SUPPORTING INFORMATION

STA-20: An ABC-6 Zeotype Structure Prepared by Co-Templating and Solved via a Hypothetical Structure Database and STEM-ADF Imaging

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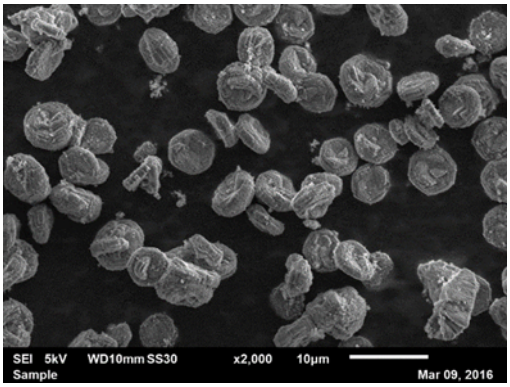

Figure S1. SEM images of SAPO STA-20 synthesised with TrMA and diDABCO-C6.

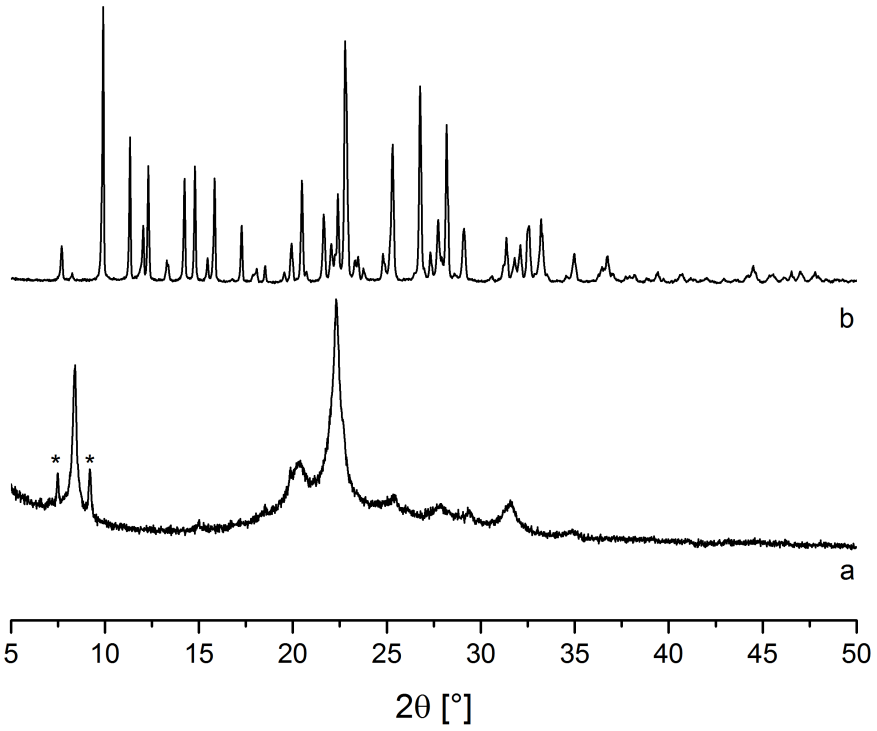

Figure S2. PXRD patterns of the respective synthesis of STA-20 performed in the absence of (a) TrMA and (b) SiO_2.

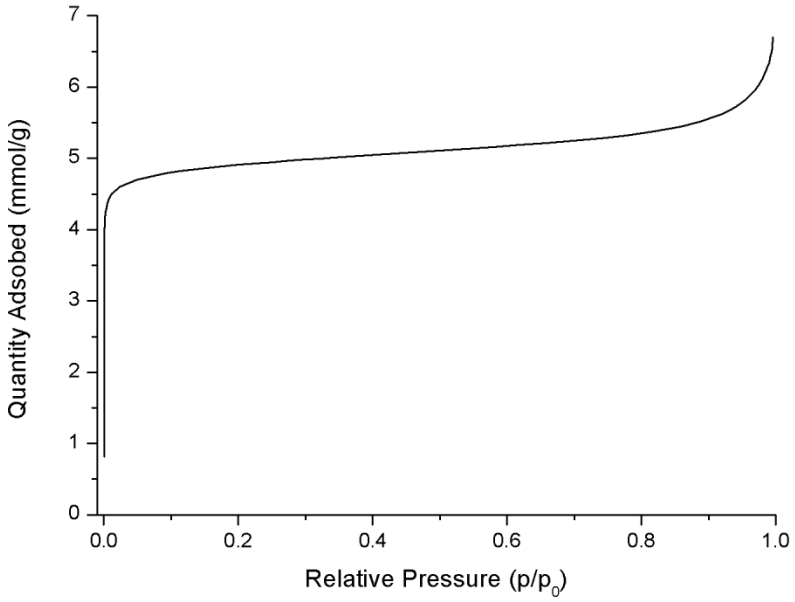

Figure S3. Isotherms for the adsorption of N_2 at -196.15 °C on calcined SAPO STA-20.

