255	0.1322	0.1618(5)	0.005	18
H20	0.4702	0.6506	0.1639	0.1618(5)	0.005	18
H21	0.3222	0.5754	0.1654	0.1618(5)	0.005	18
H22	0.32619	0.74921	0.18711	0.1618(5)	0.005	18
H23	0.47421	0.81706	0.18841	0.1618(5)	0.005	18
H24	0.31772	0.591	0.21921	0.1618(5)	0.005	18
H25	0.46503	0.66924	0.22293	0.1618(5)	0.005	18
H26	0.30757	0.75875	0.24105	0.1618(5)	0.005	18
H27	0.45301	0.82698	0.24714	0.1618(5)	0.005	18
H28	0.24625	0.51162	0.26405	0.1618(5)	0.005	18
H29	0.17182	0.58172	0.27316	0.1618(5)	0.005	18
H30	0.21765	0.43801	0.31172	0.1618(5)	0.005	18
H31	0.14216	0.50665	0.32118	0.1618(5)	0.005	18
H32	0.46307	0.61221	0.2732	0.1618(5)	0.005	18
H33	0.53399	0.74935	0.28846	0.1618(5)	0.005	18
H34	0.50087	0.67345	0.33646	0.1618(5)	0.005	18
H35	0.4305	0.53702	0.32093	0.1618(5)	0.005	18
H36	0.27614	0.78162	0.29584	0.1618(5)	0.005	18
H37	0.4226	0.84973	0.30211	0.1618(5)	0.005	18
H38	0.24525	0.70485	0.34369	0.1618(5)	0.005	18

H39	0.39188	0.77248	0.3497	0.1618(5)	0.005	18
H40	-0.1804	-0.6724	0.4341	0.4345(31)	0.005	18
H41	-0.3044	-0.8065	0.4321	0.4345(31)	0.005	18
H42	-0.2614	-0.719	0.3999	0.4345(31)	0.005	18

Table S7. Selected bond lengths and angles for as-prepared and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C6 as SDAs.

bond length / Å		**bond angle / °**	
Al1-O	1.741(6)	O-Al1-O	109.4(12)
Al2-O	1.758(8)	O-Al2-O	109.4(12)
Al3-O	1.732(6)	O-Al3-O	109.3(12)
Al-O (Avg.)	1.744(7)	O-T-O (Avg.)	109.4(12)
P1(Si1)-O	1.523(7)	O-P1(Si1)-O	109.4(12)
P2(Si2)-O	1.516(6)	O-P2(Si2)-O	109.4(12)
P3(Si3)-O	1.512(6)	O-P3(Si3)-O	109.0(12)
P(Si)-O (Avg.)	1.517(6)	O-P(Si)-O (Avg.)	109.3(12)
T-O (Avg.)	1.631(7)	O-T-O (Avg.)	109.3(12)

Table S8. Atomic coordinates and thermal parameters for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C6 as SDAs.

atom	***x***	***y***	***z***	**occupancy**	***U*iso**	**multiplicity**
Al1	0.9977(6)	0.2269(6)	0.25607(18)	1	0.0267(7)	18
Al2	0.2279(6)	0.9999(5)	0.81208(19)	1	0.0267(7)	18
Al3	0.0003(6)	0.2233(5)	0.03477(20)	1	0.0267(7)	18
O1	0.2595(9)	0.9975(9)	0.77505(14)	1	0.0289(12)	18
O2	0.9942(9)	0.2585(8)	0.21904(13)	1	0.0289(12)	18
O3	0.1239(5)	0.2385(6)	0.26493(25)	1	0.0289(12)	18
O4	0.8916(4)	0.0891(6)	0.26278(21)	1	0.0289(12)	18
O5	0.3060(6)	0.9788(5)	0.72242(22)	1	0.0289(12)	18
O6	0.9731(7)	0.3141(7)	0.27848(21)	1	0.0289(12)	18
O7	0.9080(5)	0.1080(5)	0.18036(24)	1	0.0289(12)	18
O8	0.9850(7)	0.3113(7)	0.16674(23)	1	0.0289(12)	18
O9	0.1130(4)	0.2404(6)	0.17852(21)	1	0.0289(12)	18
O10	-0.0016(8)	0.2479(10)	-0.00279(11)	1	0.0289(12)	18
O11	0.1295(5)	0.2456(5)	0.04587(21)	1	0.0289(12)	18
O12	0.8958(4)	0.0867(5)	0.04316(25)	1	0.0289(12)	18
P1	0.23085(18)	1.00422(18)	0.74245(18)	0.75	0.0267(7)	18
P2	1.00220(17)	0.23210(17)	0.18617(17)	0.75	0.0267(7)	18
P3	0.22758(18)	0.00421(18)	0.96382(18)	0.75	0.0267(7)	18

