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Mesoporous isocyanurate-containing organosilica-alumina composites and their thermal treatment in nitrogen for carbon dioxide sorption at elevated temperature

Chamila Gunathilake, Mahinda Gangoda and Mietek Jaroniec*

Department of Chemistry and Biochemistry, Kent State University, Kent, Ohio 44242, USA

Table S1. Amounts of the aluminum (Al-N, Al-I) and silica (ICS and AP) precursors used in synthesis.

Sample	ICS (mmol)	Al-N (mmol)	Al-I (mmol)	AP (mmol)
Pure Al	-	0.0110	-	-
Al-N-ICS10	0.0011	0.0099	-	-
Al-N-ICS10*	0.0011	0.0099	-	-
Al-N-ICS20	0.0022	0.0088	-	-
Al-N-ICS20*	0.0022	0.0088	-	-
Al-N-ICS30	0.0033	0.0077	-	-
Al-N-ICS30*	0.0033	0.0077	-	-
Al-N-ICS50	0.0055	0.0055	-	-
Al-N-ICS50*	0.0055	0.0055	-	-
Al-N-ICS80	0.0088	0.0022	-	-
Al-N-ICS80*	0.0088	0.0022	-	-
Al-0.1(N/I)-ICS10	0.0011	0.0009	0.0090	-
Al-0.1(N/I)-ICS10*	0.0011	0.0009	0.0090	-
Al-1(N/I)-ICS10	0.0011	0.00495	0.00495	-
Al-1(N/I)-ICS10*	0.0011	0.00495	0.00495	-
Al-10(N/I)-ICS10	0.0011	0.0090	0.0009	-
Al-10(N/I)-ICS10*	0.0011	0.0090	0.0009	-
Al-0.1(N/I)-ICS20	0.0022	0.0008	0.0080	-
Al-0.1(N/I)-ICS20*	0.0022	0.0008	0.0080	-
Al-1(N/I)-ICS20	0.0022	0.0044	0.0044	-
Al-1(N/I)-ICS20*	0.0022	0.0044	0.0044	-
Al-10(N/I)-ICS20	0.0022	0.0080	0.0008	-
Al-10(N/I)-ICS20*	0.0022	0.0080	0.0008	-
Al-N-ICS5-AP5	0.00055	0.0099	-	0.00055
Al-N-ICS5-AP5*	0.00055	0.0099	-	0.00055
Al-N-ICS10-AP10	0.0011	0.0088	-	0.0011
Al-N-ICS10-AP10*	0.0011	0.0088	-	0.0011

Table S2. N_2 adsorption analysis for alumina-silica composites thermally treated at 700 ^{0}C.

Sample	S_{BET} (m^2/g)	V_{sp} (cm^3/g)	w_{KJS} nm	V_{mi} (cm^3/g)
Al-N-ICS10*h	336	0.87	10.0	0.02
Al-N-ICS30*h	294	0.45	5.5	0.02
Al-N-ICS80*h	295	0.25	2.7	0.02

S_{BET} - specific surface area calculated from adsorption data in relative pressure range of 0.05-0.20; V_{sp} - single point pore volume calculated at a relative pressure of ~0.98; w_{KJS} - pore width calculated at the maximum of PSD using improved KJS method; V_{mi} – micropore volume estimated by α_s-plot method.

Table S3. Room temperature (25 ^{o}C) CO_2 adsorption obtained at 1 bar pressure for alumina-organosilica composites thermally treated at 300 ^{o}C.

Sample	n_{CO2} (mmol/g)
Al-N-ICS10*	0.96
Al-N-ICS30*	0.98
Al-N-ICS80*	0.95

n_{CO2} - number of moles of CO_2 adsorbed per gram of the sample.

Table S4. CO_2 desorption, TGA and elemental analysis data for the alumina-silica composites studied.

