Supporting Information

Tailoring penta-coordinated Aluminium species on silica-alumina via flame spray pyrolysis for enhanced arenes benzylation

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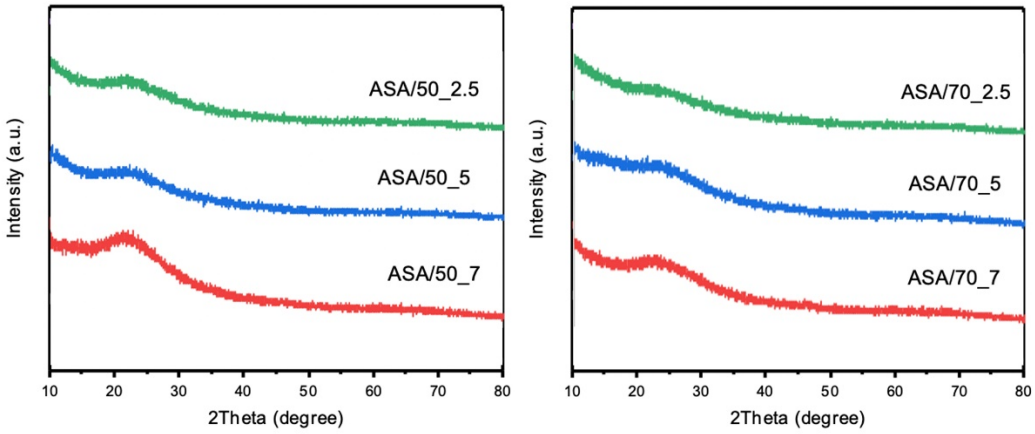

Figure S1 (A) wide-angle XRD patterns of ASA catalysts.

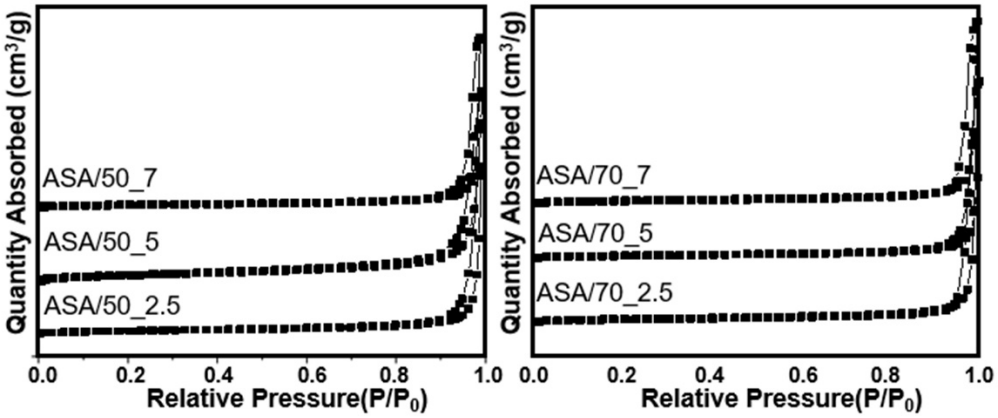

Figure S2 (A) N_2 adsorption-desorption isotherms of ASA catalysts.

Table S1. Summary of best-fit NMR parameters used to simulate the spectra of Fig.2 A-F.

	$Al^{IV}a$			$Al^{IV}b$			$Al^{V}a$			$Al^{V}b$			Al^{VI}		
	δ_{iso} (ppm)	C_{QCC} (MHz)	η_Q	δ_{iso} (ppm)	C_{QCC} (MHz)	η_Q	δ_{iso} (ppm)	C_{QCC} (MHz)	η_Q	δ_{iso} (ppm)	C_{QCC} (MHz)	η_Q	δ_{iso} (ppm)	C_{QCC} (MHz)	η_Q
ASA/50_2.5	56	3.2	0.5	41	4.7	0.5	33	2.8	0.5	18	5.0	0.5	7	3.2	0.5
ASA/50 _5	56	3.1	0.5	44	4.8	0.5	31	2.8	0.5	18	5.0	0.5	9	3.5	0.5
ASA/50 _7	54	3.4	0.5	44	4.9	0.5	30	2.9	0.5	18	5.1	0.5	9	3.5	0.5
ASA/70 _2.5	60	3.2	0.5	45	4.8	0.5	33	2.8	0.5	18	5.0	0.5	4	3.0	0.5
ASA/70 _5	60	3.4	0.5	45	4.8	0.5	33	2.8	0.5	18	5.0	0.5	4	3.0	0.5
ASA/70 _7	60	3.3	0.5	45	4.8	0.5	32	2.9	0.5	18	5.1	0.5	3	3.0	0.5

