

Predicting the Effect of Framework and Hydrocarbon Structure on The Zeolite-Catalyzed Beta-Scission

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Supporting Information

S1. Calculated Activation Enthalpy ($\Delta^\ddagger H$) and Activation Entropy ($\Delta^\ddagger S$)

Table S1. Calculated activation enthalpies and entropies of all studied hydrocarbons and zeolites in this work, with the obtained pore-confinement descriptor.

Zeolite topology	Name β -scission reactant	$\Delta^\ddagger H$ (kJ.mol ⁻¹)	$\Delta^\ddagger S$ (J.K ⁻¹ .mol ⁻¹)	$\Delta(\Sigma d^{-1})$ (Å ⁻¹)
FAU	Hex-2-ylium	67.04	-27.91	-1.300
FAU	Hept-2-ylium	69.19	-4.30	-2.012
FAU	Oct-2-ylium	61.32	-15.68	-2.701
FAU	Non-2-ylium	68.61	-19.53	-3.204
FAU	Dec-2-ylium	70.45	-22.83	-1.949
FAU	Undec-2-ylium	81.53	-14.83	-1.408
FAU	Dodec-2-ylium	88.49	-17.60	-0.758
FAU	Hex-1-ene-5-ylium	39.51	-40.45	-2.052
FAU	Hept-1-ene-6-ylium	68.90	-16.91	-1.865
FAU	Oct-1-ene-7-ylium	72.19	-21.42	-2.518
FAU	Non-1-ene-8-ylium	74.36	-15.17	-2.805
FAU	Dec-1-ene-9-ylium	70.34	-22.82	-1.481
FAU	Undec-1-ene-10-ylium	76.38	-8.53	-0.780
FAU	Dodec-1-ene-11-ylium	73.90	-27.45	-0.743
FAU	2,3,4-trimethylpent-2-ylium	55.93	2.99	-1.001
FAU	2,3,4-trimethylhex-2-ylium	60.99	16.44	-1.424
FAU	2,3,4-trimethylhept-2-ylium	60.79	15.46	-1.871
FAU	2,4,6-trimethylhept-2-ylium	76.54	17.14	-2.842
FAU	2,4,6-trimethylnon-2-ylium	83.43	11.20	-1.002
FAU	2,4-dimethylpent-2-ylium	77.07	-21.43	-1.045
FAU	2,4-dimethylhex-2-ylium	70.59	-26.02	-1.496
FAU	2,4-dimethylhept-2-ylium	73.28	-19.94	-2.823
FAU	2,4-dimethylnon-2-ylium	80.67	0.18	-1.300
MFI	Hex-2-ylium	112.90	16.01	0.120
MFI	Hept-2-ylium	111.39	37.37	0.138
MFI	Oct-2-ylium	107.53	43.42	0.269
MFI	Non-2-ylium	112.33	29.04	0.326
MFI	Dec-2-ylium	118.61	14.91	0.432
MFI	Undec-2-ylium	118.13	5.90	0.621
MFI	Dodec-2-ylium	126.29	7.28	0.763
MFI	Hex-1-ene-5-ylium	74.09	17.54	0.173
MFI	Hept-1-ene-6-ylium	123.42	33.25	0.256
MFI	Oct-1-ene-7-ylium	120.57	10.44	0.329
MFI	Non-1-ene-8-ylium	122.76	18.42	0.525
MFI	Dec-1-ene-9-ylium	110.34	22.28	0.536
MFI	Undec-1-ene-10-ylium	117.74	30.56	0.718
MFI	Dodec-1-ene-11-ylium	110.52	27.45	-0.103

MFI	2,3,4-trimethylpent-2-ylum	121.62	28.19	-0.188
MFI	2,3,4-trimethylhex-2-ylum	98.50	10.78	-0.342
MFI	2,3,4-trimethylhept-2-ylum	97.16	11.52	-0.340
MFI	2,4,6-trimethylhept-2-ylum	99.77	17.49	-0.902
MFI	2,4,6-trimethylnon-2-ylum	95.23	4.00	-0.033
MFI	2,4-dimethylpent-2-ylum	112.81	24.22	-0.167
MFI	2,4-dimethylhex-2-ylum	107.97	16.99	-0.369
MFI	2,4-dimethylhept-2-ylum	103.04	19.12	-0.872
MFI	2,4-dimethylnon-2-ylum	88.26	4.56	0.120
MOR	Hex-2-ylum	72.55	-16.32	0.158
MOR	Hept-2-ylum	70.27	-23.76	0.486
MOR	Oct-2-ylum	72.71	-29.65	0.733
MOR	Non-2-ylum	73.60	-25.05	0.996
MOR	Dec-2-ylum	74.23	-20.64	1.262
MOR	Undec-2-ylum	75.79	-17.45	1.516
MOR	Dodec-2-ylum	77.28	-15.97	1.530
MOR	Hex-1-ene-5-ylum	47.62	-13.62	0.476
MOR	Hept-1-ene-6-ylum	79.13	-4.83	0.668
MOR	Oct-1-ene-7-ylum	77.11	-16.22	0.988
MOR	Non-1-ene-8-ylum	72.39	-27.26	1.192
MOR	Dec-1-ene-9-ylum	70.86	0.66	1.503
MOR	Undec-1-ene-10-ylum	73.20	-23.93	1.595
MOR	Dodec-1-ene-11-ylum	71.74	-12.19	0.528
MOR	2,3,4-trimethylpent-2-ylum	86.30	5.72	0.674
MOR	2,3,4-trimethylhex-2-ylum	81.77	-10.16	0.875
MOR	2,3,4-trimethylhept-2-ylum	89.17	-17.48	0.911
MOR	2,4,6-trimethylhept-2-ylum	158.73	18.92	1.362
MOR	2,4,6-trimethylnon-2-ylum	163.39	14.53	0.563
MOR	2,4-dimethylpent-2-ylum	112.31	13.16	0.738
MOR	2,4-dimethylhex-2-ylum	114.91	8.81	0.970
MOR	2,4-dimethylhept-2-ylum	120.66	3.72	1.462
MOR	2,4-dimethylnon-2-ylum	126.27	17.03	0.158
TON	Hex-2-ylum	77.86	-21.16	-0.213
TON	Hept-2-ylum	88.38	-28.02	-0.265
TON	Oct-2-ylum	106.57	-24.69	-0.350
TON	Non-2-ylum	102.62	-16.32	-0.442
TON	Dec-2-ylum	99.79	-16.76	-0.590
TON	Undec-2-ylum	102.31	-6.69	-0.674
TON	Dodec-2-ylum	107.09	-15.84	-0.603
TON	Hex-1-ene-5-ylum	49.81	-27.69	-0.309
TON	Hept-1-ene-6-ylum	92.45	-17.81	-0.403
TON	Oct-1-ene-7-ylum	96.74	-20.33	-0.440
TON	Non-1-ene-8-ylum	104.18	-17.74	-0.588
TON	Dec-1-ene-9-ylum	103.20	-29.59	-0.699
TON	Undec-1-ene-10-ylum	108.42	-20.21	-0.714
TON	Dodec-1-ene-11-ylum	109.68	-16.04	0.196
TON	2,3,4-trimethylpent-2-ylum	127.34	-0.81	0.224