Sample	n_{CO2} (mmol/g)	(10^3 n_{CO2}/S_{BET}) (mmol/m^2)	Nitrogen content (mmol/g)	Carbon (%)	Al:Si ratio
Pure alumina*h	0.55	-	-	-	-
Al-N-ICS10*h	0.58	1.39	0.88	5.79	9:1
Al-N-ICS20*h	0.95	2.57	1.09	7.82	9:1
Al-N-ICS30*h	1.12	3.06	2.21	12.71	8:2
Al-N-ICS50*h	1.63	4.91	3.89	19.27	8:2
Al-N-ICS80*h	2.22	6.87	4.73	26.56	7:3
Al-10(N/I)-ICS10*h	0.81	2.62	1.85	10.28	7:3
Al-10(N/I)-ICS20*h	0.78	3.01	2.49	12.89	5:5
Al-N-ICS5-AP5*h	1.19	4.28	2.30	11.74	5:5
Al-N-ICS10-AP10*h	0.76	5.76	1.16	13.17	2:8

n_{CO2} - number of moles of CO_2 adsorbed per gram of the sample; nitrogen content was calculated using N% obtained by elemental analysis for the samples heated in flowing nitrogen up to 700 ^{o}C; carbon percentage was obtained by elemental analysis for the samples heated in flowing nitrogen up to 700 ^{o}C.

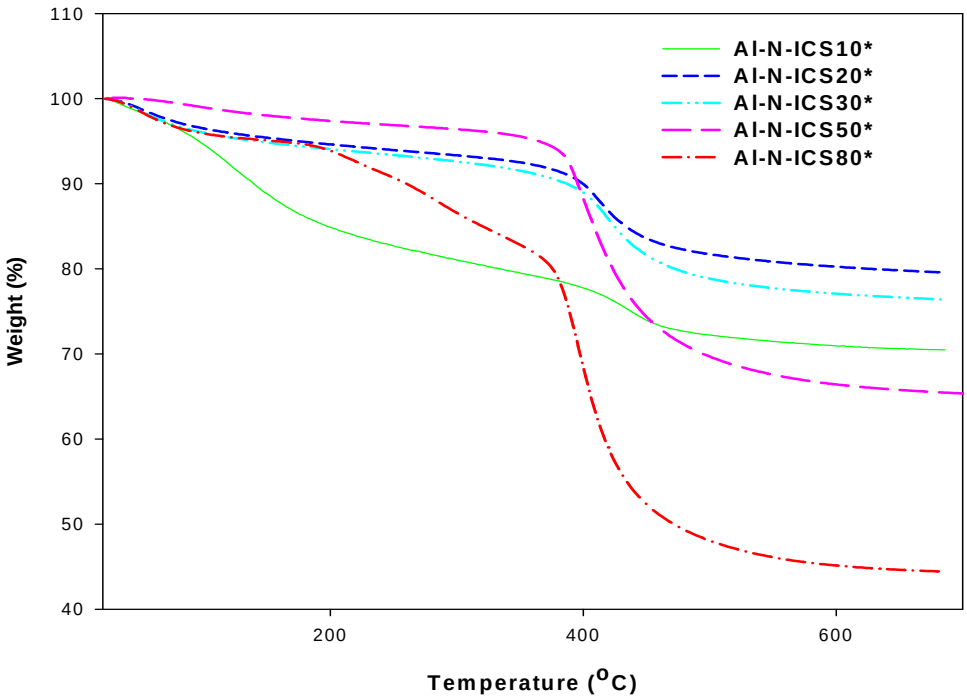


Figure S1. TG curves for alumina-silica composites with isocyanurate bridging groups for extracted-thermally treated (*) samples in flowing nitrogen at 300 °C.

