

## SUPPORTING INFORMATION

### **Understanding the structure directing action of copper-polyamine complexes in the direct synthesis of Cu-SAPO-34 and Cu-SAPO-18 catalysts for the selective catalytic reduction of NO with NH<sub>3</sub>**

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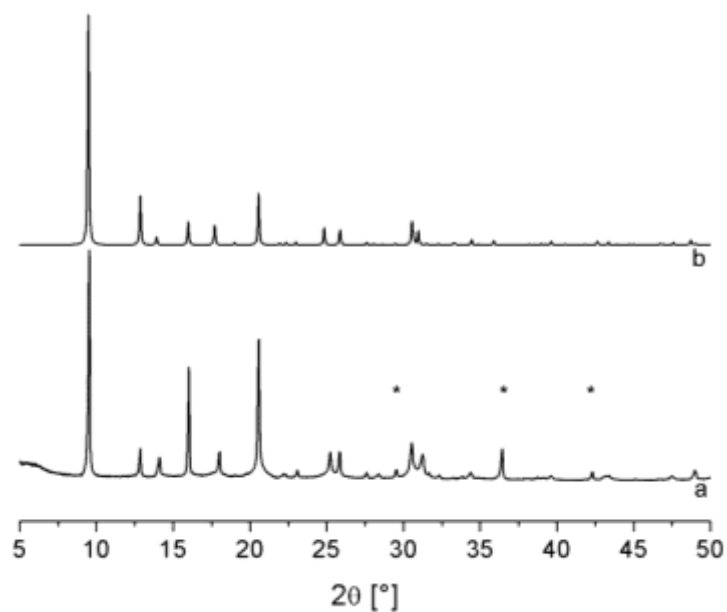
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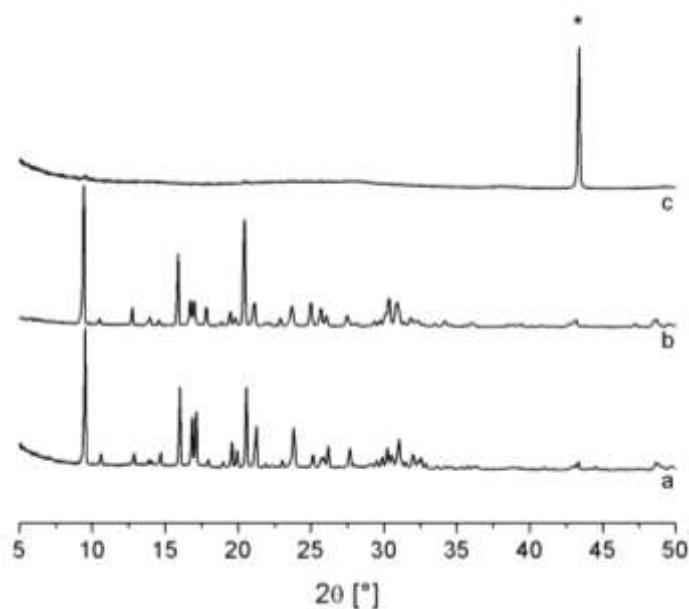
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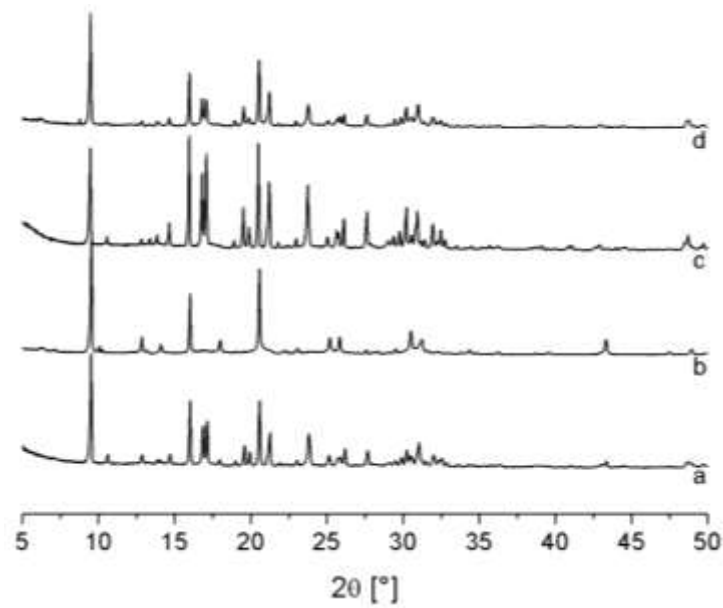
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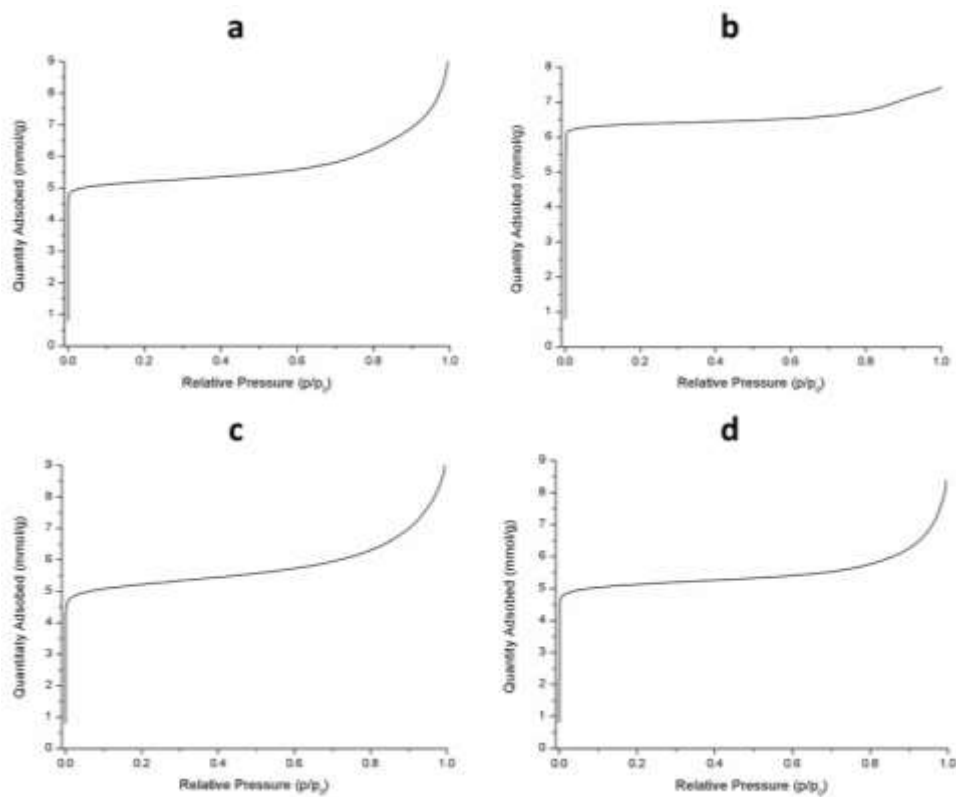
**Figure S1.** PXRD patterns of SAPO-34 synthesised using TEAOH and copper acetate without any polyamines (a). Simulated pattern of SAPO-34 has been plotted as comparison (b). The peaks marked with an \* belong to copper oxide.<sup>S1</sup>



