

Supporting Information

Table SI1. NMR-parameters obtained by simulation of the ^{27}Al MAS NMR spectra (samples **I** and **III**) at different magnetic fields using a decomposition into lines with mixed Gaussian/Lorentzian character (approximation to derive data for SORGE-method). The denotation of the species follows Table 2.

I Al: F 1:1 species #	21.1 T				17.6 T				14.1 T			
	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl
1	43.9	4.8	46.2	0.2	38.3	3.8	33.9	0	34.7	3.2	22.6	0
2	30.8	2.1	7.9	1	29.2	2.0	8.7	1	25.3	1.7	8.8	1
3	26.7	0.8	1.2	1	24.9	1.0	1.8	1	19.3	1.4	4.2	1
4	22.5	3.2	13.5	1	19.4	2.6	18.8	0.6	14.2	2.6	17.6	0.9
6	2.1	0.3	1.7	1	1.7	0.2	2.2	1	1.6	0.2	3.9	1
7	-1.3	2.3	22.4	1	-2.6	2.1	21.3	1	-4.9	2.4	25.6	1
8	-9.9	2.0	7.2	1	-11.1	2.0	13.3	0.4	-13.0	4.0	17.4	0

III Al: F 1:2 species #	21.1 T				17.6 T				14.1 T			
	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl	$\delta_{^{27}\text{Al}}$ / ppm	FWHM / kHz	intensity / %	gl
1	52.8	1.6	0.8	1	50.3	2.1	1.0	1	45.8*	2.7	1.2	1
3	37.7	7.5	20.5	1	36.5	5.5	7.6	1	34.3*	4.5	7.8	1
4	28.8	2.2	7.7	1	28.4	2.8	10.4	1	24.2	2.2	14.7	1
5	19.9	1.7	3.3	1	18.2	3.0	6.8	1	13.6	3.0	6.2	1
6	1.9	1.4	2.1	1	3.3	1.1	2.5	1	2.7	0.5	0.3	1
8	-9.2	2.2	65.7	0.3	-10.3	2.5	71.9	0.3	-9.6**	2.4	68.9	
ss +1	77.0	2.2		1	132.7	3.1		1	151.4	3.0		1
ss 0	-8.3	2.2		1	-8.1	3.1		1	-11.6	3.0		1
ss -1	-93.6	2.2		1	-148.9	3.1		1	-174.6	3.0		1

* For a full reproduction of the spectrum the assumption of a further species at $\delta_{^{27}\text{Al}} = 37.2$ ppm (species #2) with an intensity of 1% was necessary.

** The simulation of this species required a change of the model: the line was simulated for the approximation using a Czjzek distribution with following parameters:
 $\delta_{\text{iso}} = -9.6$; $v_Q = 673$ kHz; ($\eta = 0.61$).

| FWHM: full width at half maximum; gl: Gaussian/Lorentzian ratio, gl • Gaussian/[(1 - gl) • Lorentzian]; ss: spinning side band. PAGE SI 1