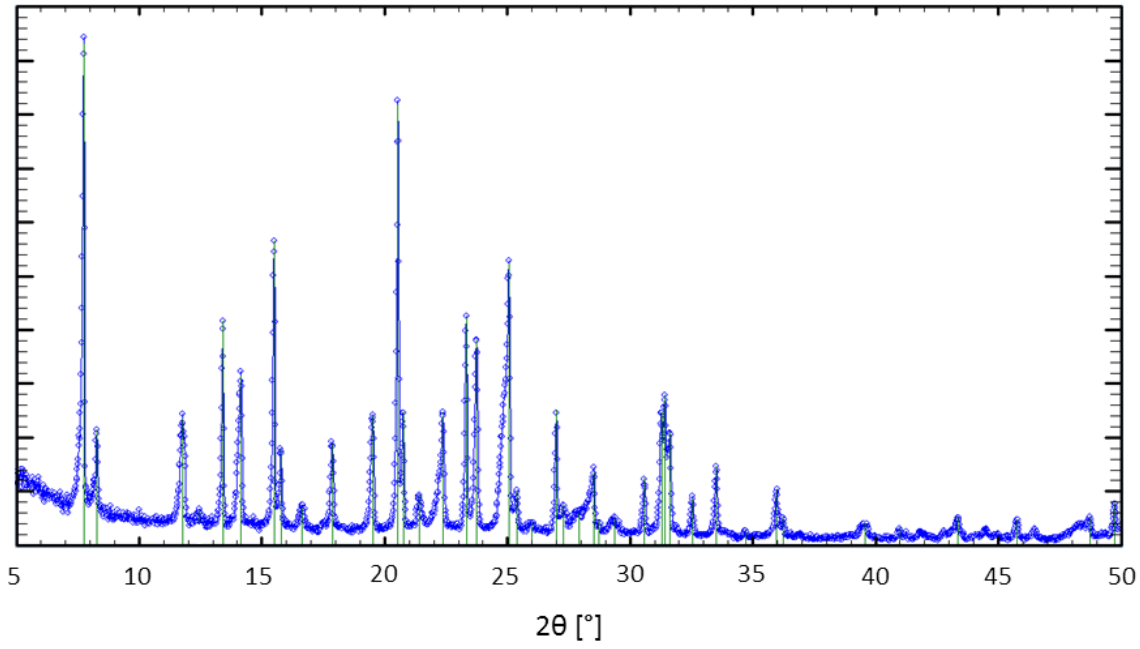

Figure S4. Indexed laboratory X-ray powder diffraction pattern of as-prepared SAPO STA-20 using the algorithm DICVOL 06 within the program FullProf.

