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Supporting information for article:

Intermolecular interactions in AST zeolites through ^{14}N NMR and DFT calculations

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Figure S1 ^{19}F NMR spectrum of Si-AST (ν_0 = 564.8 MHz, ν_{MAS} = 20 kHz, $T \approx$ 300 K). The asterisks correspond to the MAS bands.

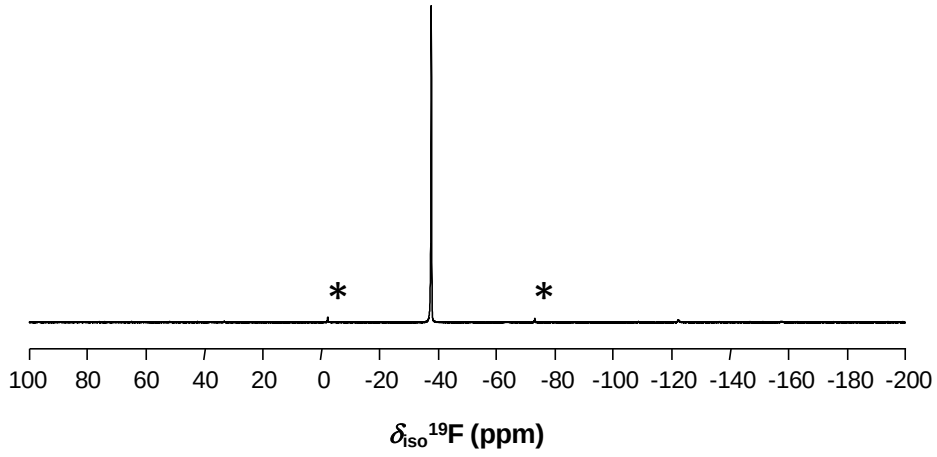
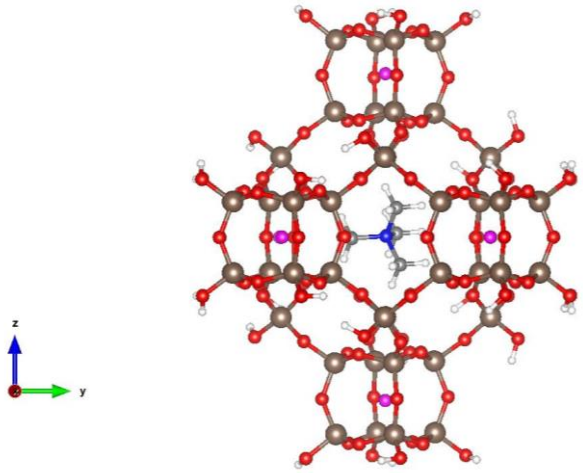
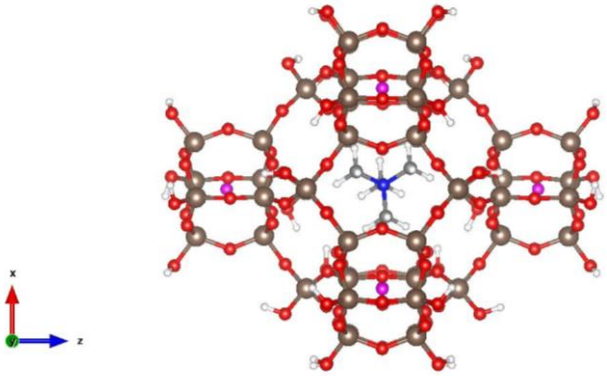


Figure S2 Schematic view of the optimized cluster following the principal coordinate axes.

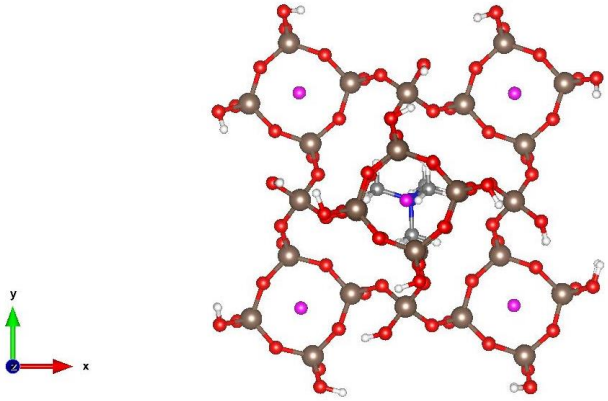
Colors convention for atoms: Si in brown, O in red, F in pink, N in blue, C in grey, H in white.