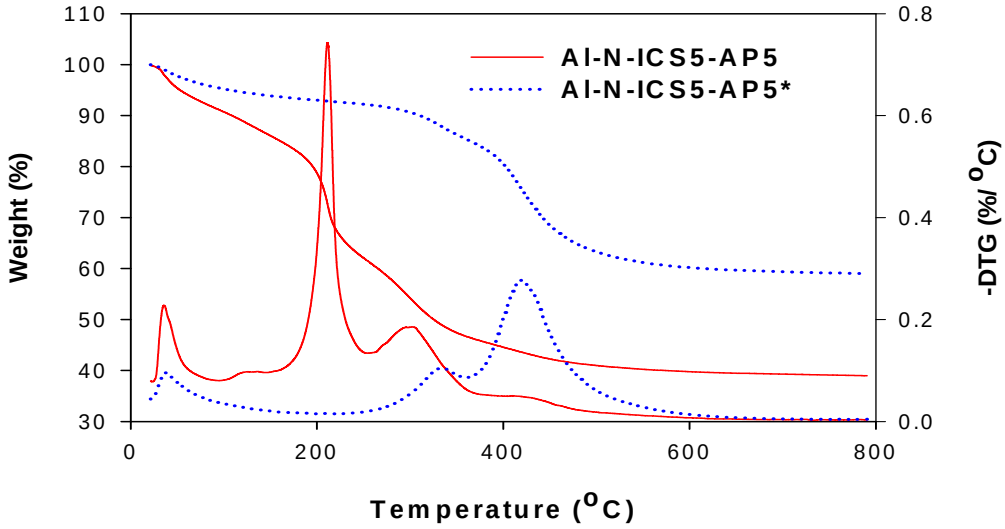


Figure S2. Extracted and extracted-thermally treated in N_2 at 300 °C (*) samples synthesized by using aluminum nonahydrate (Al-N), isocyanurate (ICS) and aminopropyl (AP) organosilanes.

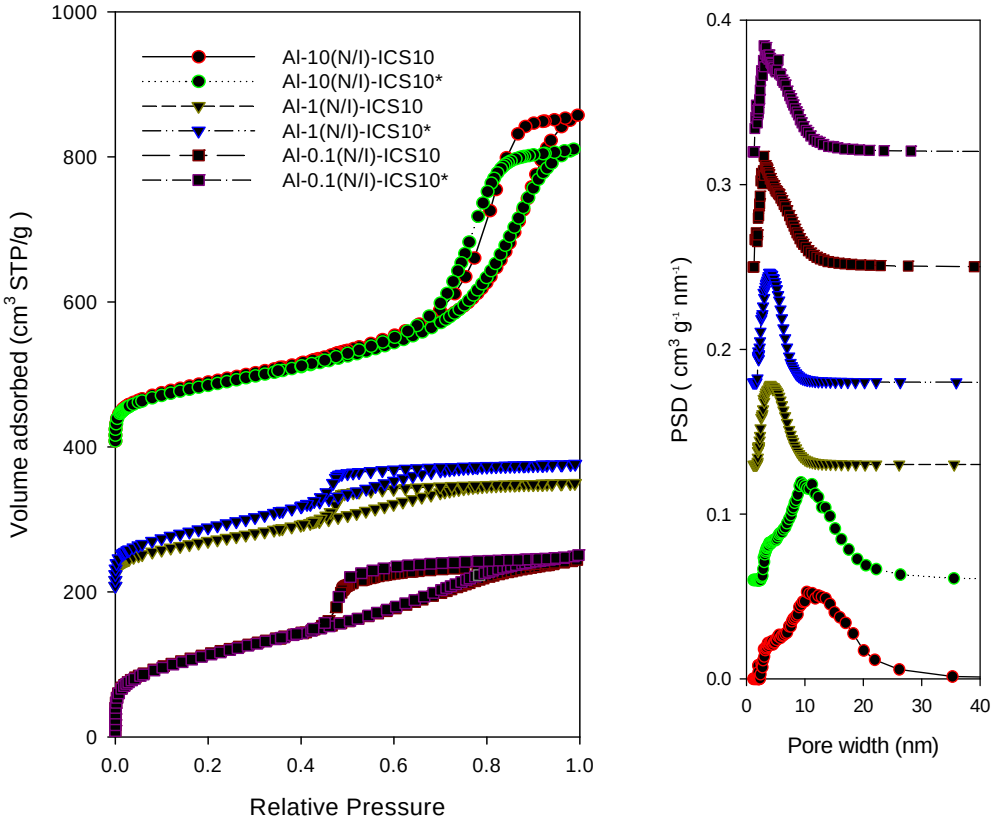


Figure S3. Nitrogen adsorption isotherms (left panel) and the PSD curves (right panel) for extracted and extracted-thermally treated in N_2 at 300 ^oC (*) samples obtained using Al-N, Al-I and ICS precursors; all isotherm and PSD curves are shifted by 200 cm^3STP/g and 0.06 cm^3/g, respectively.

