

Supporting Information for

Acidic Properties of Cage-Based, Small-Pore Zeolites
with Different Framework Topologies and Their Sili-
coaluminophosphate Analogues

Naonobu Katada,^{,†} Kazuma Nouno,[†] Jun Kyu Lee,[‡] Jiho Shin,[‡] Suk Bong Hong,[‡] Miki Niwa[§]*

[†] Department of Chemistry and Biotechnology, Graduate School of Engineering, Tottori University, 4-101 Koyama-cho Minami, Tottori 680-8552, Japan

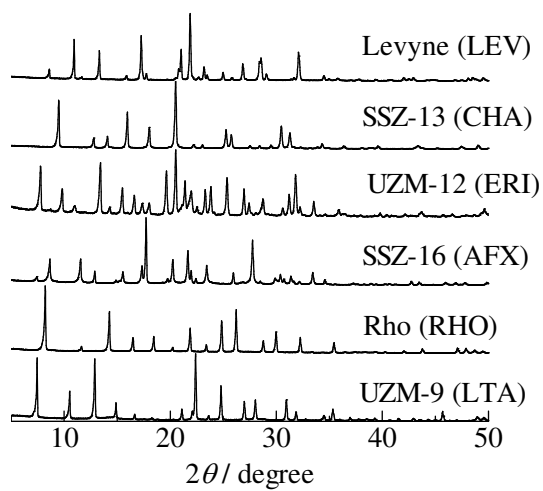
[‡] Department of Chemical Engineering and School of Environmental Science and Engineering, POSTECH, Pohang 790-784, Korea

[§] Nagoya Industrial Science Research Institute, 2F Noah Yotsuya Bldg., 1-13 Yotsuya-dori, Chikusa-ku, Nagoya 464-0819, Japan

Table S1 Geometric parameters after optimization

Model			T _n - O _a	T _s -O _a	T _s -T _n	T _n - O _{b1}	T _n - O _{b2}	T _n - O _{b3}	O _{b1} - T _{c1}	O _{b2} - T _{c2}	O _{b3} - T _{c3}	T _s O _a T _n	T _n O _{b1} T _{c1}	T _n O _{b2} T _{c2}	T _n O _{b3} T _{c3}
			/ Å									/ degree			
CHA	SiO ₂	Si1O1Si1	1.64	1.64	3.154	1.628	1.639	1.627	1.628	1.639	1.627	148.1	149.9	145.1	146.9
	AS	Al1O1HSi1	1.723	1.941	3.358	1.613	1.613	1.607	1.646	1.659	1.641	132.7	161.6	150.7	145.9
	AlPO ₄	Al1O1P1	1.751	1.544	3.282	1.755	1.755	1.767	1.547	1.546	1.558	169.9	132.0	137.9	140.0
	SAPO	Al1O1HSi1	1.857	1.813	3.314	1.734	1.753	1.748	1.557	1.563	1.555	129.1	149.2	136.8	161.8
	SiO ₂	Si1O3Si1	1.628	1.628	3.145	1.627	1.639	1.64	1.627	1.639	1.64	149.9	145.1	148.1	146.9
	AS	Al1O3HSi1	1.711	1.895	3.329	1.61	1.621	1.612	1.659	1.656	1.647	134.71	155.7	141.2	144.1
	AlPO ₄	Al1O3P1	1.755	1.546	3.102	1.755	1.751	1.767	1.547	1.544	1.558	140.0	132.0	169.9	137.9
	SAPO	Al1O3HSi1	1.834	1.769	3.254	1.749	1.741	1.738	1.56	1.554	1.564	129.1	126.7	167.1	140.3
RHO	SiO ₂	Si1O2Si1	1.645	1.645	3.126	1.645	1.637	1.637	1.645	1.637	1.637	143.7	143.7	149.4	149.4
	AS	Al1O2HSi1	1.731	1.956	3.404	1.626	1.62	1.616	1.653	1.666	1.658	134.8	154.1	149.3	147.2
	AlPO ₄	Al1O2P1	1.745	1.544	3.185	1.745	1.748	1.748	1.544	1.545	1.545	151.0	151.0	135.3	135.3
	SAPO	Al1O2HSi1	1.854	1.804	3.295	1.76	1.755	1.751	1.56	1.571	1.563	128.5	142.7	144.2	146.5
ERI	SiO ₂	Si1O1Si1	1.63	1.63	3.048	1.621	1.643	1.622	1.63	1.643	1.622	138.5	143.0	137.6	156.1
	AS	Al1O1HSi1	1.715	1.925	3.261	1.626	1.636	1.601	1.653	1.662	1.648	127.2	136.1	167.6	131.3
	AlPO ₄	Al1O1Si1	1.759	1.551	2.983	1.739	1.772	1.741	1.543	1.5561	1.54	128.6	148.1	130.0	138.8
	SAPO	Al1O1HSi1	1.843	1.799	3.197	1.759	1.785	1.734	1.56	1.575	1.551	122.8	135.0	125.8	169.3