TON	2,3,4-trimethylhex-2-ylum	142.30	-33.49	0.292
TON	2,3,4-trimethylhept-2-ylum	182.20	-20.27	0.255
TON	2,4,6-trimethylhept-2-ylum	175.07	-33.47	0.417
TON	2,4,6-trimethylnon-2-ylum	159.46	-30.35	0.016
TON	2,4-dimethylpent-2-ylum	164.71	-22.91	0.110
TON	2,4-dimethylhex-2-ylum	169.06	-25.67	0.211
TON	2,4-dimethylhept-2-ylum	181.20	-31.33	0.270
TON	2,4-dimethylnon-2-ylum	188.34	-43.31	-0.213

S2. Zeolite Frameworks

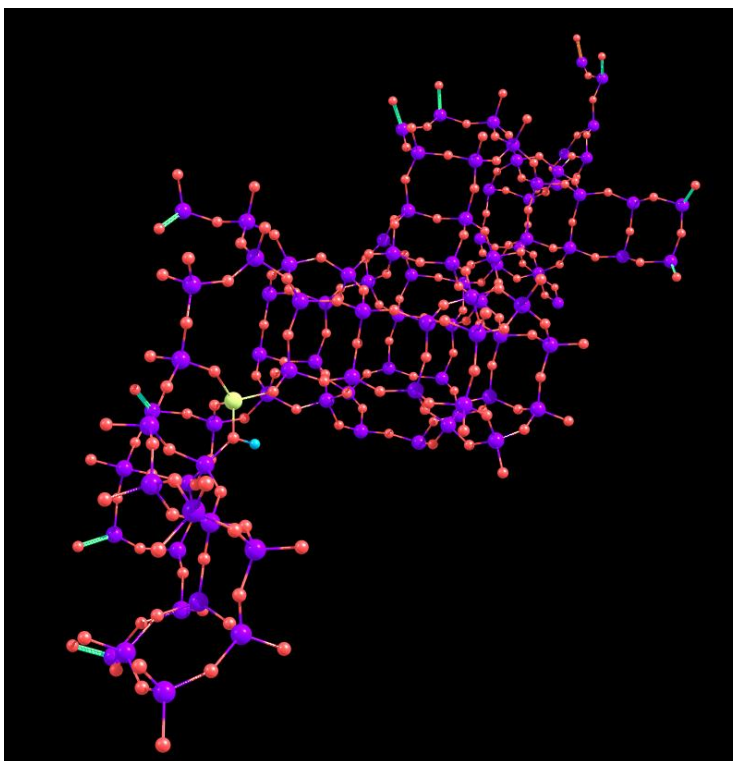


Figure S1. Illustrative FAU unit cell

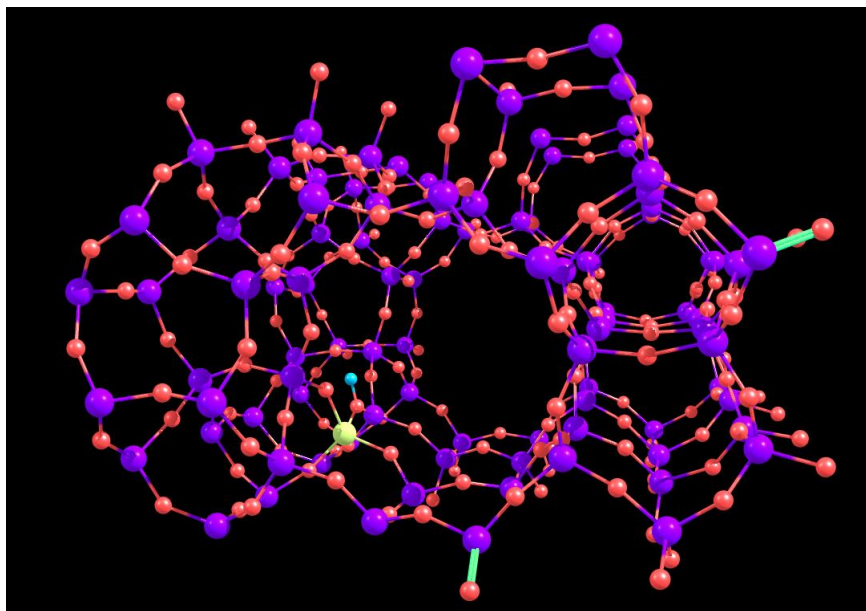


Figure S2. Illustrative MFI unit cell

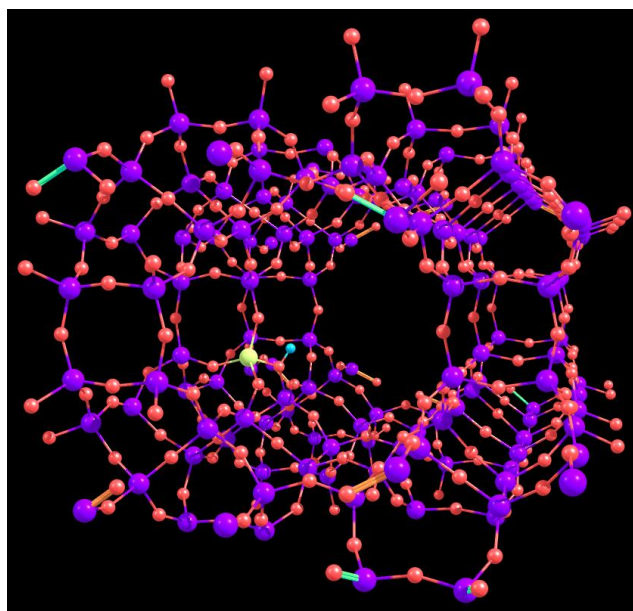


Figure S3. Illustrative MOR unit cell

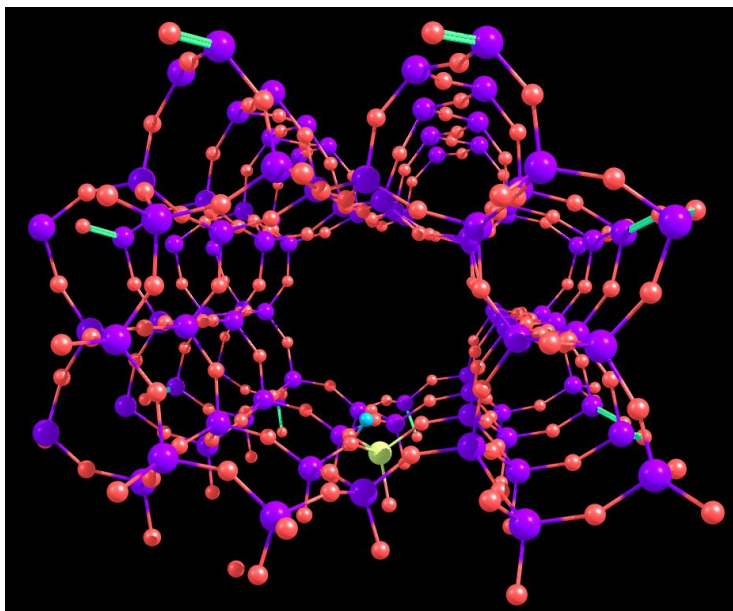


Figure S4. Illustrative TON unit cell

S3. FAU Correlation Linear Hydrocarbons

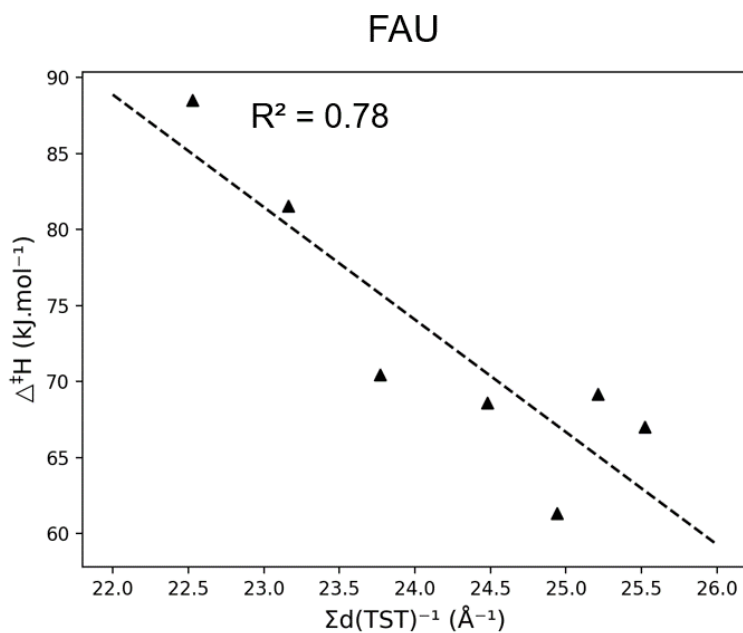


Figure S5. Correlation between the activation enthalpy ($\Delta^{\ddagger}H$) and the stabilization descriptor of the transition state $\Sigma d(\text{TST})^{-1}$ for linear carbenium ions, together with the R^2 -value.