View perpendicular to x axis.



View perpendicular to y axis.



View perpendicular to z axis.

Table S1 Atomic coordinates of the optimized cluster.

Atom	*x(A)*	*y(A)*	*z(A)*
Si1	2.1447	0.5206	14.9878
Si2	6.9653	8.6350	14.9855
Si3	8.5198	2.1550	15.0093
Si4	0.3998	6.9558	14.9945
Si5	6.9742	8.6465	11.8855
Si6	2.1323	0.5243	11.8827
Si7	0.4062	6.9532	11.8834
Si8	8.5055	2.1726	11.9000
Si9	6.7392	4.8911	7.9624
Si10	2.3836	4.0844	8.0229
Si11	4.1565	6.6577	8.0315
Si12	4.9657	2.3082	7.9521
Si13	2.3883	4.0923	18.8577
Si14	6.7421	4.9019	18.9245
Si15	4.9678	2.3174	18.9243
Si16	4.1595	6.6667	18.8544
Si17	4.4674	-0.0308	9.9454
Si18	4.5434	9.1156	9.9641
Si19	-0.0462	4.5368	16.9261
Si20	9.1136	4.4809	16.9397
Si21	-0.0442	4.5338	9.9625
Si22	9.1058	4.4816	9.9574
Si23	4.4775	-0.0278	16.9346
Si24	4.5447	9.1128	16.9083
Si25	2.1134	9.5567	14.9908
Si26	6.8818	-0.5008	15.0073
Si27	-0.5200	2.1445	14.9989
Si28	9.5601	6.9110	14.9959
Si29	6.8718	-0.4841	11.8835
Si30	2.1138	9.5587	11.8841
Si31	9.5671	6.9182	11.8799
Si32	-0.5285	2.1489	11.8902
Si33	11.1820	0.5031	14.9912
Si34	-2.2231	8.6596	14.9932
Si35	8.6868	11.2531	15.0031
Si36	0.5084	-2.1462	14.9911
Si37	-2.2182	8.6555	11.8797
Si38	11.1739	0.5202	11.8833
Si39	0.4967	-2.1430	11.8815
Si40	8.6971	11.2642	11.8972
Si41	11.2713	9.5319	14.9990
Si42	-2.1348	-0.5455	14.9995
Si43	-0.5178	11.2536	14.9846
Si44	9.5623	-2.1349	14.9826
Si45	-2.1439	-0.5416	11.8956
Si46	11.2791	9.5401	11.9040
Si47	9.5580	-2.1159	11.8810
Si48	-0.5176	11.2538	11.8886
Si49	6.6593	4.9110	22.0493
Si50	2.3389	4.1574	21.9616
Si51	4.1250	6.6886	21.9722
Si52	4.8771	2.3633	22.0366
Si53	2.3384	4.1562	4.9187
Si54	6.6597	4.9149	4.8380
Si55	4.8803	2.3655	4.8410
Si56	4.1237	6.6891	4.9133
O1	8.4181	2.7444	13.4576
O2	0.5087	6.3801	13.4397
O3	6.3896	8.4581	13.4336
O4	2.7232	0.5423	13.4329
O5	3.4688	0.8582	15.9374
O6	5.6458	8.3332	15.9507
O7	8.2025	3.4711	15.9680
O8	0.7179	5.6305	15.9500
O9	5.6580	8.3506	10.9159
O10	3.4468	0.8602	10.9223
O11	0.7309	5.6238	10.9355
O12	8.1907	3.4971	10.9520
O13	7.2998	1.0904	11.5672
O14	1.6269	8.0137	11.5168
O15	8.0398	7.4382	11.4824
O16	1.0575	1.7469	11.5947
O17	1.6305	8.0087	15.3551
O18	7.3216	1.0656	15.3455
O19	1.0676	1.7399	15.2875
O20	8.0285	7.4243	15.3880
O21	2.9517	5.6023	18.4639
O22	6.1797	3.3859	18.5384
O23	3.4547	2.8731	18.5149
O24	5.6737	6.0978	18.4842
O25	6.1925	3.3640	8.3250
O26	2.9345	5.6026	8.4057
O27	5.6605	6.0722	8.4167
O28	3.4585	2.8742	8.3705
O29	-0.7706	2.6776	13.4458
O30	9.6773	6.3283	13.4368
O31	6.3383	-0.6907	13.4458
O32	2.6874	9.7059	13.4378
O33	8.1018	5.1939	8.8584
O34	1.0735	3.7860	8.9966
O35	3.8518	7.9886	8.9695
O36	5.2539	0.9669	8.8904
O37	1.0786	3.7917	17.8851
O38	8.1068	5.2027	18.0312
O39	5.2604	0.9788	17.9843
O40	3.8557	7.9971	17.9164
O41	3.4047	9.8757	15.9901
O42	5.6064	-0.8368	16.0152
O43	-0.8549	3.4145	16.0115
O44	9.8725	5.6245	16.0083
O45	5.5933	-0.8239	10.8818
O46	3.4067	9.8780	10.8877
O47	9.8818	5.6352	10.8627
O48	-0.8635	3.4209	10.8798
O49	7.4838	10.1830	11.5228
O50	1.6050	-0.9863	11.3833
O51	-1.1112	7.4783	11.4642
O52	10.0318	1.6621	11.4368
O53	1.6238	-0.9933	15.4863
O54	7.4729	10.1680	15.3604
O55	10.0520	1.6492	15.4601
O56	-1.1166	7.4829	15.4131
O57	4.0891	7.2622	6.4741
O58	4.0714	7.2630	20.4129
O59	5.0305	1.7581	6.3794
O60	5.0476	1.7676	20.4962
O61	1.7608	4.0175	6.4730
O62	1.7613	4.0364	20.4060
O63	7.2530	5.0288	6.3836
O64	7.2576	5.0146	20.5047
O65	-1.6234	0.9746	11.4363
O66	10.7805	7.9977	11.5012
O67	8.0329	-1.6003	11.4467
O68	1.0150	10.7412	11.4676
O69	10.7716	7.9872	15.3900
O70	-1.6135	0.9705	15.4570
O71	1.0138	10.7381	15.4078
O72	8.0342	-1.6338	15.4263
O73	8.6516	11.8588	13.4520

