Supporting information online

Table 5

Peak intensities of the specific simulations of the ^{29}Si MAS NMR spectra

Specimens	*9544*	*176*	*116*	*FB4*	*K-ASGS*	*1406*	*AGM*		*K-EU2*
							sim1	sim2	
T_1O (0Si, 4Al)	0.00	0.06	0.11	0.12	0.12	0.10	0.25	-	0.23
T_1O (1Si, 3Al)	0.00	0.44	0.92	0.99	1.36	1.04	1.98	-	1.95
T_1O (2Si, 2Al)	0.00	1.20	2.52	2.78	4.35	3.75	5.94	-	5.98
T_1O (3Si, 1Al)	0.00	1.39	2.75	3.33	3.40	5.63	7.92	20.00	7.97
T_1O (4Si, 0Al)	0.00	0.58	1.03	1.45	0.77	2.81	3.96	-	3.89
T_1m (0Si, 4Al)	0.00	0.00	0.01	0.03	0.01	0.11	0.21	-	0.27
T_1m (1Si, 3Al)	0.00	0.12	0.45	0.71	0.55	1.70	2.09	-	2.49
T_1m (2Si, 2Al)	0.00	3.13	5.46	6.32	6.44	8.32	7.51	-	8.26
T_1m (3Si, 1Al)	33.33	26.71	21.35	19.47	18.77	14.51	11.27	26.66	11.62
T_1m (4Si, 0Al)	0.00	2.38	4.40	4.81	5.91	5.38	5.63	-	5.72
T_2O (0Si, 4Al)	0.00	0.00	0.01	0.01	0.01	0.04	0.21	-	0.14
T_2O (1Si, 3Al)	0.00	0.12	0.37	0.46	0.55	0.83	2.09	-	1.66
T_2O (2Si, 2Al)	0.00	3.13	5.11	5.36	6.43	5.95	7.31	-	6.63
T_2O (3Si, 1Al)	33.33	26.71	21.62	20.13	18.77	15.32	11.27	26.66	11.00
T_2O (4Si, 0Al)	0.00	2.38	4.22	4.35	5.91	4.47	5.64	-	5.48
T_2m (0Si, 4Al)	0.00	0.03	0.09	0.14	0.08	0.33	0.42	-	0.39
T_2m (1Si, 3Al)	0.00	1.70	2.67	3.23	2.42	4.12	3.34	-	3.34
T_2m (2Si, 2Al)	33.33	26.30	20.81	18.49	18.63	13.09	9.18	26.66	9.23
T_2m (3Si, 1Al)	0.00	3.52	5.71	7.10	5.18	10.17	10.02	-	10.01
T_2m (4Si, 0Al)	0.00	0.12	0.40	0.71	0.37	2.31	3.76	-	3.73

Peak intensities in % are calculated assuming a constant Si/Al ratio of 3.0 and Loewenstein's Al-O-Al avoidance rule, after Xiao et al. (1995). The chemical shifts produced by replacement of Si by Al, to calculate different possible Si Q^4 (nAl) n = 0, 1, 2, 3, 4, was assumed ± 4.85 ppm in all cases. The δ_x values are in ppm.

Table 6. Simulation of the ^{29}Si NMR spectra of the order-disorder models

Alternative models	*Two-step Orthoclase* Fig. 2c	*One-step Orthoclase* Fig.2d	*Triclinic High sanidine* Fig. 4c	*Monoclinic High sanidine* Fig. 4d
Linewidth	1.10	1.10	1.35	1.35
t_1O	0.40	0.70	0.25	
t_1m	0.40	0.10	0.25	
t_2O	0.10	0.10	0.25	
t_2m	0.10	0.10	0.25	0.25
δT_1O (3Si,1Al)	-100.8	-101.7	-101.7	-100.6
δT_1m (3Si,1Al)	-100.8	-100.8	-100.6	-100.6
δT_2O (3Si,1Al)	-96.5	-97.8	-97.8	-97.8
δT_2m (2Si,2Al)	-91.7	-94.7	-94.7	-93.0
T_1O (0Si, 4Al)	0.06	0.12	0.31	
T_1O (1Si, 3Al)	0.97	0.99	2,47	
T_1O (2Si, 2Al)	5.15	2.96	7.41	
T_1O (3Si, 1Al)	10.14	3.95	9.88	
T_1O (4Si, 0Al)	3.90	1.98	4.94	
T_1m (0Si, 4Al)	0.06	0.03	0.31	
T_1m (1Si, 3Al)	0.97	0.78	2.47	
T_1m (2Si, 2Al)	5.15	6.37	7.41	
T_1m (3Si, 1Al)	10.14	18.15	9.88	
T_1m (4Si, 0Al)	3.90	4.68	4.94	
T_2O (0Si, 4Al)	0.30	0.03	0.31	
T_2O (1Si, 3Al)	3.48	0.78	2.47	
T_2O (2Si, 2Al)	9.15	6.31	7.41	
T_2O (3Si, 1Al)	11.67	18.15	9.88	
T_2O (4Si, 0Al)	4.62	4.68	4.94	
T_2m (0Si, 4Al)	0.30	0.22	0.31	
T_2m (1Si, 3Al)	3.48	3.71	2.47	
T_2m (2Si, 2Al)	10.26	16.42	7.41	
T_2m (3Si, 1Al)	11.67	8.49	9.88	
T_2m (4Si, 0Al)	4.62	1.17	4.94	

The letter "t" lowercase is used for the Al content in the tetrahedral sites, which are named with "T" uppercase. Peak intensities in % are calculated assuming a constant Si/Al ratio of 3.0 and Loewenstein's Al-O-Al avoidance rule, after Xiao et al. (1995). The chemical shifts produced by replacement of Si by Al, to calculate different possible Si Q^4 (nAl) n = 0, 1, 2, 3, 4, was of ± 4.85 ppm in all cases. The δ_x values are in ppm.