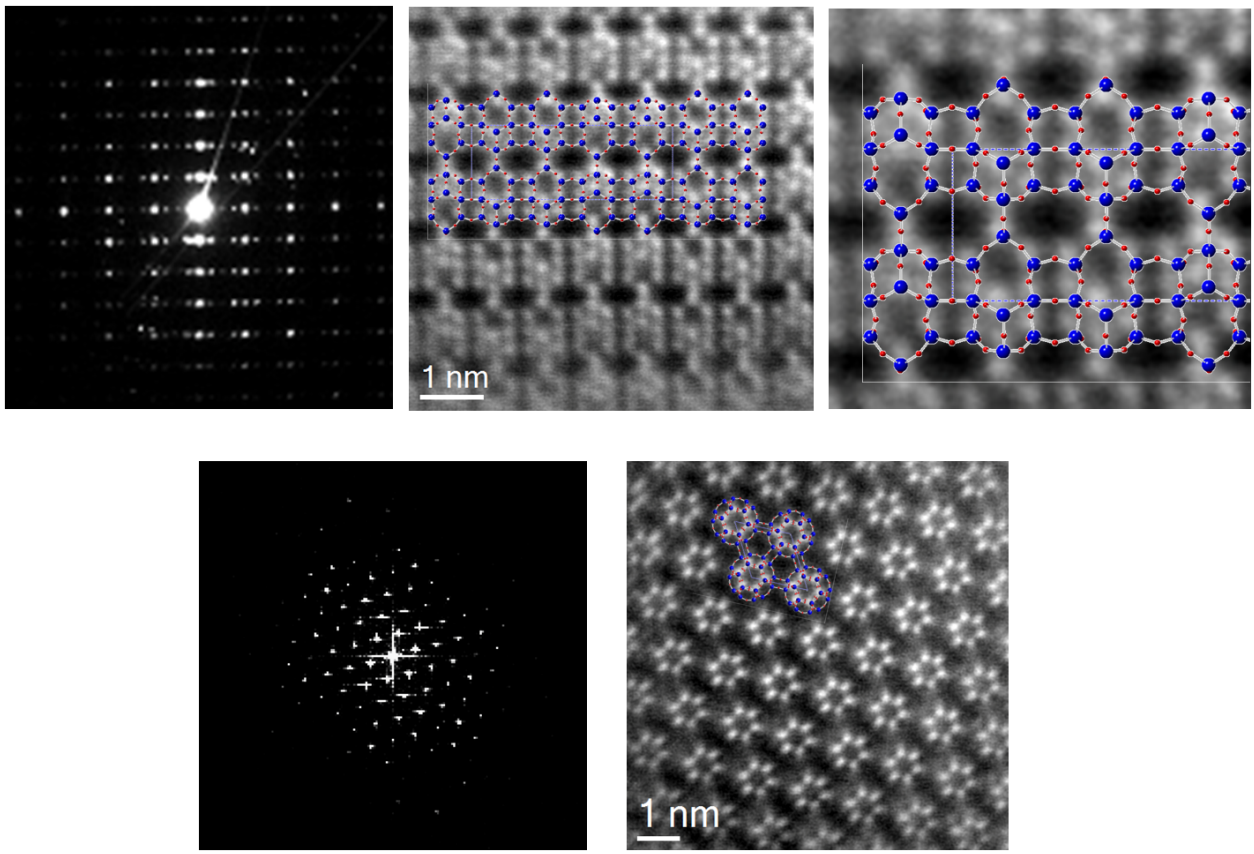

Figure S5. Associated electron diffraction patterns and STEM ADF images, with superposed figures of the STA-20 framework structure, taken down the [100] zone axis (above) and the [001] zone axis (below).