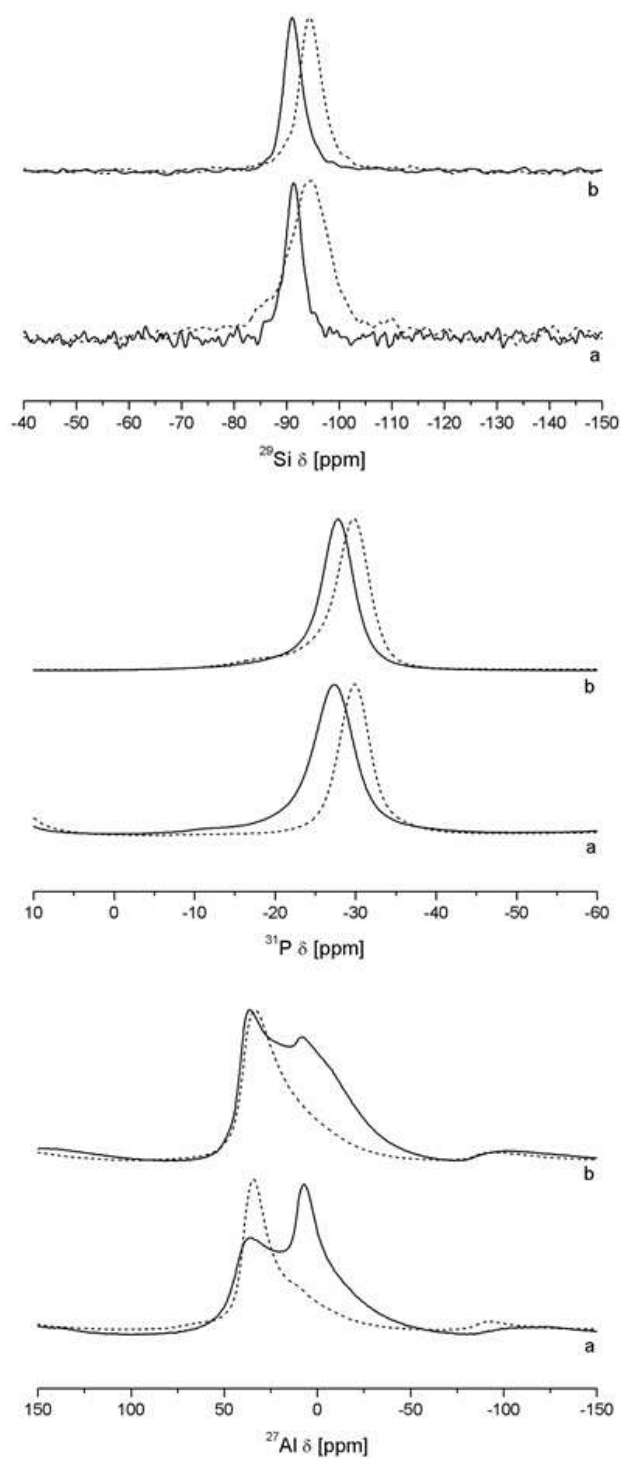
**Figure S2.** PXRD patterns of the respective synthesis of Cu-SAPO-18 performed using TEAOH as co-base/co-template agent and adding STA-7 seeds (a), without seeds (b) and without TEAOH (replaced by 232) in presence of STA-7 seeds (c). The peak marked with an \* belong to the sample holder.