O74	0.7666	-2.7023	13.4346
O75	-2.8064	8.5543	13.4360
O76	11.7503	0.7327	13.4364
O77	-1.7430	10.2023	11.4763
O78	10.7837	-1.0452	11.4985
O79	-1.0848	-1.7819	11.5298
O80	10.2226	10.7507	11.4627
O81	10.7824	-1.0611	15.3768
O82	-1.7468	10.2061	15.3971
O83	10.2099	10.7375	15.4438
O84	-1.0695	-1.7829	15.3585
O85	-0.6599	11.8496	13.4365
O86	9.7056	-2.7174	13.4276
O87	-2.7354	-0.6538	13.4493
O88	11.8623	9.7145	13.4535
O89	2.8466	5.6989	4.5126
O90	6.1283	3.3854	4.4128
O91	3.3416	2.9100	4.4554
O92	5.6304	6.1579	4.4194
O93	6.1165	3.3870	22.4787
O94	2.8555	5.6927	22.3844
O95	5.6378	6.1642	22.4570
O96	3.3333	2.8997	22.4111
O97	3.6068	-1.1798	9.0819
O98	5.2420	10.3145	9.0074
O99	-1.2100	5.2585	17.9073
O100	10.2827	3.6182	17.7755
O101	-1.2114	5.2578	8.9880
O102	10.2650	3.5990	9.1293
O103	3.6067	-1.1637	17.8059
O104	5.2583	10.3148	17.8494
O105	12.4944	0.8178	16.0036
O106	-3.5320	8.3155	15.9968
O107	8.3355	12.5490	16.0177
O108	0.8319	-3.4615	15.9983
O109	-3.5257	8.3122	10.8748
O110	12.4700	0.8539	10.8567
O111	0.8159	-3.4535	10.8673
O112	8.3571	12.5695	10.8907
O113	12.6285	9.7456	15.9838
O114	-3.4671	-0.8128	16.0016
O115	-0.7430	12.6068	15.9734
O116	9.8200	-3.4830	15.9662
O117	-3.4821	-0.8045	10.9006
O118	12.6409	9.7571	10.9261
O119	9.8096	-3.4521	10.8814
O120	-0.7481	12.6062	10.9002
O121	7.9717	5.1659	23.0822
O122	0.9897	3.9449	22.9602
O123	3.8510	8.0342	22.9589
O124	5.0642	1.0504	23.0854
O125	0.9912	3.9505	3.9153
O126	7.9722	5.1820	3.8083
O127	5.0721	1.0556	3.7888
O128	3.8406	8.0342	3.9282