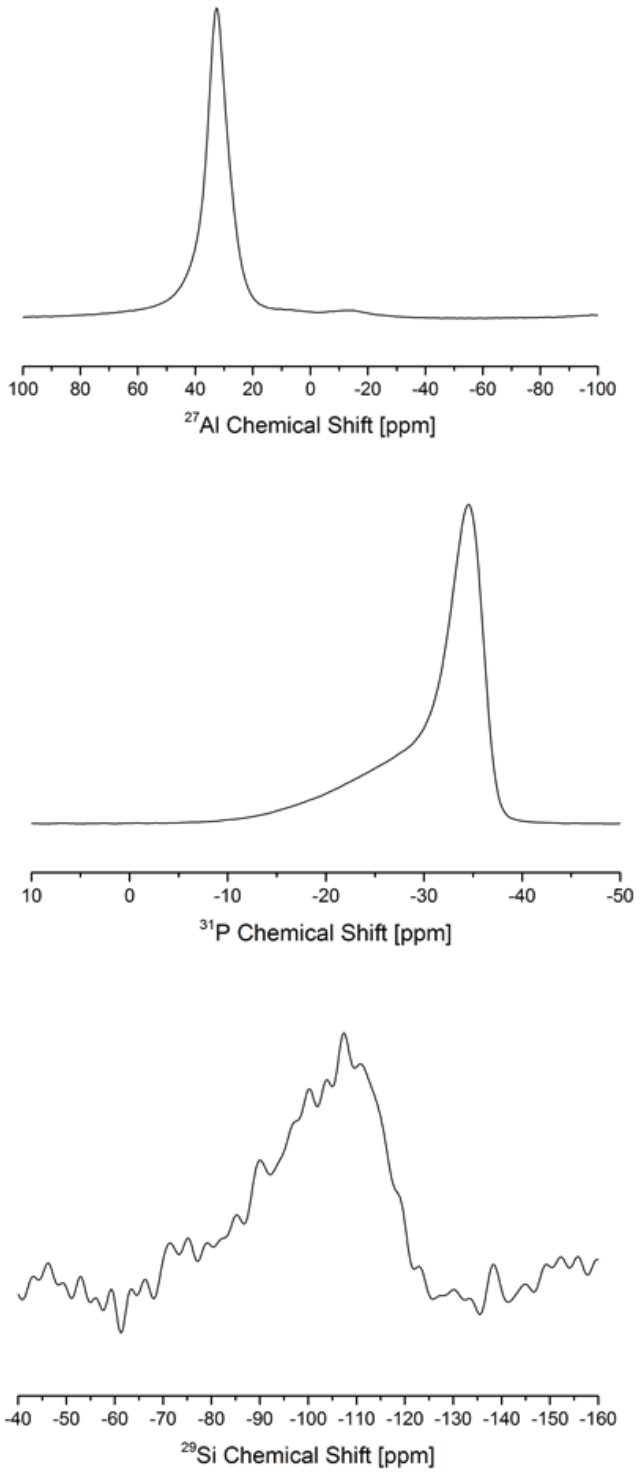

Figure S6. Solid-state NMR spectra of calcined, dehydrated SAPO STA-20, stabilised against water adsorption by hexane adsorption after calcination. (Top) ^{27}Al, (middle), ^{31}P and (bottom) ^{29}Si.

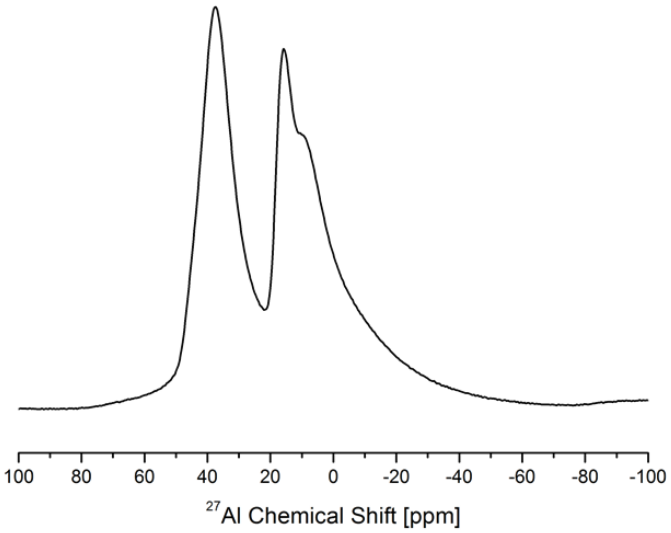

Figure S7. ^{27}Al MAS NMR spectrum of as-prepared SAPO STA-20.

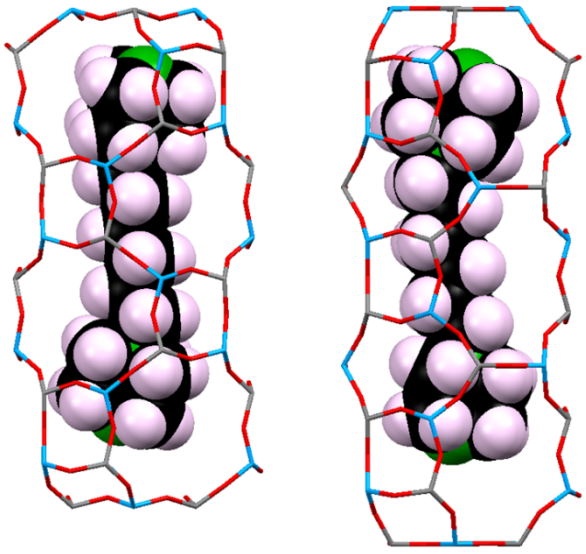

Figure S8. Minimum energy configurations of diDABCO-C6 in (left) $AlPO_4$ (SFW) and (right) $AlPO_4$ (STA-20). (Al light blue, P dark grey, O red, C black, N green, H light pink).