Si1	0.23085(18)	1.00422(18)	0.74245(18)	0.25	0.0267(7)	18
Si2	1.00220(17)	0.23210(17)	0.18617(17)	0.25	0.0267(7)	18
Si3	0.22758(18)	0.00421(18)	0.96382(18)	0.25	0.0267(7)	18

Table S9. Selected bond lengths and angles for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C6 as SDAs.

bond length / Å		**bond angle / °**	
Al1-O	1.726(7)	O-Al1-O	109.5(5)
Al2-O	1.726(7)	O-Al2-O	109.5(5)
Al3-O	1.728(8)	O-Al3-O	109.5(5)
Al-O (Avg.)	1.727(7)	O-T-O (Avg.)	109.5(5)
P1(Si1)-O	1.529(6)	O-P1(Si1)-O	109.4(5)
P2(Si2)-O	1.529(6)	O-P2(Si2)-O	109.5(5)
P3(Si3)-O	1.528(7)	O-P3(Si3)-O	109.5(5)
P(Si)-O (Avg.)	1.529(6)	O-P(Si)-O (Avg.)	109.5(5)
T-O (Avg.)	1.628(7)	O-T-O (Avg.)	109.5(5)

Table A10. atomic coordinates and thermal parameters for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C7 as SDAs.

atom	***x***	***y***	***z***	**occupancy**	***U*iso**	**multiplicity**
Al1	0.9967(7)	0.2299(6)	0.25537(20)	1	0.0307(7)	18
Al2	0.2274(7)	0.9984(6)	0.81183(21)	1	0.0307(7)	18
Al3	-0.0062(7)	0.2195(6)	0.03494(22)	1	0.0307(7)	18
O1	0.2601(9)	0.9949(10)	0.77463(15)	1	0.0336(13)	18
O2	0.9946(11)	0.2626(9)	0.21835(14)	1	0.0336(13)	18
O3	0.1234(5)	0.2386(7)	0.26402(28)	1	0.0336(13)	18
O4	0.8943(5)	0.0930(6)	0.26237(22)	1	0.0336(13)	18
O5	0.3017(7)	0.9803(6)	0.72069(23)	1	0.0336(13)	18
O6	0.9750(7)	0.3189(8)	0.27802(24)	1	0.0336(13)	18
O7	0.9090(5)	0.1080(5)	0.18070(27)	1	0.0336(13)	18
O8	0.9867(8)	0.3099(8)	0.16572(26)	1	0.0336(13)	18
O9	0.1149(4)	0.2395(7)	0.17832(23)	1	0.0336(13)	18
O10	-0.0081(9)	0.240(1)	-0.00326(13)	1	0.0336(13)	18
O11	0.1209(6)	0.2398(5)	0.04688(22)	1	0.0336(13)	18
O12	0.8930(5)	0.0845(5)	0.04500(25)	1	0.0336(13)	18
P1	0.22808(19)	1.00042(19)	0.74221(19)	0.75	0.0307(7)	18
P2	1.00363(19)	0.23155(19)	0.18562(19)	0.75	0.0307(7)	18
P3	0.22756(20)	0.00574(20)	0.96292(20)	0.75	0.0307(7)	18
Si1	0.22808(19)	1.00042(19)	0.74221(19)	0.25	0.0307(7)	18
Si2	1.00363(19)	0.23155(19)	0.18562(19)	0.25	0.0307(7)	18
Si3	0.22756(20)	0.00574(20)	0.96292(20)	0.25	0.0307(7)	18

Table S11. Selected bond lengths and angles for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C7 as SDAs.

bond length / Å		bond angle / °	
Al1-O	1.726(8)	O-Al1-O	109.5(6)
Al2-O	1.726(9)	O-Al2-O	109.5(6)
Al3-O	1.727(8)	O-Al3-O	109.5(6)
Al-O (Avg.)	1.726(8)	O-T-O (Avg.)	109.5(6)
P1(Si1)-O	1.531(7)	O-P1(Si1)-O	109.5(6)
P2(Si2)-O	1.531(7)	O-P2(Si2)-O	109.5(6)
P3(Si3)-O	1.532(8)	O-P3(Si3)-O	109.4(6)
P(Si)-O (Avg.)	1.531(7)	O-P(Si)-O (Avg.)	109.5(6)
T-O (Avg.)	1.629(8)	O-T-O (Avg.)	109.5(6)

Table S12. Atomic coordinates and thermal parameters for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C8 as SDAs.