S4. 95%-Confidence Interval Slope and Intercept of Correlation with Pore Confinement Descriptor

Table S2. Intercepts and slopes of correlation between activation enthalpy and pore confinement descriptor of the linear carbenium ions (depicted in Figure 3) with 95%-confidence intervals.

	Intercept	Slope
FAU	87.5 ± 18.2	-8.0 ± 7.2
MFI	107.0 ± 6.8	-21.9 ± 15.4
MOR	70.2 ± 2.8	3.7 ± 2.7
TON	74.0 ± 15.1	49.0 ± 31.6

Table S3. Intercepts and slopes of correlation between activation enthalpy and pore confinement descriptor of the branched carbenium ions (depicted in Figure 5) with 95%-confidence intervals.

	Intercept	Slope
FAU	69.3 ± 18.5	3.8 ± 10.5
MFI	113.4 ± 1.8	28.8 ± 3.7
MOR	103.9 ± 8.0	15.7 ± 8.0
TON	151.3 ± 10.0	-95.3 ± 55.2

S5. Activation Enthalpy Unsaturated Hydrocarbons

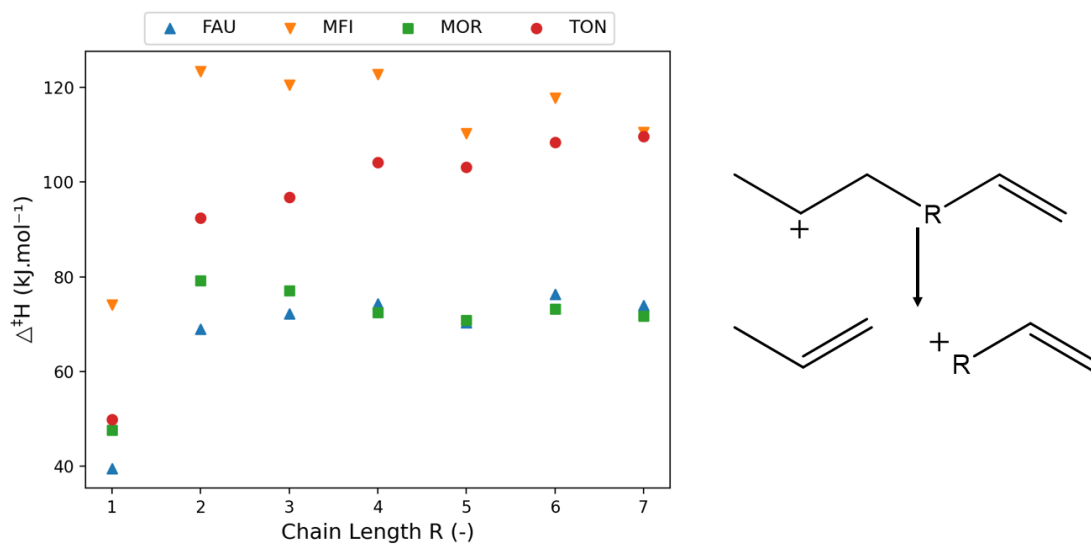


Figure S6. The variation of activation enthalpy ($\Delta^\ddagger H$) with increasing chain length of branched components (left) or the depicted reaction template (right).