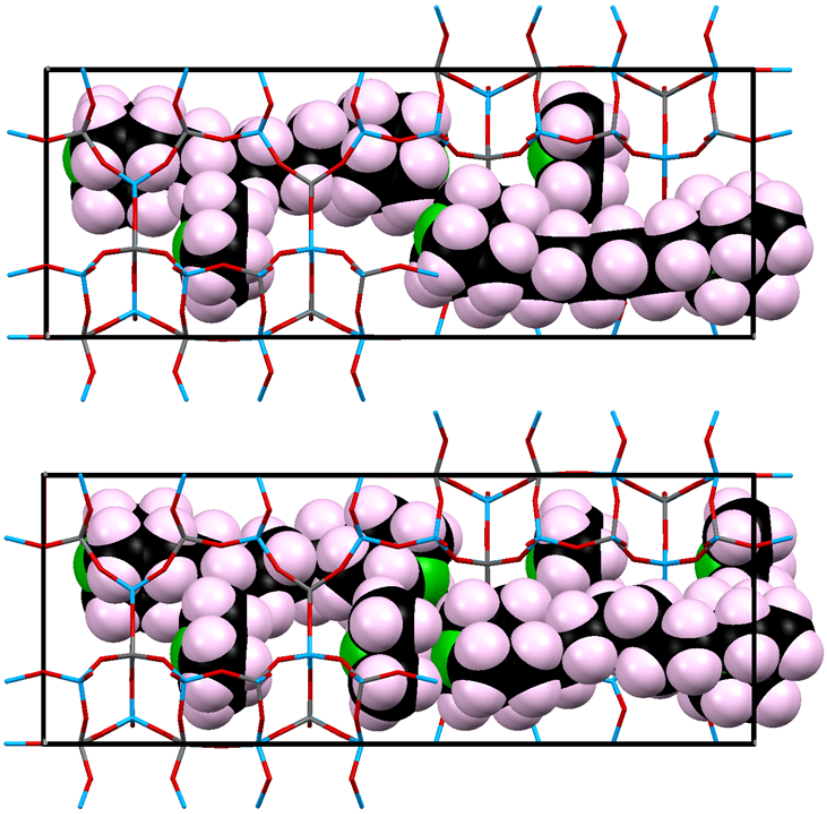

Figure S9. Energy-minimised configurations of diDABCO-C6 and TrMA included in the *sta-20* and *gme* cages (top) and TrMA molecule included into each *sta-20* cage along with the diDABCO-C6 molecule (bottom). (Al light blue, P dark grey, O red, C black, N green, H light pink).

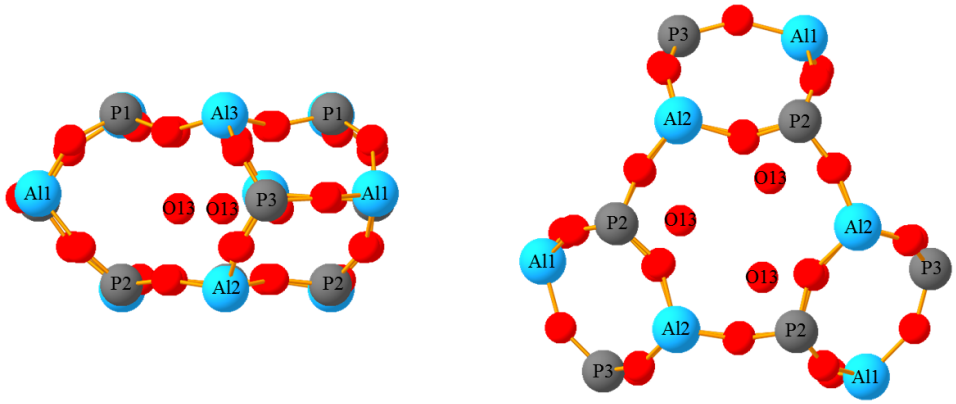

Figure S10. Bridging hydroxyl O atom positions found to be occupied in the *can* cages of SAPO STA-20 viewed down the *a*-axis (left) and *c*-axis (right). (Al light blue, P dark grey, O red).

Table S1. Syntheses from gel composition 1.0$Al(OH)_3$ · *a* H_3PO_4 · *b* SiO_2 · 0.1 (diDABCO-C6)Br_2 · *c* TrMA · *d* TBAOH · 40 H_2O with 2 wt. % of SAPO-56 seeds with respect to SiO_2 (when *b* = 0.2).

