

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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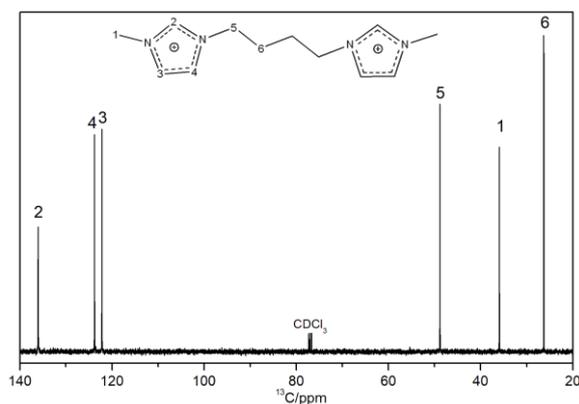


Figure S1. ¹³C NMR spectra of the pristine SDA, 4BI.

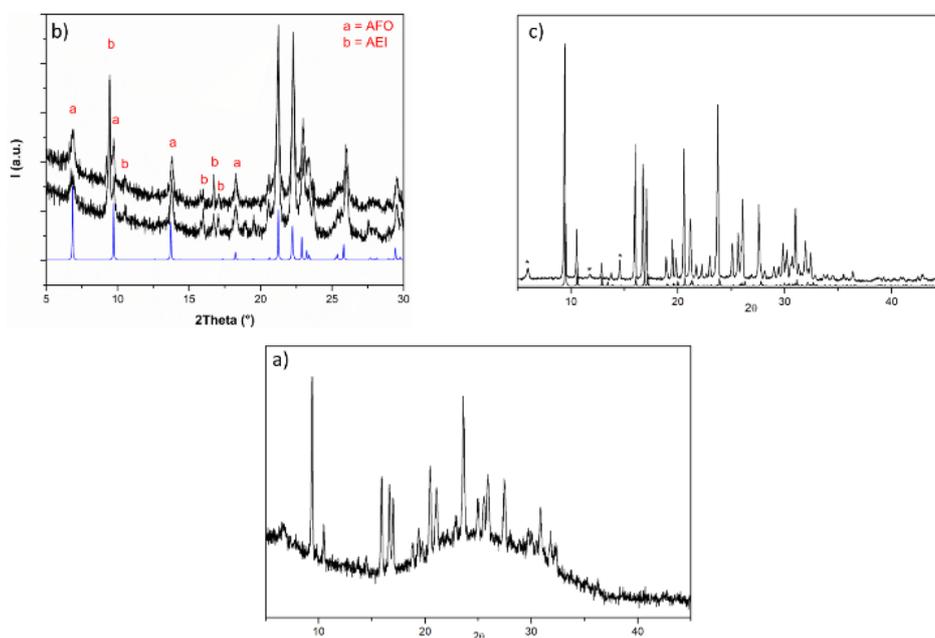


Figure S2. XRD patterns of mixture phases. a) AEI+amorphous mixture. b) AFO(+AEI) mixture. From bottom to top: simulated XRD from IZA date base, XRD of AFO(+AEI) mixture. c) AEI(+AFO) mixture. From bottom to top: simulated XRD from IZA date base, XRD of AEI(+AFO) mixture. *Reflections belonging to AFO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

Table S2. AEI structure. hkl assignment.

h	k	l	d observed	d calculated	2θ 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

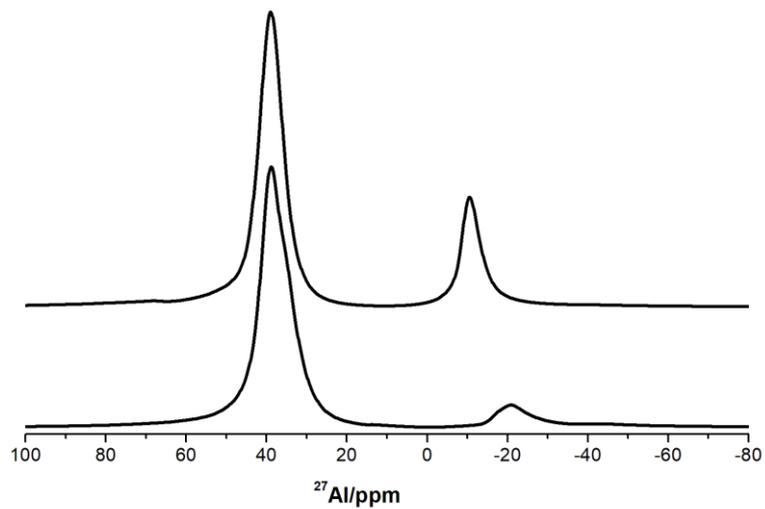


Figure S4. ^{27}Al NMR spectra of CHA calcined (bottom) and as made (top).

