

SUPPLEMENTARY INFORMATION

Disproportionation mechanism of methylchlorosilanes catalyzed by different clusters $\text{AlCl}_3/\text{ZSM-5}$

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Table S1. The coordinates of optimized geometries of 3T cluster AlCl₃/ZSM-5 catalyst

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.356267	0.819574	-1.389526
2	8	0	-1.075067	2.702105	0.187123
3	8	0	0.206402	0.015571	0.857493
4	8	0	-2.369978	0.093896	-0.278822
5	14	0	-0.285100	-0.967376	2.195420
6	1	0	0.930177	-1.265571	3.004869
7	1	0	-1.244134	-0.148859	2.991340
8	1	0	-0.934318	-2.217479	1.720809
9	14	0	-3.841953	-0.620614	-0.627181
10	1	0	-3.797885	-2.094112	-0.355350
11	1	0	-4.933989	-0.038432	0.221876
12	1	0	-4.227828	-0.422611	-2.063747
13	13	0	-0.968193	1.038772	-0.132824
14	1	0	-1.607432	3.293130	0.750083
15	1	0	0.445905	1.241583	-2.268954
16	13	0	1.547566	-0.074482	-0.353296
17	17	0	1.887814	-2.149234	-0.974040
18	17	0	3.328386	1.108014	0.112459

Table S2. The coordinates of optimized geometries of 4T cluster AlCl₃/ZSM-5 catalyst

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	1.050371	1.293610	-2.229262
2	1	0	1.639697	1.304732	-3.006737
3	8	0	2.427296	0.097349	0.079097
4	8	0	-0.068376	-1.055501	-0.638648
5	8	0	-0.403634	1.216641	0.165492
6	13	0	0.991815	0.448171	-0.751865
7	14	0	0.447162	2.682408	0.925678
8	1	0	1.152396	-3.216493	0.270668
9	1	0	-0.760858	-3.492961	-1.247321
10	1	0	1.369431	2.633602	2.096823
11	14	0	3.887593	-0.015773	0.888301
12	1	0	4.072588	-1.386401	1.467023
13	1	0	5.037040	0.241885	-0.041674
14	1	0	3.975396	0.981328	2.005361
15	14	0	0.659873	2.909652	0.439823
16	1	0	1.421829	3.505032	0.690220
17	1	0	1.407323	3.044608	1.722462
18	1	0	0.693536	3.522700	0.559061
19	13	0	-1.436789	-0.267563	0.244376
20	17	0	-3.285496	-0.061516	-0.910883
21	17	0	-1.659153	-1.091197	2.264287

Table S3. The coordinates of optimized geometries of 6T cluster AlCl₃/ZSM-5 catalyst

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.092442	0.452197	0.876363
2	8	0	-1.038052	1.355290	1.092298
3	14	0	-1.083423	-0.768619	-2.101704

4	1	0	-0.689078	-2.070187	-2.694470
5	1	0	-0.991682	0.369155	-3.052304
6	14	0	-2.581520	1.423766	1.707328
7	1	0	-2.599487	0.953061	3.122549
8	1	0	-3.112168	2.814513	1.614560
9	8	0	1.106571	2.351306	-0.618506
10	8	0	1.599068	-0.017412	0.995306
11	14	0	1.753372	3.688014	-1.391823
12	1	0	1.859252	3.458899	-2.869924
13	1	0	0.901436	4.903250	-1.175726
14	1	0	3.125306	3.993552	-0.867520
15	14	0	2.739662	0.388886	2.236198
16	1	0	4.014524	0.842315	1.615369
17	1	0	2.122002	1.481609	3.040108
18	1	0	2.949112	-0.826891	3.071321
19	8	0	-2.585466	-0.835362	-1.419453
20	13	0	0.352454	1.055296	0.163698
21	14	0	-3.917194	-0.689621	-0.396781
22	1	0	-5.064965	-0.216813	-1.217457
23	1	0	-4.195120	-2.024772	0.199051
24	8	0	-3.566619	0.418608	0.791811
25	13	0	1.312453	1.486152	0.024569
26	17	0	3.045779	1.994710	1.261486
27	17	0	0.390748	-3.136607	1.081483