Run nº	Al source	Si source	TBAOH source	*a*	*b*	*c*	d	temp. (°C)	time (days)	Stirring (rpm)	product (topology type)
1	Aldrich[1]	Aldrich[2]	Aldrich[3]	0.8	0.2	0.13	0.28	190	7	static	STA-18 + STA-20
2	Aldrich	Aldrich	Aldrich	0.7	0.3	0.52	0.0	190	7	static	STA-20 + SAPO-43
3	Aldrich	Aldrich	Aldrich	0.8	0.2	0.52	0.0	160	7	static	STA-20 + SAPO-43 + AlPO-21
4	Aldrich	Aldrich	Aldrich	0.8	0.2	0.42	0.08	160	7	static	STA-20 + SAPO-43
5	Aldrich	PX-30[4]	Aldrich	0.8	0.2	0.42	0.08	160	1	30	STA-20
6	Aldrich	PX-30	Aldrich	0.9	0.1	0.42	0.08	160	1	30	STA-20
7	Alfa[5]	Cabosil[6] M5	Aldrich	0.9	0.1	0.42	0.08	160	1	30	STA-20
8	Alfa	PX-30	Aldrich	0.9	0.1	0.42	0.08	160	1	30	STA-20 + unckown impurity
9	Aldrich	Cabosil M5	Sachem[7]	0.9	0.1	0.42	0.08	160	1	30	STA-20 + SAPO-43
10	Aldrich	PX-30	Sachem[7]	0.9	0.1	0.42	0.08	160	1	30	STA-20 + SAPO-43 + AlPO-21
11	Alfa	Cabosil M5	Sachem	0.9	0.1	0.42	0.08	160	1	30	STA-20
12	Alfa	PX-30	Sachem	0.9	0.1	0.42	0.08	160	1	30	STA-20 + AlPO-21
13	Alfa	Cabosil M5	Sachem	0.8	0.2	0.42	0.08	160	1	30	STA-20
14	Alfa	PX-30	Sachem	0.8	0.2	0.42	0.08	160	1	30	STA-20
15	Alfa		Sachem	1.0	0.0	0.42	0.08	160	2	30	AlPO-21 + STA-20
16	Alfa	Cabosil M5	Sachem	0.9	0.1	0	0.28	160	1	30	SAPO-31

[1] Aluminum hydroxide, Sigma Aldrich.

[2] Silica (fumed), powder 0.007 μm, Sigma Aldrich.

[3] Tetrabutylammonium hydroxide, 40 wt. % in H_2O, Sigma Aldrich.

[4] Ludox PX-30 Colloidal Silica, 30 wt. % (aq.) Grace Davison.

[5] Aluminium hydroxide, Alfa Aesar.

[6] Fumed silica, Cabosil M5, > 99.8%, Cabot.

[7] Tetrabutylammonium hydroxide, 55 wt. % in H_2O, Sachem.

Table S2. Atomic coordinates and thermal parameters for as-prepared and dehydrated SAPO STA-20.

Atom	x	y	z	Occupancy	U_{iso}	Multiplicity
Al1	0.33229(34)	0.4202(4)	0.11992(28)	1	0.02125(34)	12
Al2	0.2374(7)	0.9976(5)	0.20425(25)	1	0.02125(34)	12
Al3	0.2375(7)	1.0057(6)	0.05597(24)	1	0.02125(34)	12
O1	0.3252(6)	0.3566(5)	0.07025(19)	1	0.0342(10)	12
O2	0.3053(5)	0.31873(35)	0.16132(15)	1	0.0342(10)	12
O3	0.6694(6)	0.6486(6)	0.58589(24)	1	0.0342(10)	12
O4	0.6752(7)	0.6454(6)	0.66792(22)	1	0.0342(10)	12
O5	0.2597(7)	0.2521(7)	-0.00021(13)	1	0.0342(10)	12
O6	0.1071(4)	0.2054(5)	0.05884(23)	1	0.0342(10)	12
O7	0.2215(4)	0.4603(5)	0.12329(33)	1	0.0342(10)	12
O8	0.1070(4)	0.1985(6)	0.19534(31)	1	0.0342(10)	12
O9	0.2531(6)	0.1387(6)	0.06785(23)	1	0.0342(10)	12
O10	0.2513(6)	0.1268(5)	0.19046(24)	1	0.0342(10)	12
O11	0.46621(32)	0.5432(4)	0.1277625)	1	0.0342(10)	12
O12	0.2815(7)	0.2868(6)	0.24262(13)	1	0.0342(10)	12
O13	0.11174(9)	1.10762(9)	0.13067(24)	0.26	0.0218	12
P1	0.23786(33)	0.23759(34)	0.05077(15)	0.80	0.02125(34)	12
P2	0.23536(33)	0.23529(34)	0.19677(15)	0.80	0.02125(34)	12
P3	0.66706(33)	0.57509(34)	0.62467(15)	0.80	0.02125(34)	12
Si1	0.23786(33)	0.23759(34)	0.05077(15)	0.20	0.02125(34)	12
Si2	0.23536(33)	0.23529(34)	0.19677(15)	0.20	0.02125(34)	12
Si3	0.66706(33)	0.57509(34)	0.62467(15)	0.20	0.02125(34)	12
C1	0.6931	0.4535	0.1125	0.16	0.005	12
C2	0.6936	0.4477	0.1639	0.16	0.005	12
C3	0.5532	0.2392	0.1607	0.16	0.005	12
C4	0.5523	0.2468	0.1094	0.16	0.005	12
C5	0.7586	0.3132	0.1077	0.16	0.005	12
C6	0.7605	0.3079	0.1589	0.16	0.005	12
C7	0.6748	0.3214	0.2276	0.16	0.005	12
C8	0.5984	0.3595	0.2542	0.16	0.005	12
C9	0.5606	0.2951	0.2988	0.16	0.005	12
C10	0.6647	0.3339	0.3305	0.16	0.005	12
C11	0.6334	0.2413	0.3668	0.16	0.005	12
C12	0.7244	0.2892	0.4049	0.16	0.005	12
C13	0.6378	0.4	0.4389	0.16	0.005	12
C14	0.5974	0.4278	0.4833	0.16	0.005	12
C15	0.5532	0.241	0.5131	0.16	0.005	12
C16	0.59	0.2093	0.4688	0.16	0.005	12
C17	0.7841	0.3753	0.4778	0.16	0.005	12
C18	0.7462	0.4077	0.5217	0.16	0.005	12
C19	0.6659	0.2299	0.9839	0.48	0.005	12
C20	0.7532	0.3026	0.747	0.50	0.005	12
H1	0.7793	0.5249	0.1004	0.16	0.005	12
H2	0.6267	0.4761	0.101	0.16	0.005	12
H3	0.78	0.5167	0.1769	0.16	0.005	12
H4	0.6263	0.4676	0.1769	0.16	0.005	12
H5	0.5331	0.1495	0.1708	0.16	0.005	12
H6	0.4813	0.2514	0.1736	0.16	0.005	12
H7	0.5308	0.1612	0.0943	0.16	0.005	12
H8	0.482	0.2647	0.0984	0.16	0.005	12
H9	0.8457	0.3808	0.0948	0.16	0.005	12