(A)



(B)

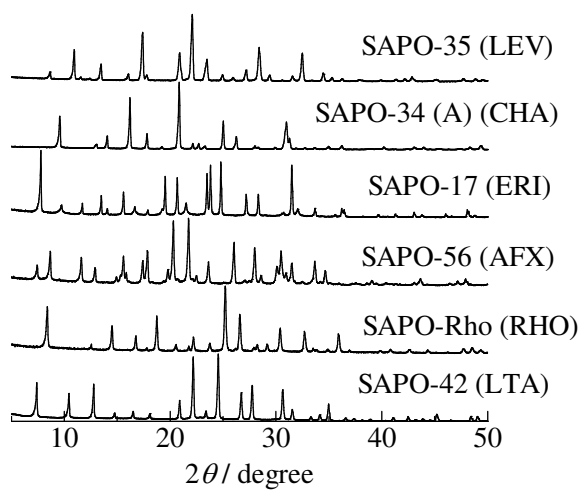


Figure S1 Powder XRD patterns of synthesized AS (A) and SAPO (B) materials.

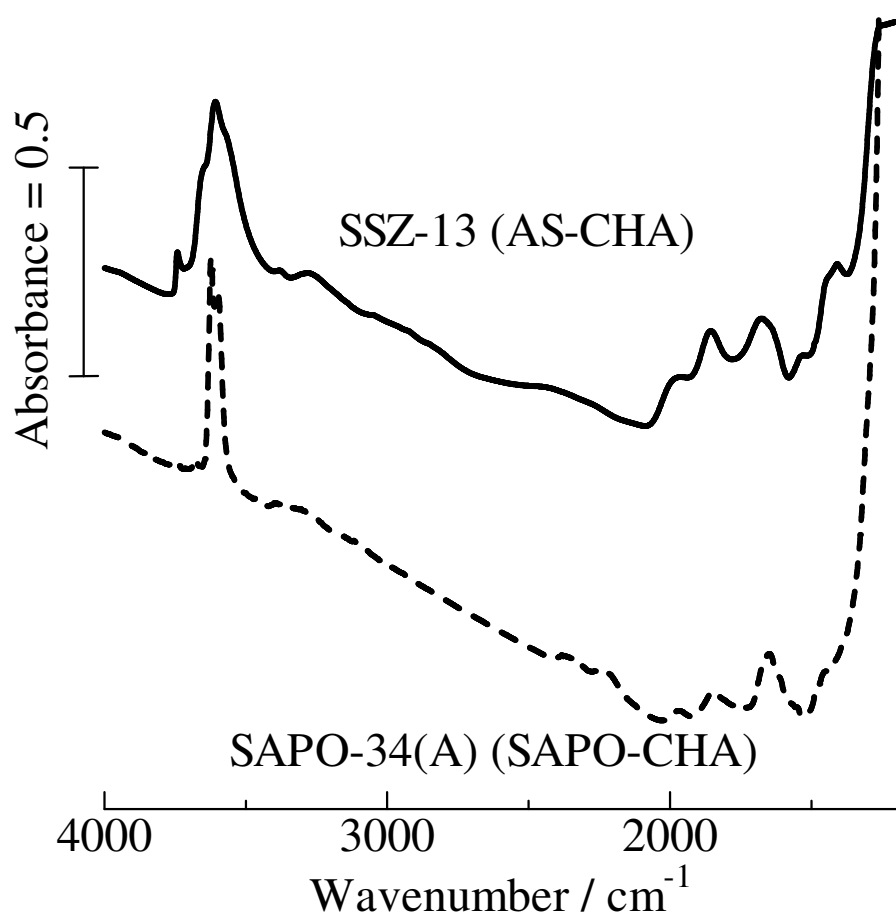


Figure S2 Examples of IR spectra of small-pore zeolitic materials after evacuation at 773 K.