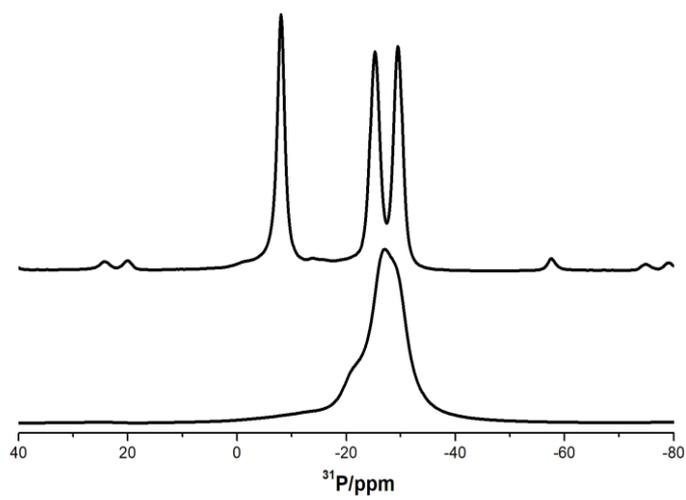


Figure S5. ^{31}P NMR spectra of CHA calcined (bottom) and as made (top).

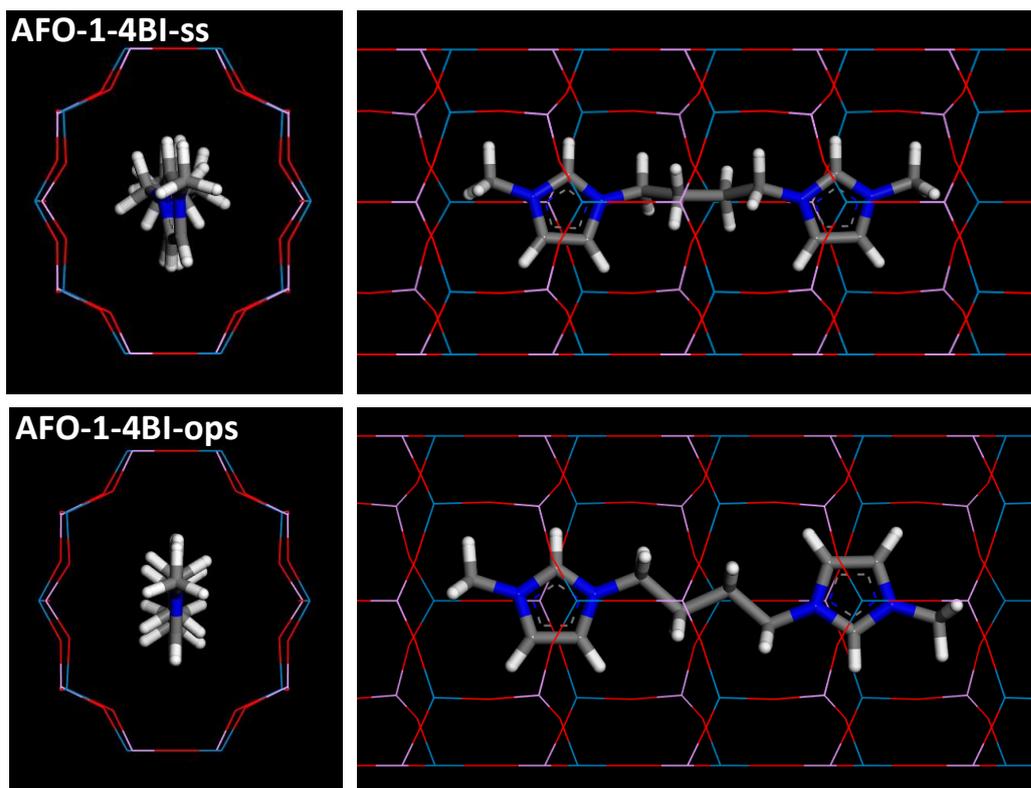


Figure S6. Location of 1 4BI cation in 'ss' (top) or 'ops' (bottom) conformations within the 1D channels of AFO framework