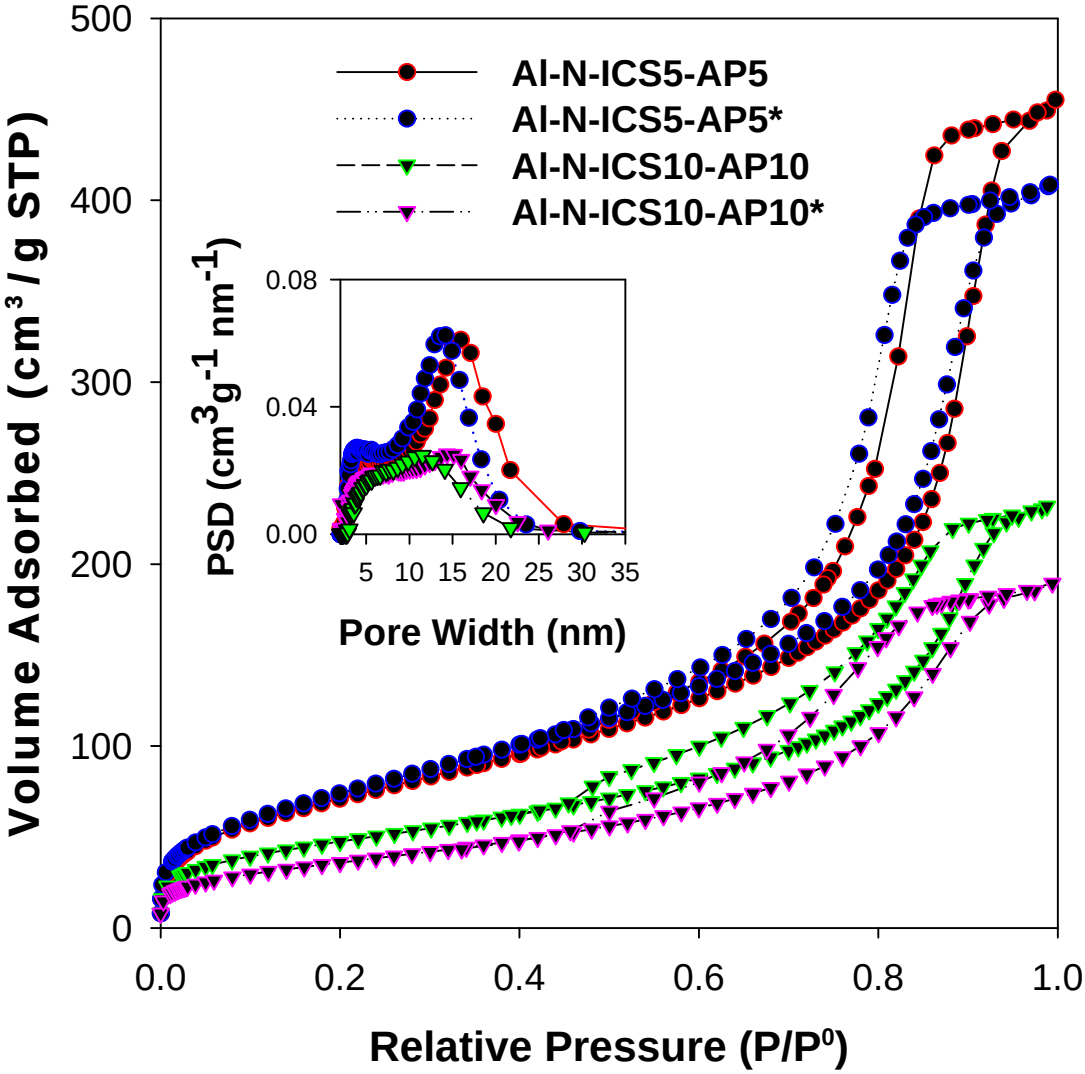
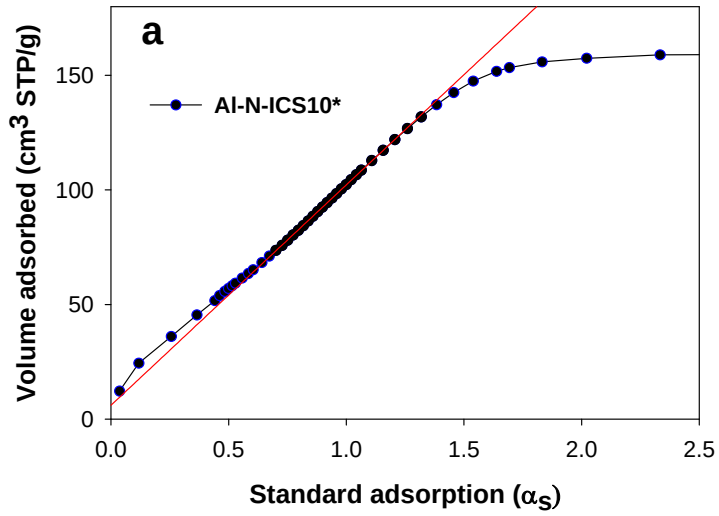
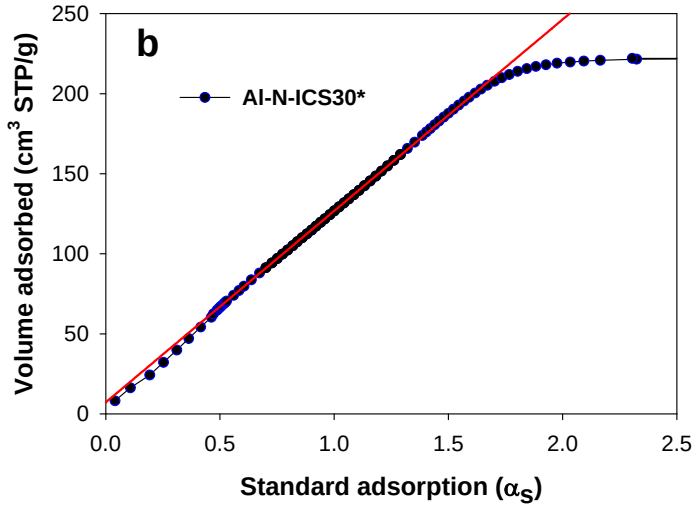