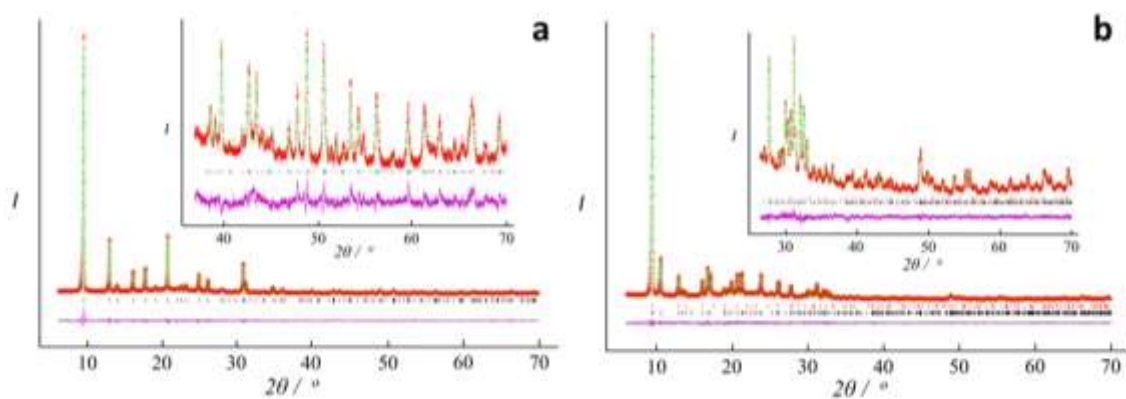
**Figure S3.** PXRD patterns of Cu and Ni SAPO-18 synthesised using as starting gel  $\text{Al}(\text{OH})_3 : 0.61 \text{H}_3\text{PO}_4 : 0.2 \text{SiO}_2 : 40 \text{H}_2\text{O} : 0.06 \text{Cu}^{2+}$  ( $0.1 \text{Ni}^{2+}$ ) : 0.2 '232' (a for copper, c for nickel) and  $\text{Al}(\text{OH})_3 : 0.8 \text{H}_3\text{PO}_4 : 0.2 \text{SiO}_2 : 40 \text{H}_2\text{O} : 0.1 \text{M}^{2+}$ -232 (b for copper, d for nickel). TEAOH and STA-7 seeds were used with copper as reported in the experimental section.