S6. TON Position Unsaturated

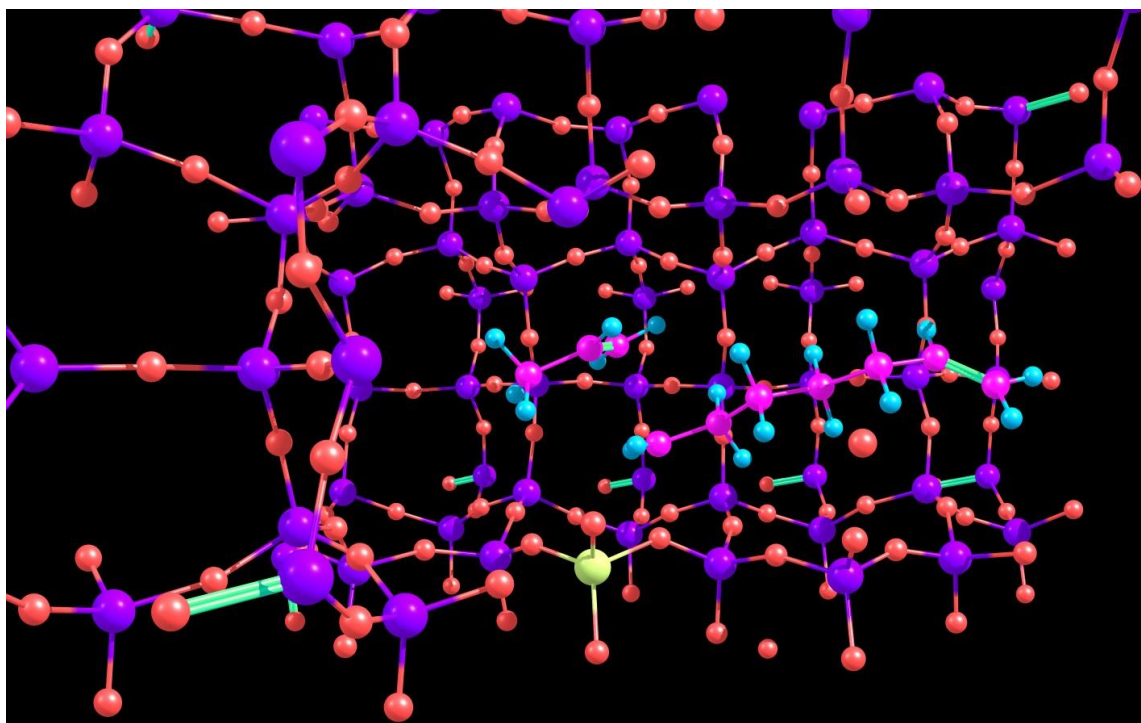


Figure S7. Geometry of the dec-1-ene-9-ylum transition state in TON-framework. Some silicon and oxygen atoms of the TON framework have been removed for visibility.

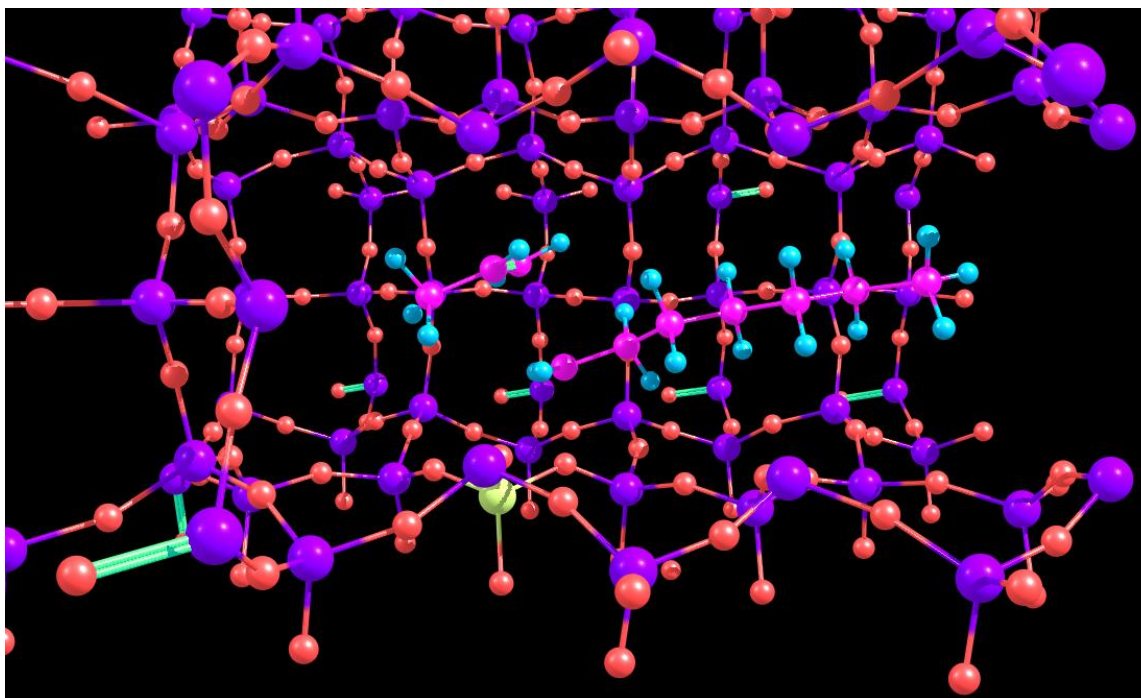


Figure S8. Geometry of the dec-2-ylum transition state in TON-framework. Some silicon and oxygen atoms of the TON framework have been removed for visibility.