F1	-0.0013	-0.0899	13.4405
F2	-0.0752	9.1219	13.4403
F3	9.1099	0.0215	13.4448
F4	9.1400	9.0948	13.4442
F5	4.5039	4.5167	6.3155
F6	4.5018	4.5245	20.5687
N1	4.6986	4.5504	13.4915
C1	5.4681	5.0048	14.7207
C2	5.3133	5.1637	12.2450
C3	3.2525	5.0015	13.6047
C4	4.7482	3.0425	13.3928
H1	2.7470	-1.3727	9.5186
H2	5.2215	10.0421	8.0667
H3	-0.9103	5.2617	18.8404
H4	10.4962	2.7782	17.3109
H5	-0.8977	5.3052	8.0610
H6	10.4584	2.7521	9.5896
H7	2.7548	-1.3690	17.3596
H8	5.2744	10.0379	18.7889
H9	12.7960	1.7444	15.9173
H10	-3.2981	7.5587	16.5734
H11	7.5521	12.3243	16.5619
H12	1.7768	-3.7119	15.9635
H13	-3.2991	7.5457	10.3084
H14	12.7033	1.8037	10.8710
H15	1.7628	-3.6980	10.8888
H16	7.5805	12.3505	10.3350
H17	12.6325	9.0536	16.6749
H18	-3.5587	-0.0621	16.6225
H19	-0.0067	12.6564	16.6155
H20	9.1156	-3.5224	16.6446
H21	-3.5831	-0.0464	10.2902
H22	12.6570	9.0551	10.2453
H23	9.1200	-3.4678	10.1874
H24	-0.0226	12.6504	10.2456
H25	8.4668	4.3320	23.2137
H26	0.6531	4.8195	23.2397
H27	4.6972	8.4766	23.1690
H28	4.1794	0.7451	23.3723
H29	0.6712	4.8266	3.6209
H30	8.4886	4.3587	3.6939
H31	4.1889	0.7325	3.5165
H32	4.6793	8.4980	3.7351
H33	4.7456	4.8072	11.3635
H34	5.2559	6.2663	12.3175
H35	6.3706	4.8393	12.1687
H36	5.4013	6.1069	14.8117
H37	5.0276	4.5185	15.6138
H38	6.5262	4.6961	14.6159
H39	3.2250	6.1040	13.6755
H40	2.6964	4.6810	12.7027
H41	2.7950	4.5594	14.5122
H42	5.8047	2.7191	13.3238
H43	4.1966	2.7109	12.4937
H44	4.2886	2.6025	14.2965

Table S2 Selection of bond angles of TMA inside the optimized cluster.

Bonds	*angle (°)*
C1-N1-C2	109.76
C1-N1-C3	109.45
C1-N1-C4	109.54
C2-N1-C3	109.05
C2-N1-C4	109.62
C3-N1-C4	109.41
N1-C1-H36	109.47
N1-C1-H37	108.62
N1-C1-H38	108.90
N1-C2-H33	108.41
N1-C2-H34	109.12
N1-C2-H35	108.93
N1-C3-H39	108.95
N1-C3-H40	109.37
N1-C3-H41	109.60
N1-C4-H42	109.07

Table S3 Bond lengths of TMA inside the optimized cluster.

Bond	*d (Å)*
N1-C1	1.520
N1-C2	1.519
N1-C3	1.519
N1-C4	1.512
C1-H36	1.108
C1-H37	1.108
C1-H38	1.107
C2-H33	1.107
C2-H34	1.107
C2-H35	1.109
C3-H39	1.105
C3-H40	1.107
C3-H41	1.108
C4-H42	1.107
C4-H43	1.106
C4-H44	1.105