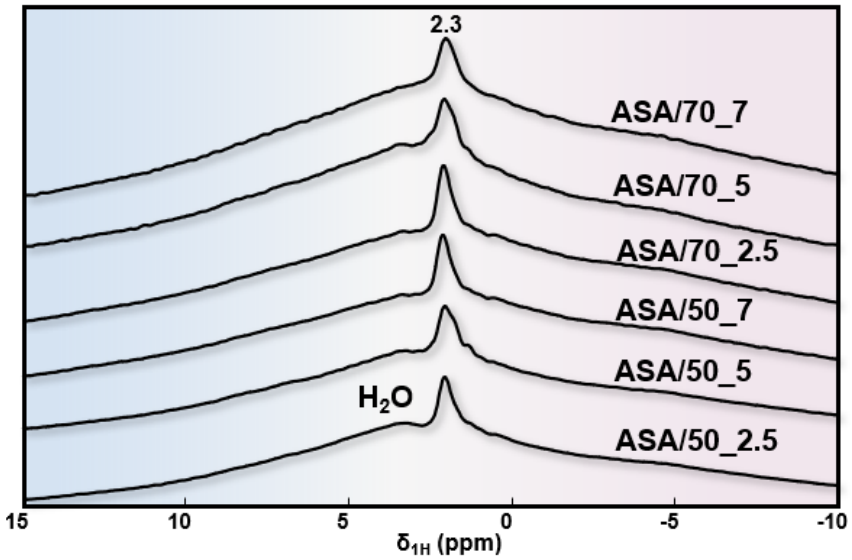

Figure S3. ^{1}H single-pulse MAS NMR spectra on dehydrated ASAs. All samples dehydrated at 573 K under a vacuum for 12 h.

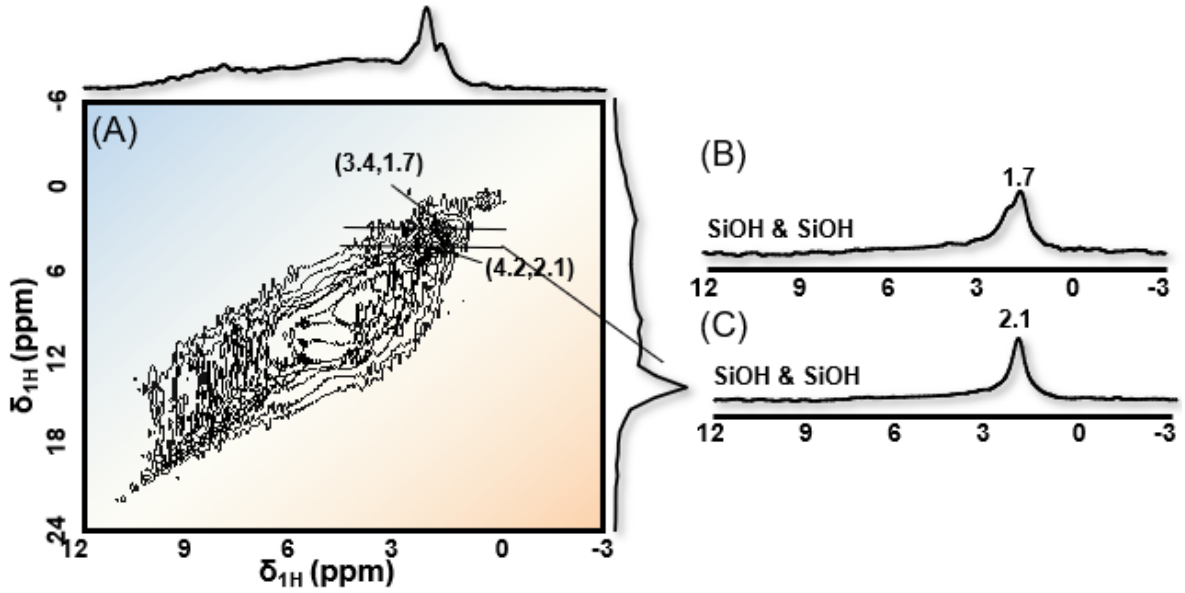

Figure S4. (A) 2D ^{1}H DQ-SQ NMR spectrum of representative ASA/70_ 7 catalyst. (B–C) Rows extracted from the 2D spectrum corresponding to the various auto-correlations and cross peaks. All rows are plotted with the same intensity scale.