S7. MFI Position 2,3,4-trimethylpent-2-ylum

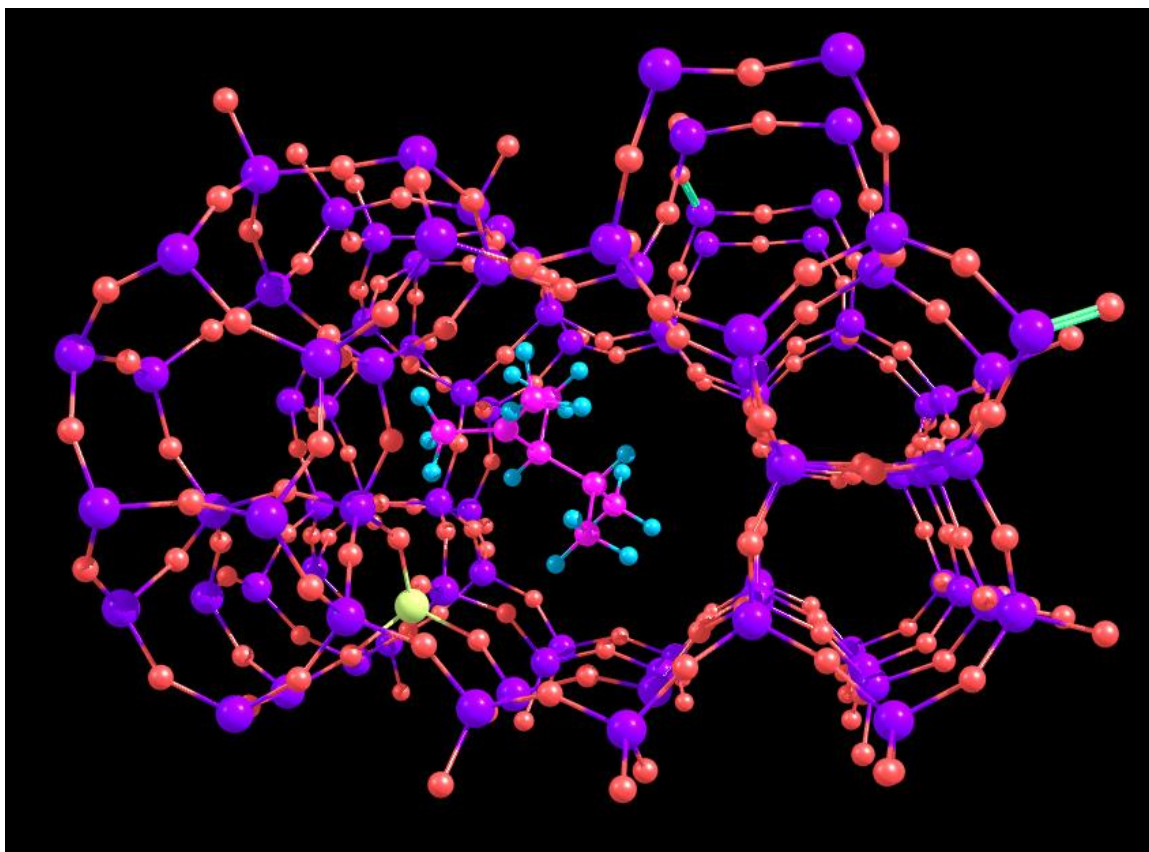


Figure S9. Geometry of the 2,3,4-trimethylpent-2-ylum in MFI indicating the “perfect fit”.

S8. Correlation Pore Stabilization Descriptor Unsaturated Hydrocarbons

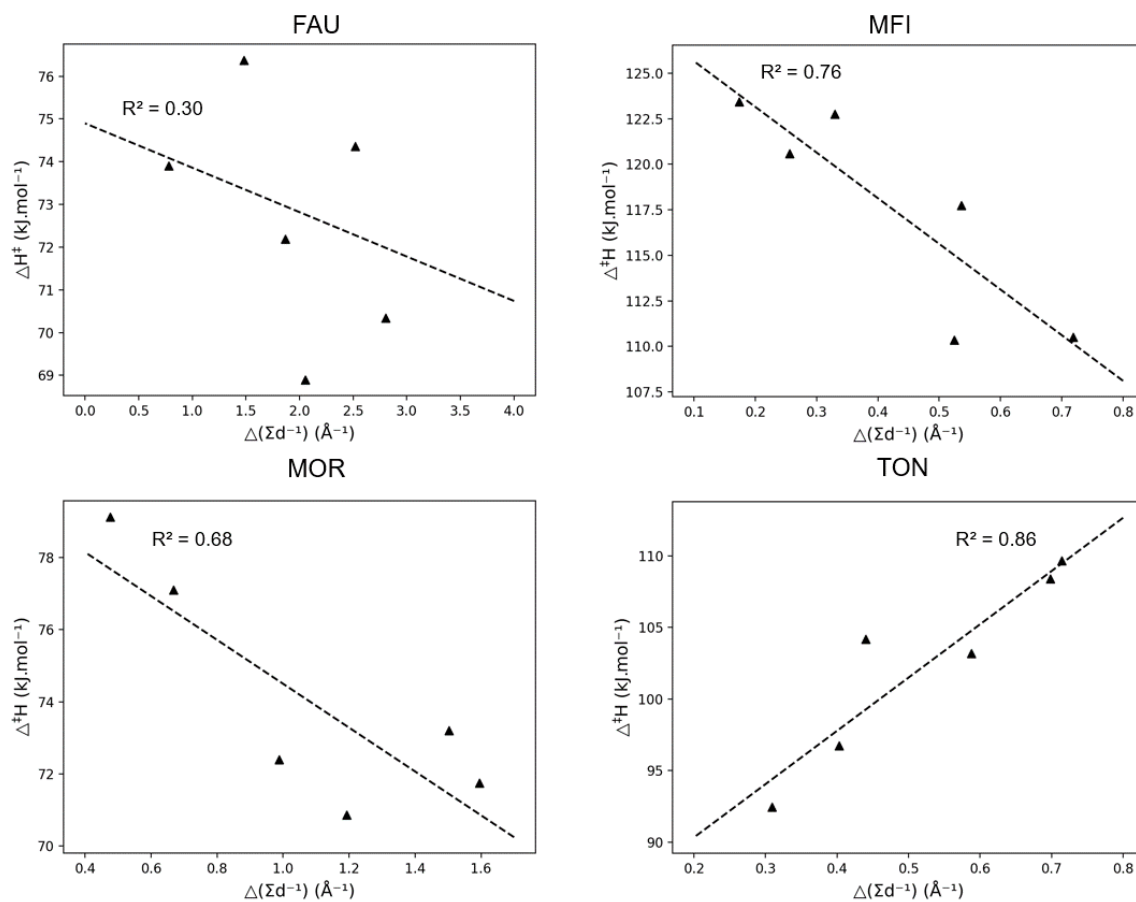


Figure S10. Correlation between the activation enthalpy ($\Delta^\ddagger H$) and the pore stabilization descriptor $\Delta(\Sigma d^{-1})$ for unsaturated carbenium ions, together with the R^2 -value.