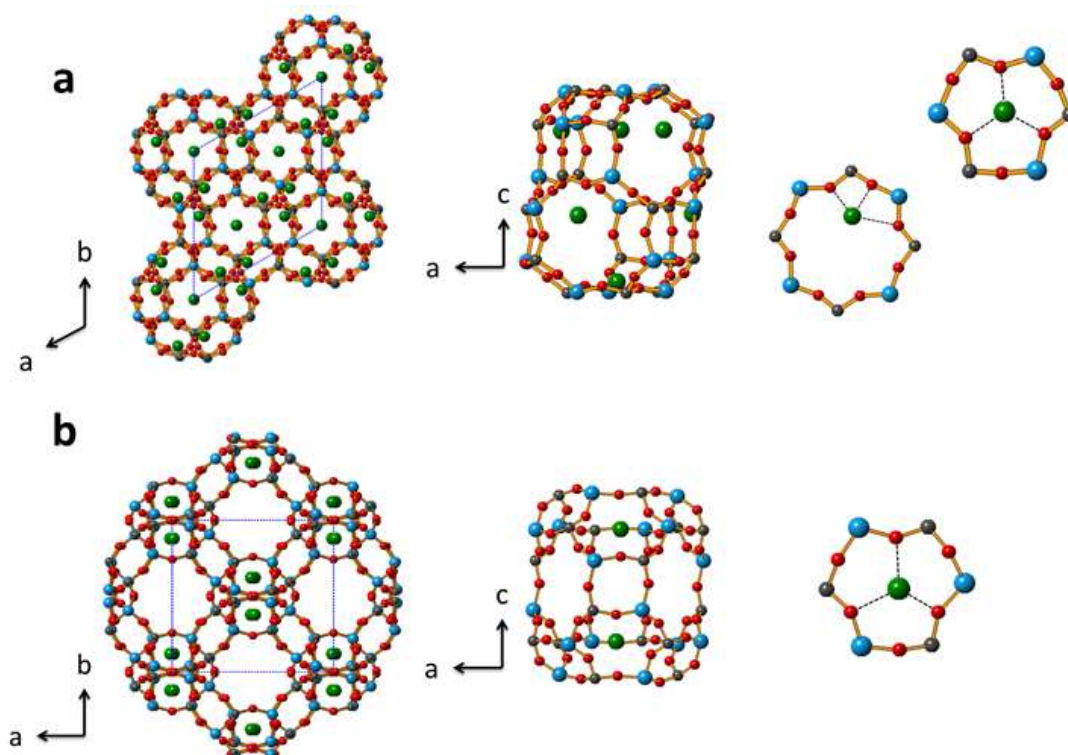
**Figure S4.** Isotherms for the adsorption of  $\text{N}_2$  at  $-196 \text{ }^\circ\text{C}$  on calcined Cu-SAPO-34 (a), Ni-SAPO-34 (b), Cu-SAPO-18 (c), Ni-SAPO-18 (d) showing uptakes of 5.2, 6.3, 5.1 and 5.0  $\text{mmol g}^{-1}$  at  $P/P_0 = 0.2$ , respectively.



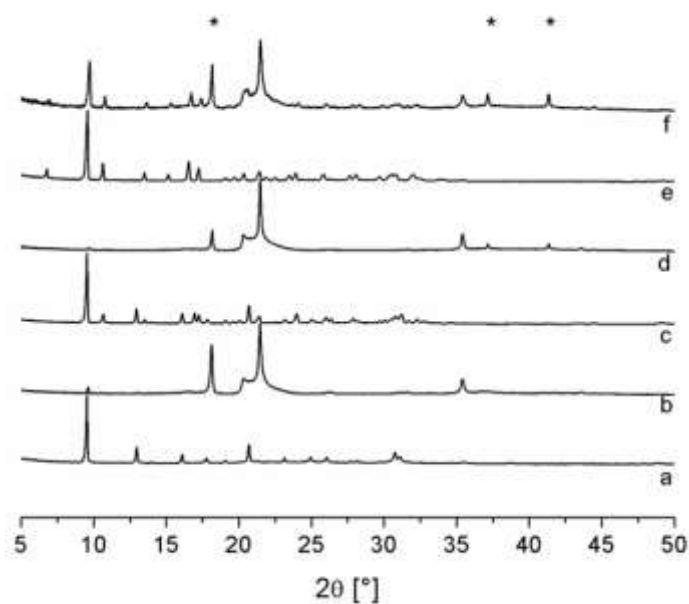
**Figure S5.** Solid-state MAS NMR spectra for dehydrated as-prepared (solid line) and calcined (dashed line) Ni-SAPO-34 (a) and Ni-SAPO-18 (b).  $^{29}\text{Si}$ , (middle)  $^{31}\text{P}$  and (bottom)  $^{27}\text{Al}$ .



**Figure S6.** Rietveld plots for calcined, dehydrated Ni-SAPO-34 (a) and Ni-SAPO-18 (b). Observed data (red crosses), calculated fit (green line), and difference plot (purple line). Peak positions are marked in black in (a) while in (b) SAPO-18 peak markers are marked in black and SAPO-34 in red.



**Figure S7.** Structures of calcined Ni-SAPO-34 (a) and Ni-SAPO-18 (b) viewed down the  $c$ -axis showing all symmetry related positions of Ni<sup>2+</sup> cations and down the  $b$ -axis showing the local environments of Ni<sup>2+</sup> site. Note that only a small fraction of these sites is occupied. (Al light blue, P dark gray, O red, Ni green).