Figure S4. N_2 adsorption isotherms and the PSD curves (inset) for extracted and extracted-thermally treated in N_2 at 300 ^oC (*) samples prepared by using Al-N, ICS and AP precursors.


a
Al-N-ICS10*
Volume adsorbed (cm3 STP/g)
Standard adsorption (αS)
0
50
100
150
0.0
0.5
1.0
1.5
2.0
2.5


b
Al-N-ICS30*
Volume adsorbed (cm3 STP/g)
Standard adsorption (αS)
0
50
100
150
200
250
0.0
0.5
1.0
1.5
2.0
2.5

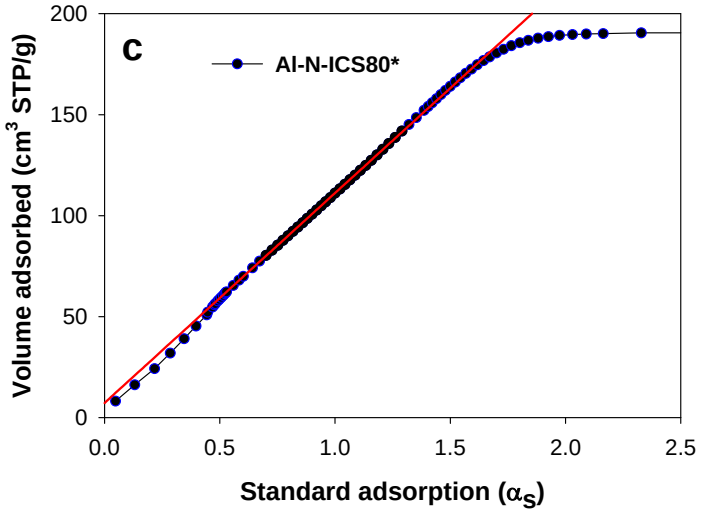

c
Al-N-ICS80*
Volume adsorbed (cm3 STP/g)
Standard adsorption (αS)
0
50
100
150
200
0.0
0.5
1.0
1.5
2.0
2.5

Figure S5. α_s-plots for a) Al-N-ICS10*, b) Al-N-ICS30*, and c) Al-N-ICS80*.