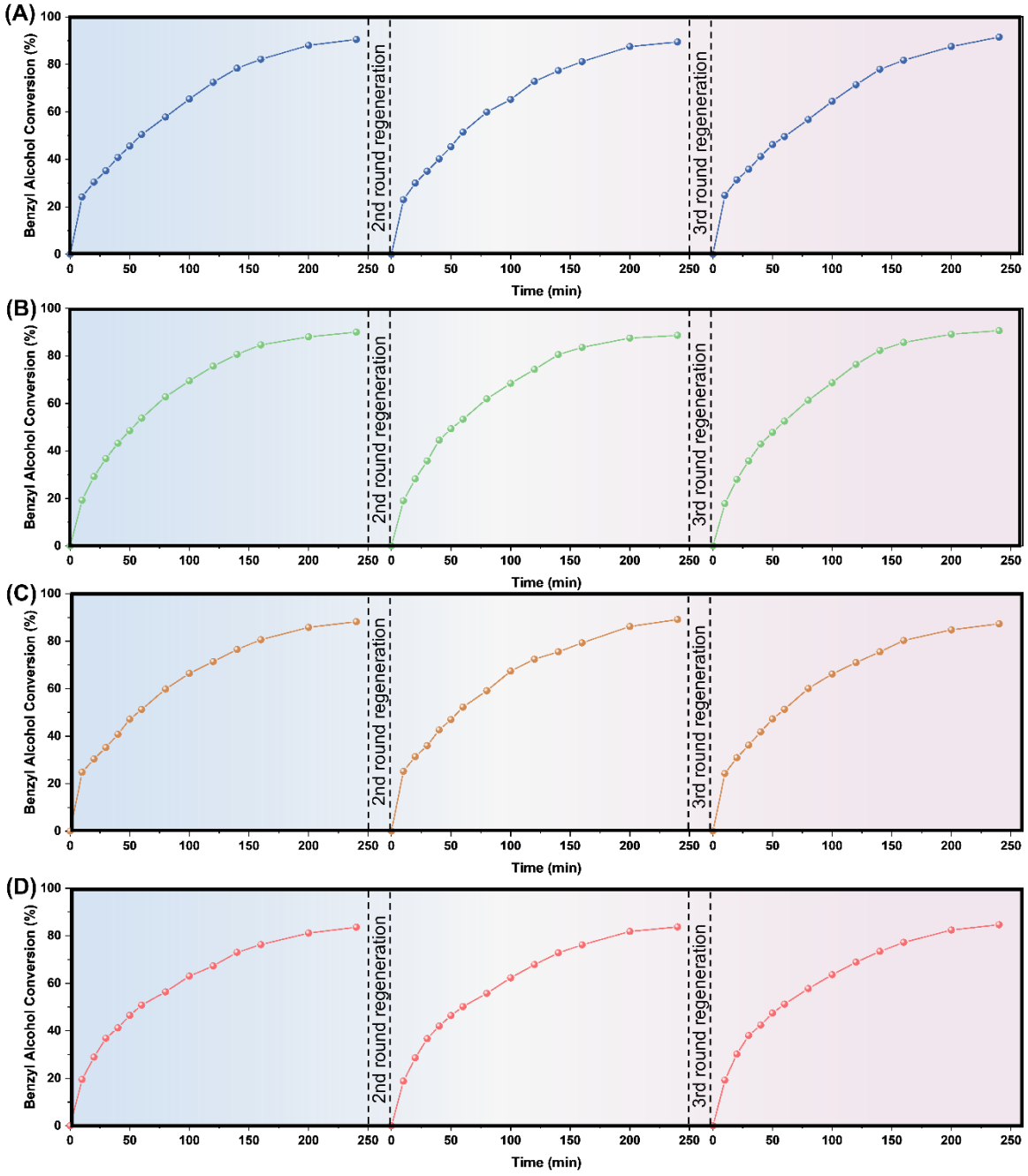

Figure S5. Catalysts regeneration test for benzyl alcohol conversion in the benzylation of different arenes over ASA/70_7: (A) benzene, (B) toluene, (C) p-xylene, and (D) mesitylene.