**Figure S8.** PXRD patterns of fresh and hydrothermally treated (900 °C for 1 h) Cu-SAPO-34, (a and b), Cu-SAPO-18, (c and d), Cu-SAPO STA-7, (e and f). The peaks marked by an asterisk belong to the Teflon disk used during the measurements.

**Table S1.** Typical wavelengths in nm for UV-visible maxima for Cu and Ni complexes with amino and aza chelating agents.

metal complex	coordination geometry	$\lambda_{\text{max}}$ (nm)
$[\text{Cu}-(\text{DETA})_2]^{2+\text{a}}$	octahedral	630 <sup>S2</sup>
$[\text{Cu}-(\text{TETA})]^{2+\text{a}}$	distorted square planar	587 <sup>S2</sup>
$[\text{Cu}-(\text{EN})_2]^{2+\text{a}}$	square planar	547 <sup>S2</sup>
$[\text{Cu}-(\text{TEPA})]^{2+\text{a}}$	square pyramidal	645 <sup>S2</sup>
$[\text{Ni}-(\text{DETA})_2]^{2+\text{b}}$	octahedral	350, 543, 871 <sup>S3</sup>
$[\text{Ni}-(\text{cyclam})]^{2+\text{c}}$	square planar	454 <sup>S4</sup>

Visible absorption spectra collected at 25 °C in H<sub>2</sub>O (a) and CH<sub>3</sub>CN (c).

Diffuse reflectance UV–visible spectra of as-prepared  $[\text{Ni}(\text{DETA})_2]^{2+}$ -UT-6 (b).

**Table S2.** EPR fitted parameters for Cu-TETA and Cu-232 complexes contained within SAPO-34 and SAPO-18 respectively.

sample	species weight (%)	$g_{\parallel}$	$g_{\perp}$	$A_{\parallel}$ (MHz)	$A_{\perp}$ (MHz)	lw (MHz)
Cu-TETA hydrated	50	2.204	2.067	408	72	450
	50	2.194	2.040	529	60	195
Cu-232 hydrated	75	2.198	2.044	410	40	440
	25	2.189	2.038	564	79	185
Cu-TETA dehydrated	60	2.225	2.052	359	79	390
	40	2.204	2.044	529	60	170
Cu-232 dehydrated	50	2.206	2.059	351	50	420
	50	2.174	2.026	570	42	280
Cu-TETA rehydrated	50	2.204	2.067	408	72	450
	50	2.194	2.040	529	60	195
Cu-232 rehydrated	75	2.196	2.047	432	22	440
	25	2.191	2.040	570	83	185

lw: linewidth

**Table S3.** EPR fitted parameters for the calcined and hydrate Cu-SAPO-34 and Cu-SAPO-18.

sample	species weight (%)	$g_1$	$g_2$	$g_3$	$A_1$ (MHz)	$A_2$ (MHz)	$A_3$ (MHz)	lw <sub>1</sub> (MHz)	lw <sub>2</sub> (MHz)	lw <sub>3</sub> (MHz)	$g$	A (MHz)	lw (MHz)
Cu-SAPO-34	55	2.064	2.113	2.390	36	53	392	150	400	330			
calcined hydrate	45										2.170	95	925
Cu-SAPO-18	60	2.068	2.093	2.375	36	76	392	150	400	330			
calcined hydrate	40	2.191	2.040	570	83						2.165	95	950

lw: linewidth



**Table S4.** Atomic coordinates and thermal parameters for calcined and dehydrated Cu-SAPO-34.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>U</i> <sub>iso</sub>	Multiplicity
Al1	0.2384(12)	0.2391(13)	0.0767(13)	1	0.0325(12)	9
Al2	0.7651(12)	0.7681(14)	0.8742(13)	1	0.0325(12)	9
P1	-0.0020(8)	0.2226(8)	0.0854(8)	1	0.0325(12)	9
P2	0.9915(8)	0.7673(8)	0.8699(8)	0.7	0.0325(12)	9
O1	0.9987(21)	0.2484(14)	0.9895(12)	1	0.0447(18)	9
O2	0.1175(10)	0.2441(16)	0.1089(16)	1	0.0447(18)	9
O3	0.2020(11)	0.1043(12)	0.1021(17)	1	0.0447(18)	9
O4	0.3098(11)	0.0167(11)	0.1533(14)	1	0.0447(18)	9
O5	0.9913(18)	0.7300(12)	0.9636(12)	1	0.0447(18)	9
O6	0.8788(11)	0.7545(15)	0.8408(17)	1	0.0447(18)	9
O7	0.8050(11)	0.9084(13)	0.8530(17)	1	0.0447(18)	9
O8	0.6897(11)	0.9984(11)	0.8027(13)	1	0.0447(18)	9
Si1	-0.0020(8)	0.2226(8)	0.0854(8)	0.3	0.0325(12)	9
Si2	0.9915(8)	0.7673(8)	0.8699(8)	0.3	0.0325(12)	9
Cu1	0.5414(21)	-0.0357(20)	0.0297(20)	0.155	0.0325(12)	9