H10	0.7416	0.2283	0.0932	0.16	0.005	12
H11	0.8496	0.3741	0.1691	0.16	0.005	12
H12	0.7455	0.2201	0.1691	0.16	0.005	12
H13	0.7673	0.3775	0.2391	0.16	0.005	12
H14	0.6509	0.23	0.237	0.16	0.005	12
H15	0.64772	0.45625	0.2597	0.16	0.005	12
H16	0.5175	0.3406	0.236	0.16	0.005	12
H17	0.4959	0.3144	0.3149	0.16	0.005	12
H18	0.5135	0.1982	0.2931	0.16	0.005	12
H19	0.6879	0.4209	0.3449	0.16	0.005	12
H20	0.7446	0.346	0.3131	0.16	0.005	12
H21	0.633	0.1637	0.3517	0.16	0.005	12
H22	0.5422	0.2077	0.3785	0.16	0.005	12
H23	0.8071	0.3673	0.393	0.16	0.005	12
H24	0.7514	0.2231	0.4119	0.16	0.005	12
H25	0.7071	0.4831	0.4236	0.16	0.005	12
H26	0.5621	0.3627	0.4156	0.16	0.005	12
H27	0.6438	0.5236	0.489	0.16	0.005	12
H28	0.5027	0.4005	0.482	0.16	0.005	12
H29	0.5677	0.1948	0.5412	0.16	0.005	12
H30	0.4579	0.2107	0.5128	0.16	0.005	12
H31	0.6215	0.1462	0.4752	0.16	0.005	12
H32	0.5107	0.1618	0.4477	0.16	0.005	12
H33	0.8576	0.4563	0.4628	0.16	0.005	12
H34	0.8204	0.3165	0.4851	0.16	0.005	12
H35	0.7975	0.5041	0.5268	0.16	0.005	12
H36	0.7653	0.3669	0.5505	0.16	0.005	12
H37	0.6577	0.2211	1.0205	0.48	0.005	12
H38	0.5921	0.1505	0.9686	0.48	0.005	12
H39	0.7482	0.2328	0.9736	0.48	0.005	12
H40	0.7528	0.2997	0.7839	0.5	0.005	12
H41	0.7341	0.2159	0.7341	0.5	0.005	12
H42	0.8425	0.3681	0.7355	0.5	0.005	12
N1	0.6675	0.34	0.0932	0.16	0.005	12
N2	0.6692	0.3297	0.1785	0.16	0.005	12
N3	0.6828	0.3175	0.4467	0.16	0.005	12
N4	0.6199	0.3689	0.5206	0.16	0.005	12
N5	0.6667	0.3333	0.9683	0.28	0.005	4
N6	0.6667	0.3333	0.7301	0.5	0.005	4

