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Supporting Information

Structure-directing study of 1-methylimidazolium-based dication with tetramethylene as spacer length in the synthesis of microporous silicoaluminophosphates

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Figure S1. ¹³C NMR spectra of the pristine SDA, 4BI.



Figure S2. XRD patterns of mixture phases. a) AEI+amorphous mixture. b) AFO(+AEI) mixture. From bottom to top: simulated XRD from IZA date base, XRD of AFO(+AEI) mixture. c) AEI(+AFO) mixture. From bottom to top: simulated XRD from IZA date base, XRD of AEI(+AFO) mixture. *Reflections belonging to AFO phase.



Figure S3. XRD of the triclinic CHA structure, as-made and calcined.

 Table S1. CHA structure. hkl assignment

h	k	Ι	d observed	d calculated	20 observed	2θ calculated	2θ difference
1	0	0	9.21013	9.20644	9.595	9.599	-0.004
0	1	0	9.07520	9.06234	9.738	9.752	-0.014
0	0	1		9.06934		9.745	-0.006
0	1	1	7.18357	7.18776	12.311	12.304	0.007
1	-1	0	6.53592	6.53050	13.537	13.548	-0.011
1	1	0	6.39198	6.38861	13.843	13.85	-0.007
0	1	-1	5.84332	5.84085	15.150	15.157	-0.006
1	-1	-1	5.78900	5.78897	15.293	15.293	0
1	1	1	5.55321	5.54972	15.947	15.957	-0.01
1	1	-1	4.94938	4.94774	17.907	17.913	-0.006
1	-1	1	4.91603	4.91643	18.030	18.028	1E-3
2	0	0	4.60102	4.60322	19.276	19.266	0.009
0	2	1	4.43361	4.43212	20.011	20.018	-0.007
0	1	2		4.43458		20.006	0.004
2	0	-1	4.16069	4.16034	21.338	21.34	-0.002
1	0	-2	4.12171	4.12206	21.542	21.541	0.002
1	-1	-2	4.06836	4.06400	21.828	21.852	-0.024
2	1	0		4.06819		21.829	-1E-3
1	0	2	4.01641	4.01597	22.114	22.117	-0.002
2	-1	-1	3.95510	3.95531	22.462	22.46	1E-3
1	1	2	3.92691	3.92987	22.625	22.608	0.017
2	1	1	3.80166	3.80206	23.381	23.378	0.002
0	2	-1	3.75638	3.75771	23.667	23.658	0.008

h	k	Ι	d observed	d calculated	20 observed	2θ calculated	2θ difference
0	1	1	9.32179	9.32918	9.48	9.472	0.008
2	0	0		9.34067		9.461	0.019
1	1	1	8.33922	8.34632	10.6	10.591	0.009
0	2	0	6.84652	6.84891	12.92	12.915	0.005
0	0	2	6.3705	6.37049	13.89	13.89	0
0	2	1	6.0294	6.03256	14.68	14.672	0.008
1	0	2		6.02955		14.68	0
1	1	2	5.52111	5.51857	16.04	16.047	-0.007
2	2	0		5.52325		16.034	0.006
2	0	2	5.26369	5.26299	16.83	16.832	-0.002
3	1	1	5.17818	5.17931	17.11	17.106	0.004
0	2	2	4.6647	4.66459	19.01	19.01	0
4	0	0		4.67033		18.987	0.023
1	2	2	4.52788	4.52564	19.59	19.6	-0.01
3	0	2	4.45361	4.45306	19.92	19.922	-0.002
0	3	1	4.29985	4.29827	20.64	20.648	-0.008
1	3	1	4.17777	4.18882	21.25	21.193	0.057
2	2	2		4.17316		21.274	-0.024
4	1	1		4.17624		21.258	-0.008
0	1	3	4.05705	4.05649	21.89	21.893	-0.003
1	1	3	3.96582	3.96411	22.4	22.41	-0.01
2	0	3	3.85544	3.86613	23.05	22.985	0.065
4	2	0		3.85859		23.031	0.019
4	0	2	3.76682	3.76656	23.6	23.602	-0.002
3	2	2	3.73098	3.73332	23.83	23.815	0.015
5	0	0		3.73627		23.796	0.034
2	1	3	3.72482	3.72077	23.87	23.896	-0.026
3	2	2		3.73332		23.815	0.055
1	2	3	3.54084	3.54384	25.13	25.108	0.022

 Table S2. AEI structure. hkl assignment.



Figure S4. ²⁷Al NMR spectra of CHA calcined (bottom) and as made (top).



Figure S5. ³¹P NMR spectra of CHA calcined (bottom) and as made (top).



Figure S6. Location of 1 4BI cation in 'ss' (top) or 'ops' (bottom) conformations within the 1D channels of AFO framework



Figure S7. Location of 1 4BI cation in 'ss' (top) or 'ops' (bottom) conformations within the 1D channels of AFO framework



Figure S8. DFT-optimized locations of 1 4BI cation in the triclinic CHA framework in 'span-x' (left) or 'span-z' (right) orientations



Figure S9. Possible locations of one 4BI cation within the AEI framework.



Figure S10. Most stable location of two 4BI cation with two imidazolium rings of adjacent cations sharing a cavity within the AEI framework.



Figure S11. Final most stable location of two 4BI cation within the AEI framework.