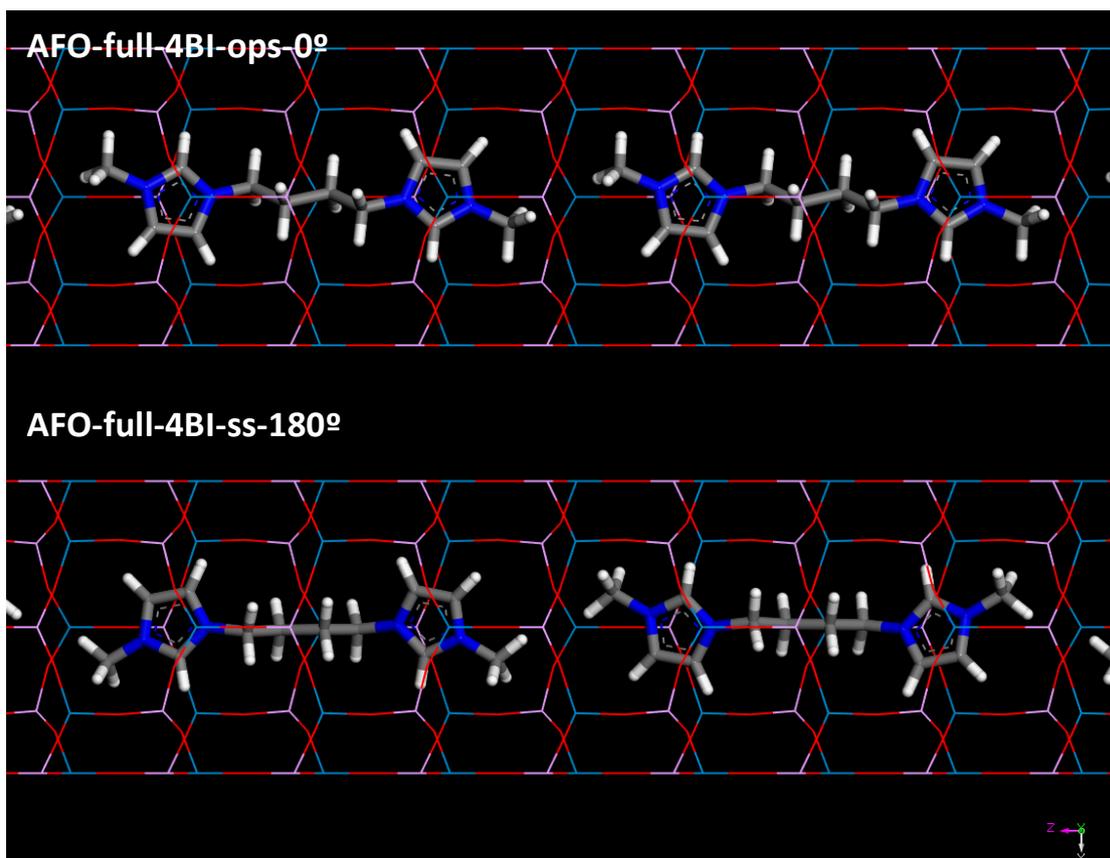


Figure S7. Location of 1 4BI cation in 'ss' (top) or 'ops' (bottom) conformations within the 1D channels of AFO framework