Table S3. Atomic coordinates and thermal parameters for calcined and dehydrated SAPO STA-20.

atom	*x*	*y*	*z*	occupancy	*U*iso	multiplicity
Al1	0.3319(4)	0.4190(4)	0.12439(20)	1	0.0058(5)	12
Al2	0.2361(4	1.0020(5)	0.19874(19)	1	0.0058(5)	12
Al3	0.2317(5)	0.9920(6)	0.05009(16)	1	0.0058(5)	12
O1	0.3207(7)	0.3343(7)	0.17161(28)	1	0.0095(11)	12
O2	0.3185(7)	0.3409(7)	0.17161(28)	1	0.0095(11)	12
O3	0.6770(6)	0.6414(5)	0.58240(20)	1	0.0095(11)	12
O4	0.6767(6)	0.6491(5)	0.66494(22)	1	0.0095(11)	12
O5	0.2745(10)	0.2646(10)	0.00421(12)	1	0.0095(11)	12
O6	0.1139(4)	0.2003(5)	0.0593(4)	1	0.0095(11)	12
O7	0.2213(4)	0.4542(6)	0.1231(4)	1	0.0095(11)	12
O8	0.1088(4)	0.2002(5)	0.1936(4)	1	0.0095(11)	12
O9	0.2504(7)	0.1260(6)	0.06391(32)	1	0.0095(11)	12
O10	0.2499(8)	0.1348(7)	0.1842(4)	1	0.0095(11)	12
O11	0.4663(3)	0.5452(4)	0.12401(24	1	0.0095(11)	12
O12	0.2781(10)	0.2685(11)	0.24729(13)	1	0.0095(11)	12
P1	0.2386(3)	0.2303(3)	0.05157(14)	0.95	0.0058(5)	12
P2	0.2373(3)	0.2359(3)	0.20008(14)	0.95	0.0058(5)	12
P3	0.6670(3)	0.5735(3)	0.62448(14	0.95	0.0058(5)	12
Si1	0.2386(3)	0.2303(3)	0.05157(14)	0.05	0.0058(5)	12
Si2	0.2373(3)	0.2359(3)	0.20008(14)	0.05	0.0058(5)	12
Si3	0.6670(3)	0.5735(3)	0.62448(14)	0.05	0.0058(5)	12

Table S4. Selected bond lengths and angles for as-prepared and dehydrated SAPO STA-20.

bond length / Å		bond angle / °	
Al1-O	1.729 (80)	O-Al1-O	108.4(4)
Al2-O	1.736(90)	O-Al2-O	108.7(5)
Al3-O	1.708(80)	O-Al3-O	111.8(5)
Al-O(Avg.)	1.724(80)	O-Al-O (Avg.)	109.6(5)
P1(Si1)-O	1.505(5)	O-P1(Si1)-O	110.3(4)
P2(Si2)-O	1.509(5)	O-P2(Si2)-O	110.2(4)
P3(Si3)-O	1.507(6)	O-P3(Si3)-O	111.1(4)
P(Si)-O(Avg.)	1.507(5)	O-P(Si)-O (Avg.)	110.5(4)
T-O(Avg.)	1.6155(40)	O-T-O (Avg.)	110.1(5)

Table S5. Selected bond lengths and angles for calcined and dehydrated SAPO STA-20.

bond length / Å		bond angle / °	
Al1-O	1.726(4)	O-Al1-O	109.5(3)
Al2-O	1.727(5)	O-Al2-O	109.5(3)
Al3-O	1.722(6)	O-Al3-O	109.5(4)
Al-O (Avg.)	1.725(5)	O-Al-O (Avg.)	109.5(3)
P1(Si1)-O	1.511(5)	O-P1(Si1)-O	109.5(4)
P2(Si2)-O	1.519(5)	O-P2(Si2)-O	109.4(4)
P3(Si3)-O	1.533(5)	O-P3(Si3)-O	109.9(4)
P(Si)-O (Avg.)	1.521(5)	O-P(Si)-O (Avg.)	109.6(4)
T-O (Avg.)	1.623(5)	O-T-O (Avg.)	109.5(4)