S9. Correlation Pore Stabilization Descriptor Branched Hydrocarbons

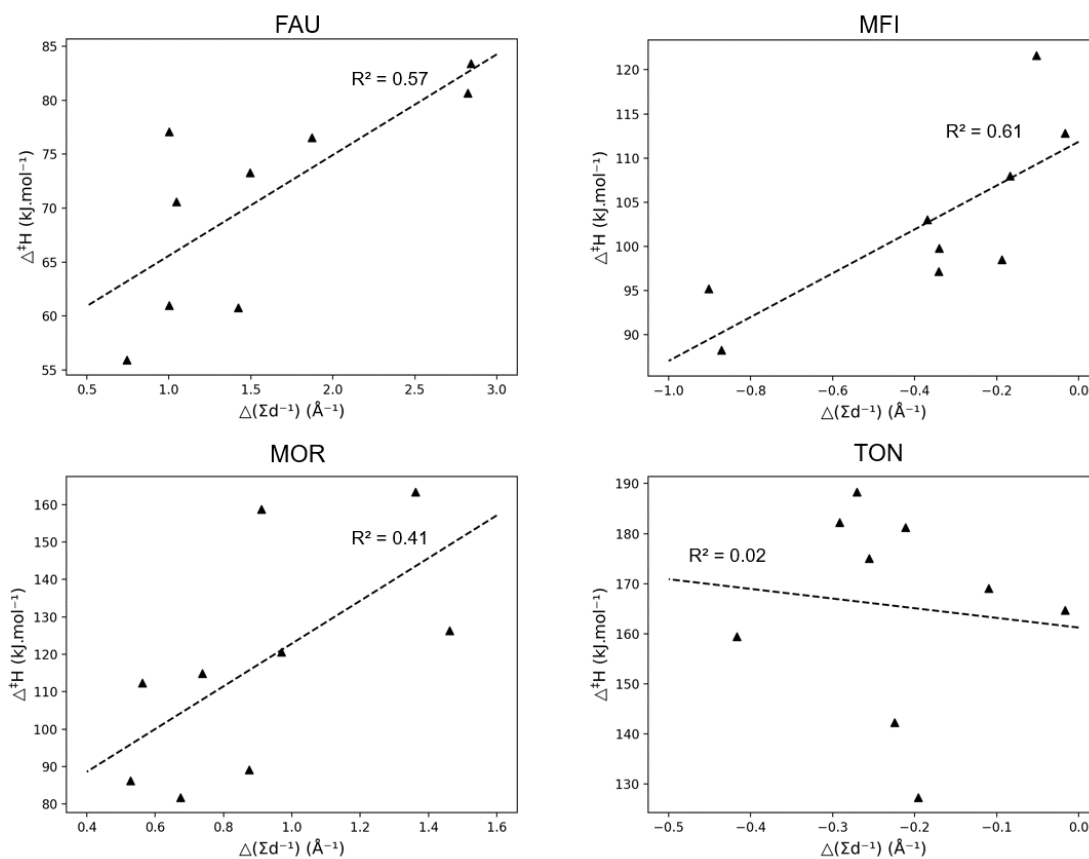


Figure S11. Correlation between the activation enthalpy ($\Delta^\ddagger H$) and the pore stabilization descriptor $\Delta(\Sigma d^{-1})$ for branched carbenium ions, together with the R^2 -value.

S10. Correlation Pore Stabilization Descriptor All Hydrocarbons

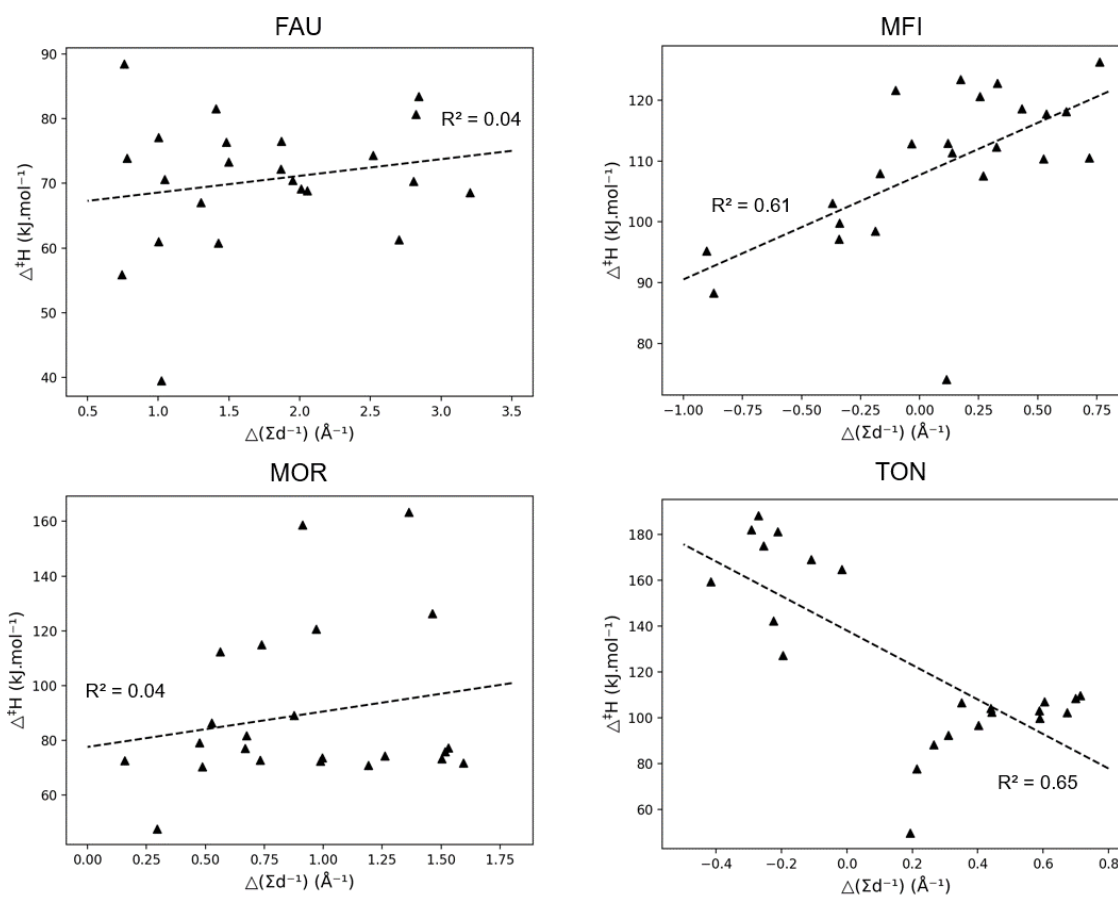


Figure S12. Correlation between the activation enthalpy ($\Delta^\ddagger H$) and the pore stabilization descriptor $\Delta(\Sigma d^{-1})$ for all carbenium ions, together with the R^2 -value.

S11. Group Additive Values

Table S4. Group additive values for kinetic group additive model for FAU and TON, excluding the pore stabilization descriptor coefficient for MFI and MOR.

$\Delta^\ddagger H$ ($\text{kJ}\cdot\text{mol}^{-1}$)	a	C_{R1}	C_{R2}	C_{R3}	C_{R4}	C_{DB}
FAU	72.4	2.3	-17.7	0	2.3	0.3
MFI	115.3	-7.0	4.6	0	-7.0	2.2
MOR	73.8	29.9	-47.0	0	29.9	0.3
TON	75.2	37.6	-22.4	0	37.6	4.6

Table S5. Group additive values for modified group additive model for FAU and TON, excluding the pore stabilization descriptor coefficient for MFI and MOR.

