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Formation Domain of SDA-Free Y Faujasite Small Crystals

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Table S1: This table represents the calculated diagram (SiO_2-H_2O-Na_2O) coordinates for each sample, their corresponding starting molar gel composition and obtained phase nature. The Al_2O_3 molar composition of the gel was kept unchanged at 0.2. SiO_2/Na_2O molar ratio varies from 0.3 to 3.8, SiO_2/Al_2O_3 molar ratio varies from 1.5 to 47 and Na_2O/H_2O molar ratio varies from 0.005 to 0.1.

Sample name	Diagram coordinates			Molar gel composition			Gel SiO_2/Na_2O molar ratio	Gel SiO_2/Al_2O_3 molar ratio	Gel Na_2O/H_2O molar ratio	Obtained phase nature
	SiO_2	Na_2O	H_2O	SiO_2	Na_2O	H_2O				
9.4-4.95-225H_2O	0.0393	0.0207	0.9400	9.4	4.95	225	1.9	47	0.022	FAU Y+amorphous
9.4-4.95-210H_2O	0.0419	0.0221	0.9360	9.4	4.95	210	1.9	47	0.024	FAU Y+amorphous
9.4-4.95-195H_2O	0.0449	0.0236	0.9315	9.4	4.95	195	1.9	47	0.025	FAU Y+amorphous
9.4-4.95-180H_2O	0.0484	0.0255	0.9261	9.4	4.95	180	1.9	47	0.028	FAU Y
9.4-4.95-165H_2O	0.0524	0.0276	0.9200	9.4	4.95	165	19	47	0.03	FAU Y
9.4-4.95-150H_2O	0.0572	0.0301	0.9127	9.4	4.95	150	1.9	47	0.033	FAU Y

9.4-4.95-135H_2O	0.0629	0.0331	0.9040	9.4	4.95	135	1.9	47	0.037	FAU Y
9.4-4.95-120H_2O	0.0700	0.0368	0.8932	9.4	4.95	120	1.9	47	0.041	FAU Y
9.4-4.95-105H_2O	0.0788	0.0415	0.8797	9.4	4.95	105	1.9	47	0.047	FAU Y
9.4-4.95-90H_2O	0.0901	0.0474	0.8625	9.4	4.95	90	1.9	47	0.055	FAU Y
9.4-4.95-80H_2O	0.0996	0.0525	0.8479	9.4	4.95	80	1.9	47	0.062	No precipitate
9.4-4.95-75H_2O	0.1052	0.0554	0.8394	9.4	4.95	75	1.9	47	0.066	No precipitate
9.4-2.48-75H_2O	0.1082	0.0285	0.8633	9.4	2.48	75	3.8	47	0.033	amorphous
0.3-0.3-64H_2O	0.0062	0.0062	0.9876	0.3	0.3	64	1	1.5	0.005	amorphous
0.6-0.6-64H_2O	0.0087	0.0087	0.9826	0.6	0.6	64	1	3	0.009	LTA
1.0-1.0-63H_2O	0.0148	0.0148	0.9704	1.0	1.0	63	1	5	0.016	FAU Y+20%LTA
1.3-1.3-62H_2O	0.0200	0.0200	0.9600	1.3	1.3	62	1	6.5	0.021	FAU Y
1.6-1.6-62H_2O	0.0247	0.0247	0.9506	1.6	1.6	62	1	8	0.026	FAU Y
0.7-2.2-62H_2O	0.0108	0.0339	0.9553	0.7	2.2	62	0.3	3.5	0.035	FAU X*+50%LTA
0.8-1.6-62H_2O	0.0123	0.0247	0.9630	0.8	1.6	62	0.5	4	0.026	FAU Y+15%LTA
1.2-2.0-62H_2O	0.0185	0.0308	0.9507	1.2	2.0	62	0.6	6	0.032	Intergrowth FAU X/EMC-2
2.1-1.8-61H_2O	0.0324	0.0277	0.9399	2.1	1.8	61	1.2	10.5	0.030	FAU Y
1.0-2.6-61H_2O	0.0176	0.0401	0.9423	1.0	2.6	61	0.4	5	0.043	FAU X*+10%LTA+ 10%SOD