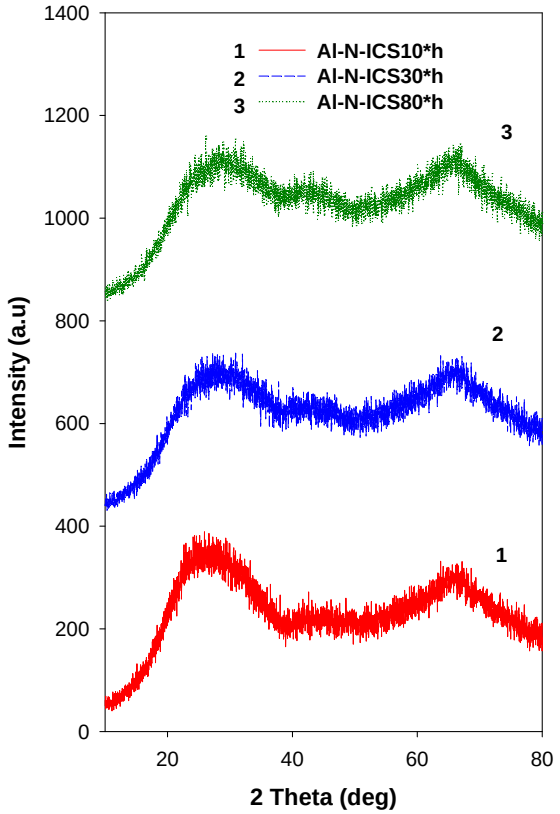


Figure S6.. Wide angle XRD profiles for the alumina-silica composites thermally treated up to 700 ^{o}C.

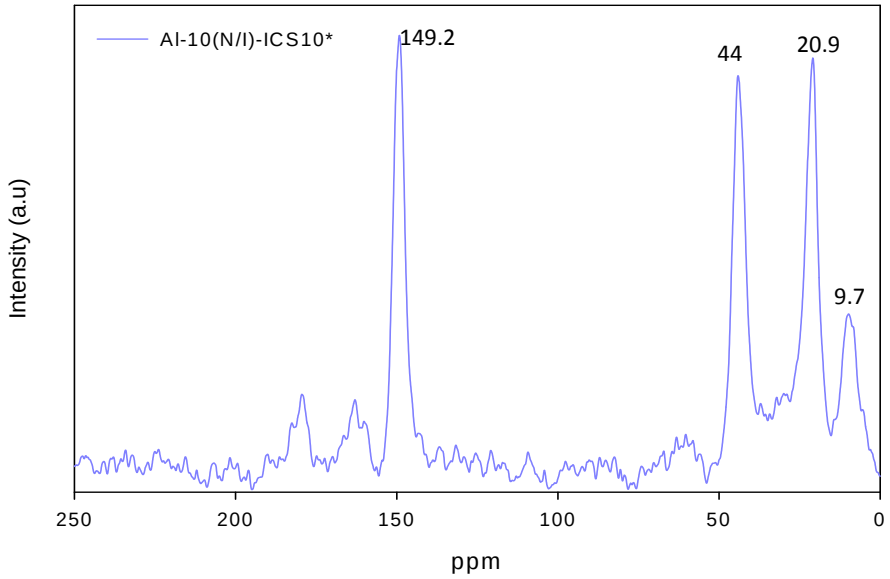


Figure S7. ^{1}H- ^{13}C CP/MAS NMR spectrum of the Al-10(N/I)-ICS-10* sample.

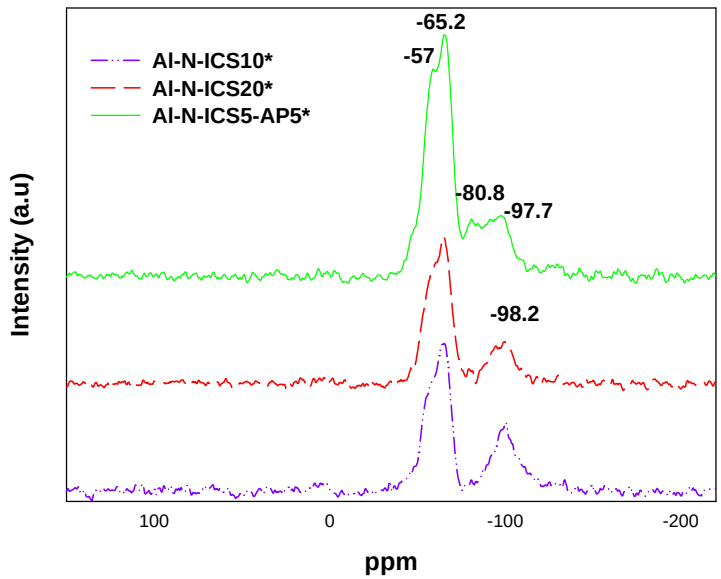


Figure S8. ^{1}H-^{29}Si-MAS NMR spectra of Al-N-ICS10*, Al-N-ICS20*and Al-N-ICS5-AP5*.