$\Delta^\ddagger H$ (kJ.mol ⁻¹)	a	C _{R1}	C _{R2}	C _{R3}	C _{R4}	C _{DB}
FAU	60.2	4.5	-14.9	2.4	4.5	-0.9
MFI	121.1	-8.2	3.2	-1.2	-8.2	2.8
MOR	64.5	31.2	-44.8	1.9	31.1	-0.6
TON	77.3	41.4	-17.6	4.1	41.3	2.6

S12. Optimized Reactant and Transition State Geometries

POSCAR geometries of the reference structures for all zeolites which offer a basis for the start of the molecular mechanics calculations.

Hex-2-ylum (FAU)							
Si	O	Al	H	C			
1.0000000000000000					0.0812831831156132	0.0173886419893669	0.9124699964914920
17.4005000000000010	0.0000000000000000	0.0000000000000000			0.4375615222540404	0.3769007369936861	0.2334085664499367
8.7151432720031057	15.0162842993351386	0.0000000000000000			0.4377539990294281	0.3812134061728474	0.7315658092417254
17.5186242368413545	10.0514156204086493	28.3978170589599976			0.6173529725192807	0.1972495268275546	0.3216628011740035
					0.6180552457598351	0.1976621638386128	0.8215308733786496
					0.2588161573356770	0.8408151721277697	0.0014190102657114
					0.2578605861494676	0.8402404608095796	0.5009789519180909
					0.4383350552202674	0.8414217232331858	0.0010261081404698
					0.4375051119102711	0.8406201488008308	0.5006967380383989
					0.0808469038516457	0.1970004588831495	0.3217803719417210
					0.0815067374691106	0.1969652118810570	0.8224424496820036
					0.2583743406934136	0.3757984445516639	0.2333760764491470
					0.2591838894416812	0.3754989286714007	0.7327732309030666
					0.6175691031247238	0.0168425026812068	0.4118706602320322
					0.6193754157438872	0.0172458623439511	0.9113814110898630
					0.6172188148982156	0.1972204766844604	0.2334293162106645
					0.6178464036983093	0.2000014200594942	0.7330198244184732
					0.3305312576986276	0.2689413300761869	0.0371190949612261
					0.32958959061581988	0.2674507254477151	0.5373248334961699
					0.2579317659765868	0.8403351781208530	0.411683176958244
					0.2588500947472651	0.8408372236595151	0.9121167243545106
					0.0810696898722611	0.0171365706266628	0.0017632000844705
					0.0803260213862705	0.0173385869127067	0.5011518866578688
					0.0812179857395326	0.3759264249052487	0.4114566057948881
					0.0810557927744143	0.3752917652627046	0.9125197893742356
					0.4382094768756088	0.0171778441623272	0.2331522671782073
					0.4384509361951313	0.0167735343433429	0.733238568168484
					0.6164079986537425	0.840562045300751	0.3216005235663267
					0.6183557956867178	0.841571394920228	0.8218350488947985
					0.25848242444174795	0.1990255533638591	0.000861032829238
					0.2578358941970738	0.1968841942484597	0.5011831671671223
					0.5085212221817725	0.4480282168053548	0.3578083662007203
					0.5104258482428821	0.4493741710776504	0.8565140561239135
					0.8662521896390155	0.0888789445571805	0.0371199076643156
					0.8655832956000921	0.0885307882932011	0.5373525323502483
					0.689184835132438	0.268401885950180	0.1260571766928614
					0.6894267580259326	0.2684216299099850	0.6255765735905601
					0.6890507439941237	0.6251545744833570	0.3571813848893688
					0.6915263673013882	0.6265088445769282	0.8577860266807819
					0.4380206192364390	0.3768260554195372	0.3215535182703969
					0.6150046997439717	0.0855961506276520	0.1120425941857596
					0.6141656571157880	0.0855083350355853	0.6121506144294516
					0.3256730137403058	0.3734182650186325	0.5002110960728432
					0.6144135118417512	0.5974431785688843	0.3557731870140441
					0.6176977726457791	0.6005933197407878	0.8553053766004093
					0.5078516653237567	0.851164400829912	0.4463492058276824
					0.5090683901306179	0.8496512077578718	0.9468632854290898
					0.0899514572449089	0.2674649985985746	0.3362358575370019
					0.0923949874908555	0.2668135261961321	0.8364866307445439
					0.2871106482302443	0.2669869272600589	0.238105560100235
					0.2867737248108136	0.2671728350598835	0.7369476531253779
					0.5093144475376502	0.0453082263884562	0.4476710178873436
					0.5102162966082910	0.0472210363096186	0.946365684909188
					0.5086906161330771	0.2682424443932933	0.2383002112842743
					0.5103936426892611	0.2722268403153436	0.7369781006933556
					0.2874560217021068	0.8487566687862313	0.4468184362974504
					0.2880029794792631	0.849585885161281	0.947160770343767
					0.0894493986795812	0.0472296612001575	0.4468562766843137
					0.0909997343383888	0.0463487826200880	0.947365146479027
					0.5086237454542192	0.2680183943390452	0.3357114855289661
					0.5113632201304101	0.2655483028453370	0.8357666781265649
					0.0919520005593448	0.2667460862694358	0.4464562573252573
					0.0896304936523571	0.2662286999321351	0.94733575745270544
					0.5074786487344791	0.0469789435507362	0.2380412878827274
					0.5078939197235505	0.0460264951987281	0.7380788881251394

0.510076054941193293 0.8498757606782719 0.3365186356659263 0.7950864574907712 0.5543087213637456 0.3393855483095417

0.5100239734369216 0.849582599594122 0.8361075271910106 0.7972704687277528 0.5549973664542150 0.8402899123947739

0.2866898993465129 0.2670428006626328 0.44628200527168265 0.3324371941111137 0.8692888585547683 0.0031073031203452

0.2861145715760867 0.2701179466082675 0.9469863404501120 0.3314873365759979 0.8684898273413582 0.5029854917335841

0.437530648109756 0.4188484953311667 0.4119602173770675 0.1081680538647757 0.0910456053752399 0.3589244580752834

0.437830040477155 0.4214168668544951 0.910660961295382 0.1092702675045380 0.0907298904504433 0.8593720121008341

0.8574682261187412 0.197407082378862 0.0233903190503922 0.3321907596049668 0.3799310645646889 0.2472299927874131