1.8-2.3-61H_2O	0.0277	0.0354	0.9369	1.8	2.3	61	0.8	9	0.038	Intergrowth FAU X/EMC-2
2.3-2.6-60H_2O	0.0354	0.0400	0.9246	2.3	2.6	60	0.9	11.5	0.043	FAU Y*+ƐGIS
2.5-1.9-60H_2O	0.0398	0.0318	0.9284	2.5	1.9	60	1.3	12.5	0.032	FAU Y
2.9-2.3-60H_2O	0.0446	0.0354	0.9200	2.9	2.3	60	1.3	14.5	0.038	FAU Y
3.6-1.0-60H_2O	0.0555	0.0154	0.9291	3.6	1.0	60	3.6	18	0.017	amorphous
1.7-2.9-60H_2O	0.0262	0.0447	0.9291	1.7	2.9	60	0.6	8.5	0.048	FAU X*+10%SOD
2.9-2.9-59H_2O	0.0447	0.0447	0.9106	2.9	2.9	59	1	14.5	0.049	FAU Y*+20%GIS
3.5-2.3-59H_2O	0.0539	0.0354	0.9107	3.5	2.3	59	1.5	17.5	0.039	FAU Y
3.6-2.9-58H_2O	0.0555	0.0447	0.8998	3.6	2.9	58	1.2	18	0.05	FAU Y*+10%GIS
4.0-3.2-58H_2O	0.0616	0.0493	0.8891	4.0	3.2	58	1.25	20	0.055	FAU Y*+15%GIS
4.2-2.8-58H_2O	0.0647	0.0431	0.8922	4.2	2.8	58	1.5	21	0.048	FAU Y
4.9-1.9-58H_2O	0.0762	0.0300	0.8938	4.9	1.9	58	2.6	24.5	0.033	amorphous
4.1-3.6-57H_2O	0.0632	0.0555	0.8813	4.1	3.6	57	1.1	20.5	0.063	FAU Y*+30%GIS+ 20%RHO
4.5-3.7-57H_2O	0.0693	0.0570	0.8737	4.5	3.7	57	1.2	22.5	0.065	FAU Y*+20%GIS+ 15%RHO
4.6-3.2-57H_2O	0.0709	0.0493	0.8798	4.6	3.2	57	1.4	23	0.056	FAU Y+10%GIS
5.2-3.2-56H_2O	0.0801	0.0493	0.8706	5.2	3.2	56	1.6	26	0.057	FAU Y+5%GIS
5.2-3.9-56H_2O	0.0800	0.0600	0.8600	5.2	3.9	56	1.3	26	0.070	FAU Y+40%GIS+ 25%RHO

6.2-2.3-56H_2O	0.1016	0.0354	0.8630	6.2	2.3	56	2.7	31	0.041	amorphous
5.8-3.6-55H_2O	0.0913	0.0592	0.8495	5.8	3.6	55	1.6	29	0.065	FAU Y+5%GIS+ƐRHO
9.4-4.95-50H_2O	0.1461	0.0769	0.7770	9.4	4.95	50	1.9	47	0.099	No precipitate

*with EMC-2 intergrowth

Percentages were determined by X-ray diffraction

Pink: zone 1 of the ternary phase diagram

Blue: zone 2 of the ternary phase diagram

Green: zone 3 of the ternary phase diagram

^{29}Al MAS NMR spectroscopy

^{27}Al (I = 5/2) magic angle spinning nuclear magnetic resonance (MAS-NMR) was carried out with a Bruker Avance II 400 spectrometer operating at B_0 = 9.4 T (Larmor frequency ν_0 = 104.2 MHz) equipped with a Bruker 4 mm double channel probe. Samples were spun at 12 kHz, and free induction decays (FID) were collected with a $\pi/12$ rf pulse (0.5 µs) and a recycle delay of 1 s. Measurements were carried out with $[Al(H_2O)_6]^{3+}$ as external standard reference.

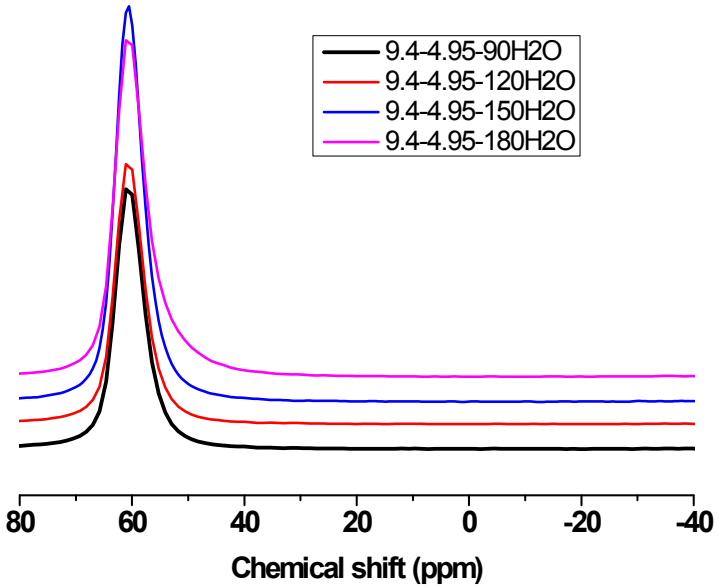

Figure S1. ^{27}Al MAS NMR spectra of the samples obtained from starting gels with the following molar compositions: 9.4 SiO_2: 0.2 Al_2O_3: 4.95 Na_2O: 90/120/150/180 H_2O.