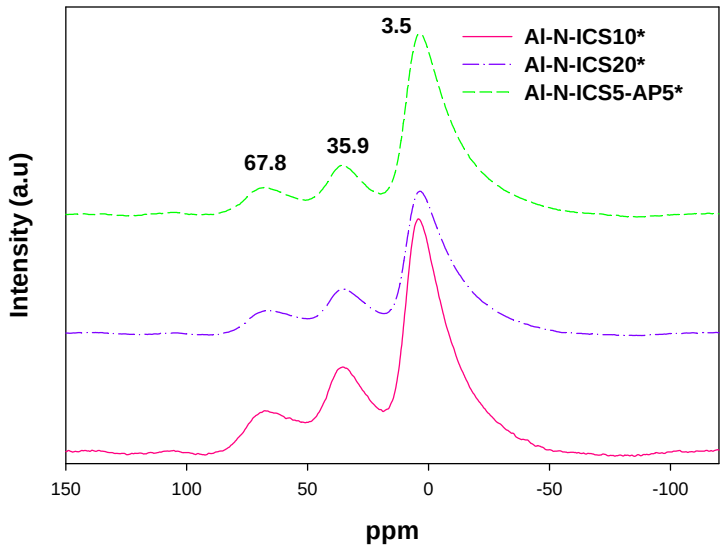


Figure S9. ^{27}Al-MAS NMR spectra of Al-N-ICS10*, Al-N-ICS20*and Al-N-ICS5-AP5*.

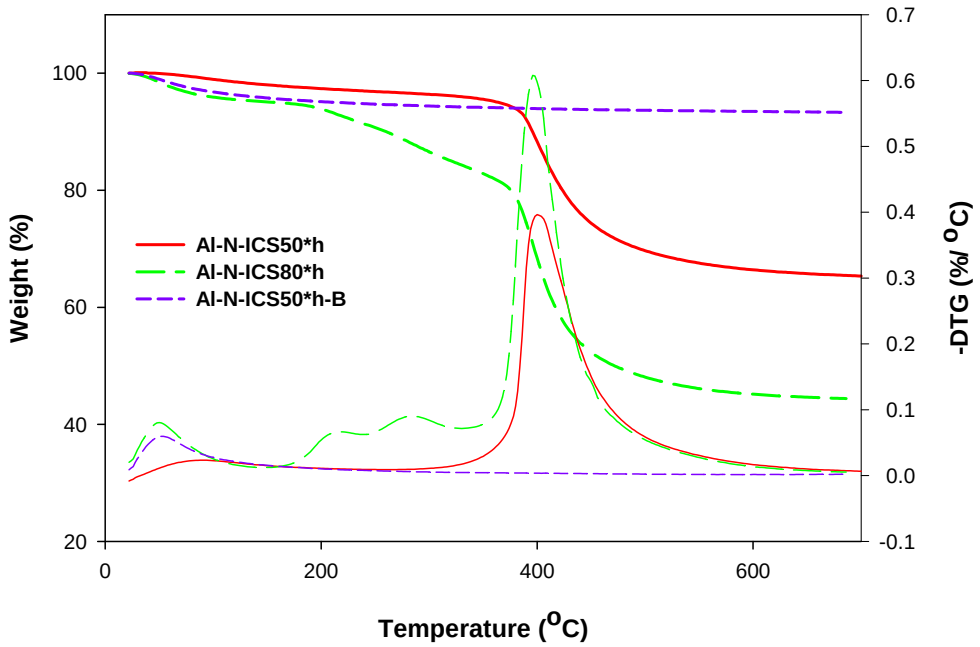


Figure S10. CO_2 desorption profiles for the Al-N-ICS80*h and Al-N-ICS50*h samples exposed to CO_2 at 120 °C and for Al-N-ICS50*h-B without passing CO_2.