**Table S5.** Selected bond lengths and angles for calcined and dehydrated Cu-SAPO-34.

Bond length / Å	Bond angle / °		
Al1-O	1.732(14)	O-Al1-O	109.4(10)
Al2-O	1.730(15)	O-Al2-O	109.4(10)
Al-O (Avg.)	1.731(15)	O-T-O (Avg.)	109.4(10)
P1(Si1)-O	1.531(15)	O-P1(Si1)-O	109.5(10)
P2(Si2)-O	1.541(15)	O-P2(Si2)-O	109.4(10)
P(Si)-O (Avg.)	1.536(15)	O-P(Si)-O (Avg.)	109.5(10)
T-O (Avg.)	1.633(15)	O-T-O (Avg.)	109.4(10)
Cu-O <sub>framework</sub>	2.56(3)		

**Table S6.** Atomic coordinates and thermal parameters for calcined and dehydrated Cu-SAPO-18.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>U</i> <sub>iso</sub>	Multiplicity
Al1	0.8930(6)	0.9612(6)	0.1670(5)	1	0.0075(6)	8
Al2	0.8830(6)	0.2227(6)	0.9409(5)	1	0.0075(6)	8
Al3	0.2278(6)	0.0967(7)	0.0491(6)	1	0.0075(6)	8
P1	0.7715(4)	0.0946(4)	0.0528(4)	0.75	0.0075(6)	8
P2	0.1099(4)	0.2289(4)	0.9351(4)	0.75	0.0075(6)	8
P3	0.1144(4)	0.9679(4)	0.1620(4)	0.75	0.0075(6)	8
O1	0.1806(9)	0.0499(10)	0.1306(6)	1	0.0190(13)	8
O2	0.1354(10)	0.1625(11)	0.0033(6)	1	0.0190(13)	8
O3	0.0041(5)	0.2566(6)	0.9458(5)	1	0.0190(13)	8
O4	0.8529(9)	0.1602(12)	0.0193(6)	1	0.0190(13)	8
O5	0.8121(9)	0.0439(10)	0.1218(6)	1	0.0190(13)	8
O6	0.0097(6)	1.0007(7)	0.1485(5)	1	0.0190(13)	8
O7	0.1372(9)	0.8613(8)	0.1317(6)	1	0.0190(13)	8
O8	0.3265(8)	0.1746(9)	0.0660(8)	1	0.0190(13)	8
O9	0.8671(7)	0.9621(7)	0.2568(4)	1	0.0190(13)	8
O10	0.8129(8)	0.3344(9)	0.9277(8)	1	0.0190(13)	8
O11	0.1250(9)	0.1636(8)	0.8679(6)	1	0.0190(13)	8
O12	0.2627(7)	-0.0104(11)	0.9977(9)	1	0.0190(13)	8
Si1	0.7715(4)	0.0946(4)	0.0528(4)	0.25	0.0075(6)	8
Si2	0.1099(4)	0.2289(4)	0.9351(4)	0.25	0.0075(6)	8
Si3	0.1144(4)	0.9679(4)	0.1620(4)	0.25	0.0075(6)	8
Cu1	0.003(5)	0.1275(12)	0.0616(11)	0.15	0.0075(6)	8

**Table S7.** Selected bond lengths and angles for calcined and dehydrated Cu-SAPO-18.

Bond length / Å		Bond angle / °	
Al1-O	1.730(9)	O-Al1-O	109.4(6)
Al2-O	1.732(9)	O-Al2-O	109.5(6)
Al3-O	1.739(9)	O-Al3-O	109.5(6)
Al-O (Avg.)	1.733(9)	O-T-O (Avg.)	109.5(6)
P1(Si1)-O	1.525(8)	O-P1(Si1)-O	109.5(6)
P2(Si2)-O	1.528(8)	O-P2(Si2)-O	109.4(6)
P3(Si3)-O	1.518(8)	O-P3(Si3)-O	109.5(6)
P(Si)-O (Avg.)	1.524(8)	O-P(Si)-O (Avg.)	109.4(6)
T-O (Avg.)	1.629(9)	O-T-O (Avg.)	109.5(6)
Cu-O <sub>framework</sub>	2.24(5)		