^{29}Si MAS NMR spectroscopy

29Si MAS NMR spectroscopy which give reliable results concerning the Si/Al molar ratio of the completely crystallized materials, was also used to confirm the results obtained from XRD refinement and XRF. The framework Si/Al molar ratio was determined using the equation ($Si/Al = \sum_{n=0}^{4} I\,Si(nAl) / \sum_{n=0}^{4} n/4\ I$, where I Si(nAl) is the intensity of the NMR signal attributed to the Si(nAl) units.[1] The spectrum was recorded on a Bruker Advance II 300 MHz spectrometer.

The Si/Al molar ratios of deduced from 29Si MAS NMR spectra are in good agreement with Si/Al molar ratio determined from XRD and XRF data's (see 29Si MAS NMR spectrum and deconvolution below).

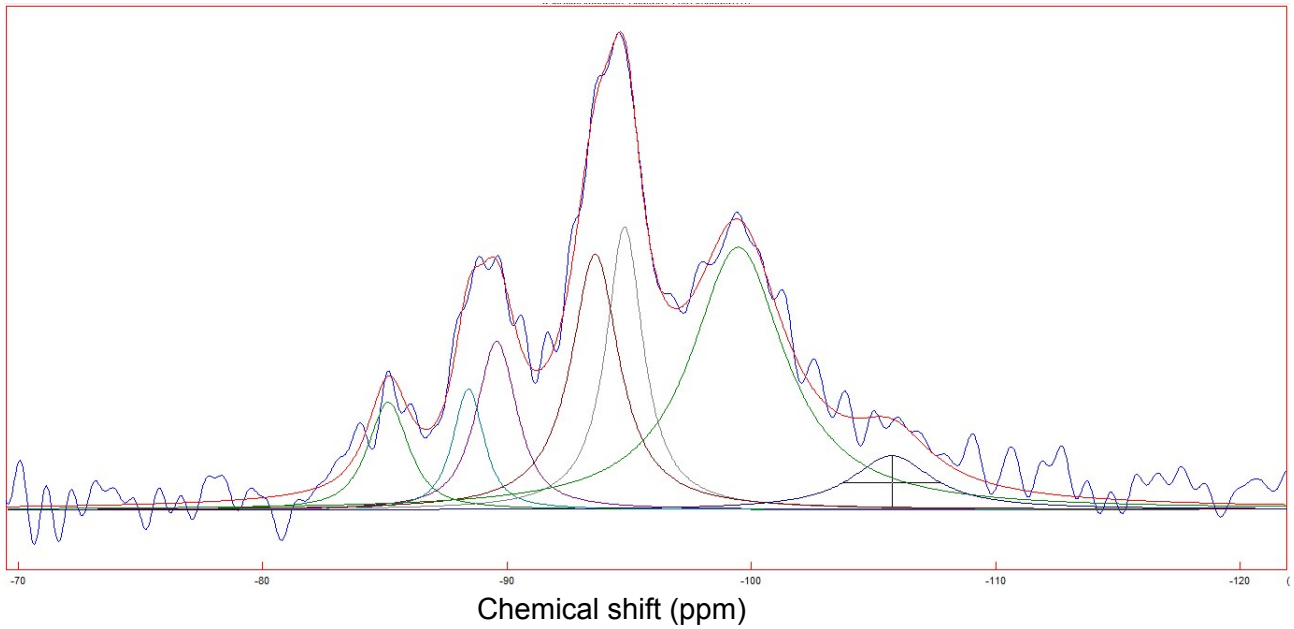

Figure S2. ^{29}Si MAS NMR spectrum with deconvolution of the sample obtained from starting gels with the following molar compositions: 9.4 SiO_2: 0.2 Al_2O_3: 4.95 Na_2O: 180 H_2O.

1- Engelhardt, G.; Lohse, U.; Lippmaa, E.; Tarmak, M.; Mägi, M. *Z. Anorg. Allg. Chem.* **1981**, *482*, 49–64.