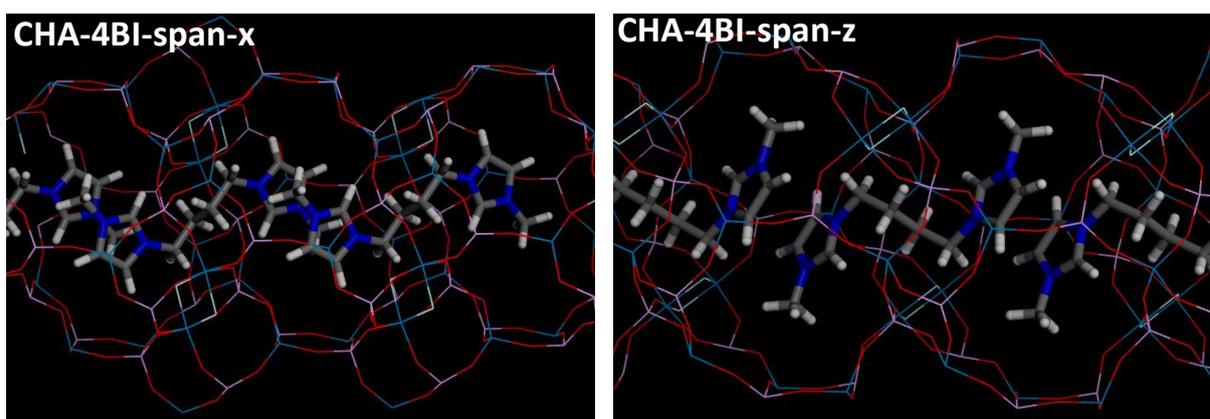


Figure S8. DFT-optimized locations of 1 4BI cation in the triclinic CHA framework in 'span-x' (left) or 'span-z' (right) orientations