**Table S8.** Crystallographic data for calcined and dehydrated Ni-SAPO-34 and Ni-SAPO-18.

	Ni-SAPO-34 <sup>a</sup>	Ni-SAPO-18 <sup>b</sup>
Chemical composition <sup>c</sup>	Ni <sub>2.6</sub> H <sub>0.7</sub> Al <sub>18</sub> Si <sub>4.413,6</sub> O <sub>72</sub> 30.4H <sub>2</sub> O	Ni <sub>2.5</sub> Al <sub>24</sub> Si <sub>5</sub> P <sub>19</sub> O <sub>96</sub> 37.2H <sub>2</sub> O
Data collection		
Wavelength / Å	1.54056	1.54056
Diffractometer	Debye-Scherrer	Debye-Scherrer
geometry		
Sample	rotating 0.5 mm capillary	rotating 0.5 mm capillary
Scanned region / 2θ°	3.0 – 70.0	5.0 – 70.0
Step size / 2θ°	0.1	0.1
Unit cell		
Chemical formula	Ni <sub>1.8</sub> Al <sub>18</sub> Si <sub>6</sub> P <sub>12</sub> O <sub>72</sub>	Ni <sub>1.4</sub> Al <sub>24</sub> Si <sub>4.8</sub> P <sub>19.2</sub> O <sub>96</sub>
Space group	R 3	C 1 2/c 1
a / Å	13.7089(2)	13.6760(3)
b / Å	13.7089(2)	12.8261(3)
c / Å	15.0663(3)	18.6162(4)
β / °		90.048(8)
Volume / Å <sup>3</sup>	2452.10(9)	3265.46(7)
Rietveld refinement		
Refined region / 2θ°	5.0 – 70.0	6.0 – 70.0
% of SAPO-34		5.8
R <sub>wp</sub>	0.056	0.036
R <sub>p</sub>	0.042	0.028
R <sub>F</sub> <sup>2</sup>	0.072	0.037
X <sup>2</sup>	3.47	1.64

(a) Ni-SAPO-34 was prepared in presence of Ni-DETA as SDA using the gel composition Al(OH)<sub>3</sub> : 0.61 H<sub>3</sub>PO<sub>4</sub> : 0.25 SiO<sub>2</sub> : 40 H<sub>2</sub>O : 0.15 Ni<sup>2+</sup>-DETA. (b) Ni-SAPO-18 was prepared in the presence of Ni-232 as SDA using the gel composition reported in the experimental section.

(c) Determined combining EDX, TGA and AAS.

**Table S9.** Atomic coordinates and thermal parameters for calcined and dehydrated Ni-SAPO-34.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>U</i> <sub>iso</sub>	Multiplicity
Al1	0.2291(9)	0.2225(11)	0.0385(12)	1	0.0483(7)	9
Al2	0.7706(10)	0.7725(11)	0.8281(11)	1	0.0483(7)	9
P1	0.0032(8)	0.2324(8)	0.0336(8)	0.667	0.0483(7)	9
P2	0.9992(8)	0.7730(8)	0.8349(8)	0.667	0.0483(7)	9
O1	-0.0037(16)	0.2628(12)	-0.0606(10)	1	0.0560(14)	9
O2	0.1167(8)	0.2432(11)	0.0613(13)	1	0.0560(14)	9
O3	0.1836(9)	0.0793(10)	0.0519(14)	1	0.0560(14)	9
O4	0.3265(9)	0.0184(8)	0.0968(10)	1	0.0560(14)	9
O5	0.9912(15)	0.7306(11)	0.9290(11)	1	0.0560(14)	9
O6	0.8902(8)	0.7645(11)	0.7985(14)	1	0.0560(14)	9
O7	0.802(1)	0.909(1)	0.8214(14)	1	0.0560(14)	9
O8	0.6672(9)	0.9698(8)	0.7763(11)	1	0.0560(14)	9
Si1	0.0032(8)	0.2324(8)	0.0336(8)	0.333	0.0483(7)	9
Si2	0.9992(8)	0.7730(8)	0.8349(8)	0.333	0.0483(7)	9
Ni1	0.0004	0.0002	0.0769(15)	0.085	0.0483(7)	9
Ni2	0.4594(26)	0.4167(25)	0.0093(27)	0.108	0.0483(7)	9