atom	*x*	*y*	*z*	occupancy	*U*iso	multiplicity
Al1	0.9947(6)	0.2237(6)	0.25578(19)	1	0.0233(6)	18
Al2	0.2283(7)	0.9997(6)	0.81163(19)	1	0.0233(6)	18
Al3	0.0044(7)	0.2271(6)	0.03462(21)	1	0.0233(6)	18
O1	0.2624(9)	1.0007(9)	0.77477(15)	1	0.0222(11)	18
O2	0.9958(9)	0.2589(9)	0.21882(14)	1	0.0222(11)	18
O3	0.1212(5)	0.2369(6)	0.26582(24)	1	0.0222(11)	18
O4	0.8881(5)	0.0883(6)	0.26233(20)	1	0.0222(11)	18
O5	0.3087(7)	0.9808(6)	0.72243(24)	1	0.0222(11)	18
O6	0.9685(7)	0.3102(7)	0.27779(22)	1	0.0222(11)	18
O7	0.9097(5)	0.1054(5)	0.18145(24)	1	0.0222(11)	18
O8	0.9826(7)	0.3062(7)	0.16624(25)	1	0.0222(11)	18
O9	0.1137(4)	0.2390(7)	0.17764(21)	1	0.0222(11)	18
O10	0.0035(9)	0.2535(9)	-0.00303(13)	1	0.0222(11)	18
O11	0.1329(5)	0.2458(5)	0.04592(21)	1	0.0222(11)	18
O12	0.9008(5)	0.0897(5)	0.04332(23)	1	0.0222(11)	18
P1	0.23270(18)	1.00583(18)	0.74208(18)	0.75	0.0233(6)	18
P2	1.00231(18)	0.22923(18)	0.18636(18)	0.75	0.0233(6)	18
P3	0.22369(19)	-0.00137(19)	0.96356(19)	0.75	0.0233(6)	18
Si1	0.23270(18)	1.00583(18)	0.74208(18)	0.25	0.0233(6)	18
Si2	1.00231(18)	0.22923(18)	0.18636(18)	0.25	0.0233(6)	18
Si3	0.22369(19)	-0.00137(19)	0.96356(19)	0.25	0.0233(6)	18

Table S13. Selected bond lengths and angles for calcined and dehydrated SAPO STA-18 (SFW) synthesised using trimethylamine and diDABCO-C8 as SDAs.

bond length / Å		bond angle / °	
Al1-O	1.722(8)	O-Al1-O	109.5(6)
Al2-O	1.727(8)	O-Al2-O	109.5(6)
Al3-O	1.734(8)	O-Al3-O	109.4(6)
Al-O (Avg.)	1.727(8)	O-T-O (Avg.)	109.5(6)
P1(Si1)-O	1.530(7)	O-P1(Si1)-O	109.4(5)
P2(Si2)-O	1.529(7)	O-P2(Si2)-O	109.5(5)
P3(Si3)-O	1.531(7)	O-P3(Si3)-O	109.4(5)
P(Si)-O (Avg.)	1.530(7)	O-P(Si)-O (Avg.)	109.4(5)
T-O (Avg.)	1.629(8)	O-T-O (Avg.)	109.5(6)

Table S14. Atomic coordinates and thermal parameters for calcined and dehydrated SAPO STA-19 (GME) synthesised using trimethylamine and $[DABCO\text{-}C6]_7$ as SDAs.

atom	*x*	*y*	*z*	occupancy	*U*iso	multiplicity
Al1	0.4409(6)	0.1069(6)	0.0852(7)	1	0.0156(12)	12
O1	0.7710(6)	0.2000(7)	0.0498(11)	1	0.0129(21)	12
O2	0.5575(7)	0.4158(8)	0.0646(11)	1	0.0129(21	12
O3	0.4114(7)	0.0758(8)	0.2540(9)	1	0.0129(21	12
O4	0.3597(7)	0.3389(11)	-0.0151(11)	1	0.0129(21	12
P1	-0.4343(4)	-0.1000(4)	0.5959(4)	0.7	0.0156(12)	12
Si1	-0.4343(4)	-0.1000(4)	0.5959(4)	0.3	0.0156(12)	12

Table S15. Selected bond lengths and angles for calcined and dehydrated SAPO STA-19 (GME) synthesised using trimethylamine and $[DABCO\text{-}C6]_7$ as SDAs.

bond length / Å		bond angle / °	
Al1-O	1.772(11)	O-Al1-O	109.2(6)
P1(Si1)-O	1.519(8)	O-P1(Si1)-O	108.9(6)
T-O (Avg.)	1.646(10)	O-T-O (Avg.)	109.0(6)