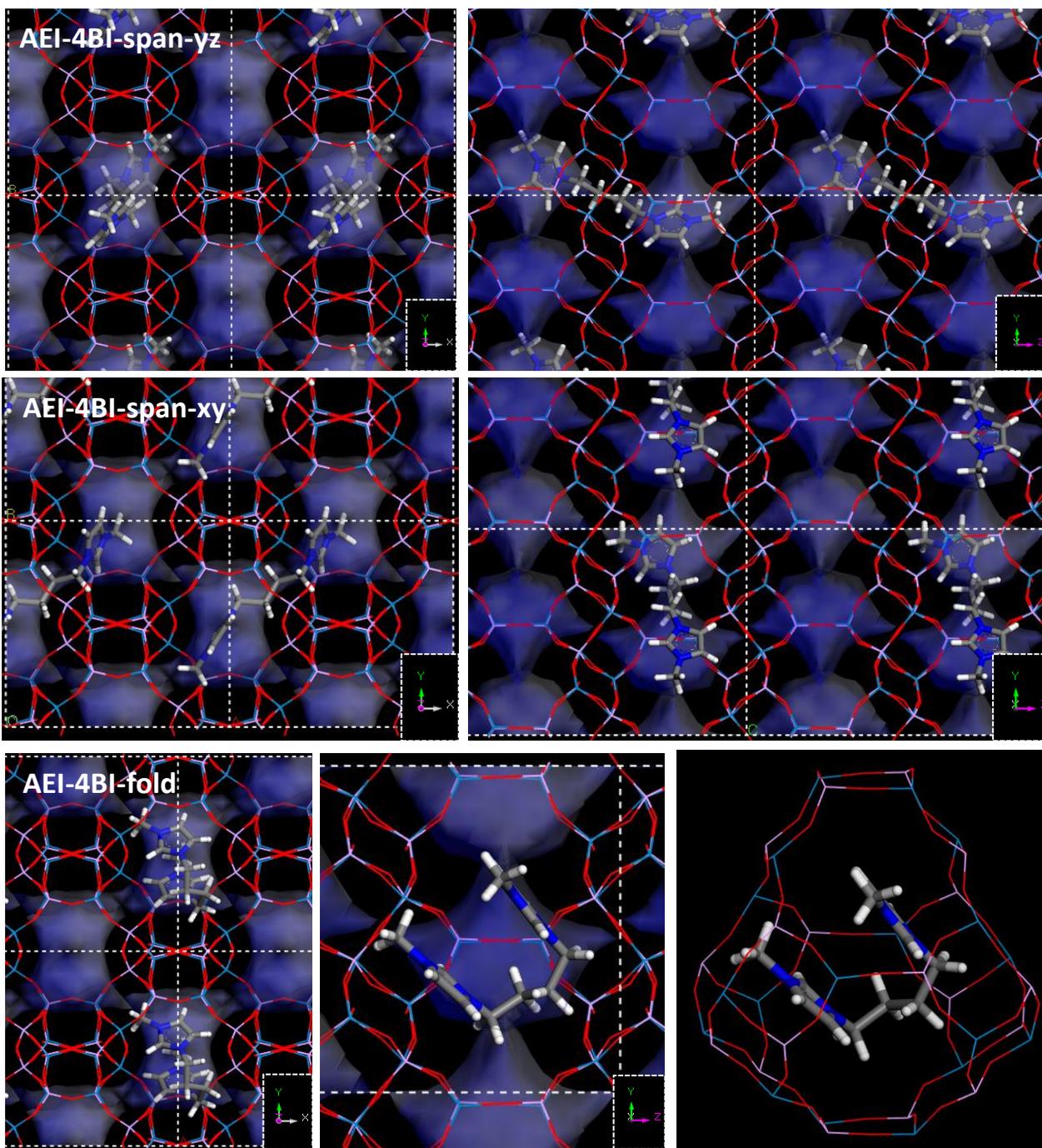


Figure S9. Possible locations of one 4BI cation within the AEI framework.

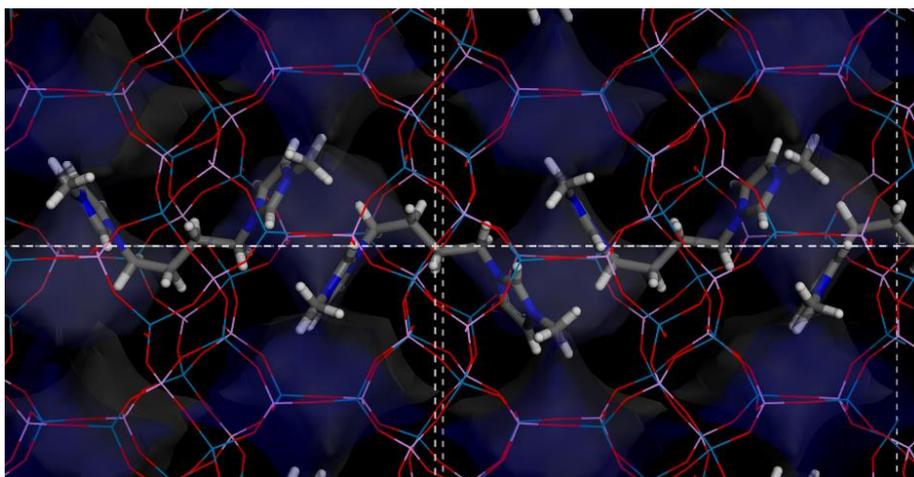


Figure S10. Most stable location of two 4BI cation with two imidazolium rings of adjacent cations sharing a cavity within the AEI framework.

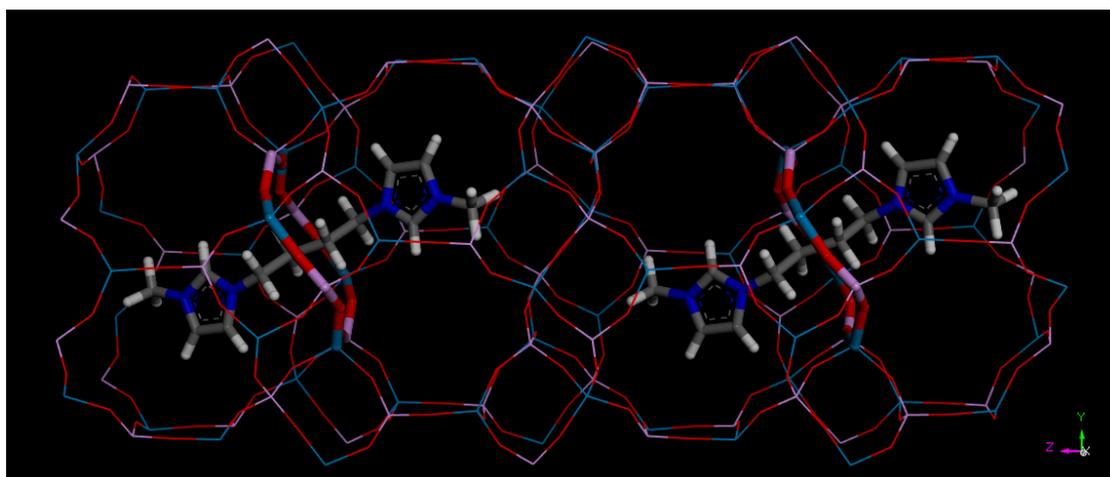


Figure S11. Final most stable location of two 4BI cation within the AEI framework.