**Table S10.** Selected bond lengths and angles for calcined and dehydrated Ni-SAPO-34.

Bond length / Å		Bond angle / °	
Al1-O	1.727(11)	O-Al1-O	109.5(8)
Al2-O	1.725(11)	O-Al2-O	109.5(8)
Al-O (Avg.)	1.726(11)	O-T-O (Avg.)	109.5(8)
P1(Si1)-O	1.537(11)	O-P1(Si1)-O	109.4(8)
P2(Si2)-O	1.533(11)	O-P2(Si2)-O	109.4(8)
P(Si)-O (Avg.)	1.535(11)	O-P(Si)-O (Avg.)	109.4(8)
T-O (Avg.)	1.630(11)	O-T-O (Avg.)	109.4(8)
Ni1-O <sub>framework</sub>	2.219(12)		
Ni2-O <sub>framework</sub>	2.16(4)		

**Table S11.** Atomic coordinates and thermal parameters for calcined and dehydrated Ni-SAPO-18.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>U</i> <sub>iso</sub>	Multiplicity
Al1	0.8903(5)	0.9578(5)	0.1666(4)	1	0.0109(7)	8
Al2	0.8789(4)	0.2208(5)	0.9389(4)	1	0.0109(7)	8
Al3	0.2296(5)	0.0944(5)	0.0503(4)	1	0.0109(7)	8
P1	0.77300(29)	0.09608(29)	0.05433(29)	0.8	0.0109(7)	8
P2	0.10860(27)	0.23014(27)	0.93642(27)	0.8	0.0109(7)	8
P3	0.11799(28)	0.97148(28)	0.16559(28)	0.8	0.0109(7)	8
O1	0.1839(7)	0.0486(8)	0.1305(5)	1	0.0197(12)	8
O2	0.1378(8)	0.1658(9)	0.0045(5)	1	0.0197(12)	8
O3	0.0025(4)	0.2594(5)	0.9445(4)	1	0.0197(12)	8
O4	0.8498(7)	0.1608(10)	0.0170(5)	1	0.0197(12)	8
O5	0.8156(7)	0.0477(8)	0.1219(5)	1	0.0197(12)	8
O6	0.0114(4)	0.9956(5)	0.1515(4)	1	0.0197(12)	8
O7	0.1385(7)	0.8614(6)	0.1346(5)	1	0.0197(12)	8
O8	0.3297(6)	0.1719(6)	0.0661(6)	1	0.0197(12)	8
O9	0.8624(5)	0.9618(6)	0.25528(30)	1	0.0197(12)	8
O10	0.8105(6)	0.3332(7)	0.9242(6)	1	0.0197(12)	8
O11	0.1278(7)	0.1640(6)	0.8700(5)	1	0.0197(12)	8
O12	0.2639(5)	-0.0096(9)	0.9951(7)	1	0.0197(12)	8
Si1	0.77300(29)	0.09608(29)	0.05433(29)	0.2	0.0109(7)	8
Si2	0.10860(27)	0.23014(27)	0.93642(27)	0.2	0.0109(7)	8
Si3	0.11799(28)	0.97148(28)	0.16559(28)	0.2	0.0109(7)	8
Ni1	0.0100(31)	0.1208(10)	0.0608(8)	0.18	0.0109(7)	8

**Table S12.** Selected bond lengths and angles for calcined and dehydrated Ni-SAPO-18.

Bond length / Å		Bond angle / °	
Al1-O	1.729(7)	O-Al1-O	109.4(5)
Al2-O	1.735(7)	O-Al2-O	109.5(5)
Al3-O	1.739(7)	O-Al3-O	109.5(5)
Al-O (Avg.)	1.735(7)	O-T-O (Avg.)	109.5(5)
P1(Si1)-O	1.517(6)	O-P1(Si1)-O	109.5(5)
P2(Si2)-O	1.527(6)	O-P2(Si2)-O	109.5(5)
P3(Si3)-O	1.514(6)	O-P3(Si3)-O	109.4(5)
P(Si)-O (Avg.)	1.519(6)	O-P(Si)-O (Avg.)	109.4(5)
T-O (Avg.)	1.627(7)	O-T-O (Avg.)	109.5(5)
Ni-O <sub>framework</sub>	2.28(3)		

## Reference

- [S1] J. D. Hanawalt, H. W. Rinn, L. K. Frevel, *Anal. Chem.*, 10 (1938) 475-512.
- [S2] T. Sawada, K. Fukumaru, H. Sakurai, *Chem. Pharm. Bull.*, 44 (1996) 1009–1016.
- [S3] R. Garcia, I.J. Shannon, A.M.Z. Slawin, W. Zhou, P.A. Cox, P.A. Wright, *Microporous Mesoporous Mater.*, 58 (2003) 91–104.
- [S4] D.J. Szalda, E. Fujita, R. Sanzenbacher, H. Paulus, H. Elias, *Inorg. Chem.*, 33 (1994) 5855–5863.