0.8567744612266063 0.1973891188062360 0.5227239971042232 0.3338140576095669 0.3787930805687287 0.7458480008441813

0.6600991262415883 0.198321577405995 0.1212528432142649 0.6209469147984670 0.0917048338752671 0.3592568139018935

0.6607473396406081 0.1972171567001896 0.6213554252288134 0.6280989917454579 0.0891079417737818 0.8580530140615700

0.4382370867927050 0.6144556046250539 0.4126342977510611 0.6206690796745220 0.0915941658051330 0.24708643302907676

0.4406175252285162 0.6163415182090961 0.9132111844587678 0.6200542762608493 0.0950398023445494 0.7454717592869953

0.4391602310348394 0.4194739426612277 0.1211875845504597 0.3314418055682558 0.8686221831094968 0.3587050173788472

0.43997767489814874 0.4169846192982852 0.6184037859013549 0.3325895642024622 0.8693749301637258 0.8589348829378932

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0.7953023359475300 0.554078749898766 0.9476072220840732 0.510479281534427 0.053092832734086 0.090336029543427

0.5096510537130451 0.0529598598566510 0.590456740249199 0.2947932066491056 0.2696888712513110 0.0900814319689464

0.2942100377983453 0.2665725278259837 0.5904472010615883 0.7950864574907712 0.5543087213637456 0.3393855483095417

Hex-2-ylium ST (FAU)

Si	O	Al	H	C
1.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000
17.400500000000000	0.000000000000000	0.000000000000000	0.000000000000000	0.000000000000000
8.7151432720031057	15.0162842993351386	0.000000000000000	0.000000000000000	0.000000000000000
17.5186242368413545	10.0514156204086493	28.3978170589599976		

Selective dynamics Direct

Si	O	Al	H	C
95	192	1	13	6
0.3303506097197888	0.6218314733959325	0.4473501417651115		
0.3345820279490384	0.6222886143770723	0.9483138119969390		
0.3323310827017395	0.4451623126205536	0.1263744602686010		
0.3315327621348078	0.4434649730014203	0.6254566083933424		
0.6897203358828121	0.0856253517784332	0.4474623948177982		
0.6919420614485444	0.0862470778422117	0.947355382586027		
0.866969680534973	0.2650765042185791	0.3578979511757951		
0.8683427094216914	0.2662929532920890	0.8582885131557739		
0.5101845365335124	0.6236967441884135	0.0378383903017705		
0.5098515374889905	0.6219055408308416	0.53572456048000416		
0.5094620737007474	0.6220290821026004	0.3582584211204784		

0.5105707878593659	0.4438787599428402	0.6238021849448103	0.43845164888254466	0.1923154293585900	0.5241238444812131
0.3319475768222748	0.6226604091321886	0.0383588422482911	0.6621605682641724	0.6129819253488429	0.4111471833767074
0.3301695071898412	0.6217678770306002	0.5371305491705340	0.6646687209965562	0.6135991415765928	0.9126941058514109
0.6901369925125079	0.26493238440452077	0.3578261967918369	0.4767687068841471	0.0178520510710186	0.0353783510890356
0.6944176950861336	0.26352408103100282	0.856490477889248	0.4745044211763728	0.0136973404826028	0.5371597053321242
0.4405825996177477	0.01681075946299627	0.000554288795627	0.2613707211407558	0.2313707211407558	0.1798755665768383
0.4391458326436620	0.0129372620423222	0.5018866434372292	0.2611630507593485	0.22736600513134301	0.6803053621328952
0.0821981111872521	0.373380192195307	0.3218873012684457	0.6874988249676383	0.7302427552335041	0.4288950000537978
0.0861553092644957	0.3720953092644957	0.8227818796383808	0.6893087967967335	0.7311256875573217	0.9298684610614283
0.2594530187556056	0.1944204055092188	0.2334948084758660	0.6878924699403872	0.01716353789383656	0.1796262141162801
0.2599960053116099	0.1931471868481876	0.7336317369335397	0.6876504678561461	0.0151728487921957	0.6796733059891920
0.6179769986177243	0.8378583024058057	0.4111554363950107	0.2609186630822054	0.4412229451370350	0.4305917322865676
0.6189926025897426	0.8385257944599258	0.9122950912655295	0.2589021745366650	0.4460541693237682	0.9316989721880791
0.6178132064044534	0.0150517640110711	0.2331481006988252	0.4734488995030702	0.7297117807102441	0.3237483851289041
0.6183508743577830	0.0153143911897310	0.7331983717055995	0.4765031974476057	0.7277930840950817	0.8245910870061088
0.2588659915057056	0.3725588704637950	0.4122249474217673	0.4744768444574711	0.4438076114787828	0.1799713232495059
0.2571851069229248	0.377966697411044	0.9122092808538861	0.4731154973771432	0.4456056688192794	0.767374230223980
0.0831904976842759	0.19464449020877318	0.0017076486819972	0.6880795635318260	0.2295373224731657	0.3230398644751149
0.0822927645002227	0.193815977088031	0.500981242906909	0.6981597925549897	0.2251696512261928	0.8213111815814817
0.5109267164548736	0.0861625372869309	0.1257840968818306	0.2630717842301180	0.7306061982993300	0.0367667900363380
0.5102458742219775	0.0840317793150668	0.6263529104559391	0.2608699928713158	0.7292796594558473	0.5365255559989183
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0.4413814451513047	0.8362489862956117	0.8226866238669835	0.4740244401375728	0.4618997749192778	0.82004366503205081
0.0814813292717159	0.0143350248468438	0.4119519811799260	0.6880740674942978	0.2297618870136577	0.1799057843863227
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0.6184192553569885	0.1943924611692310	0.3218084934989549	0.2625582383306333	0.4419665582532661	0.1801215980104345
0.6218046102508941	0.1953213752980364	0.8213268078243674	0.2634986538684459	0.4415386880311669	0.6792007320884149
0.2601246327224092	0.8382752456034611	0.0018171947484271	0.6880406448088712	0.0156345940698954	0.42973427091161339
0.2585988826864972	0.8366479127699801	0.5012753050717320	0.6889719296127970	0.0155312486747788	0.9306994222463920
0.4393665608791303	0.8391606215069043	0.0014052715561907	0.4737354901473132	0.7314685248256891	0.03668938833919
0.4386868601079866	0.8371829918731044	0.5007070052545456	0.4745154457074306	0.7291614807028992	0.5352773926784052
0.0821181610682590	0.1942364473902360	0.3220066769361934	0.4757741682639453	0.016098490987878	0.179541217618023
0.0841078098133000	0.1941821081744403	0.8227429159720459	0.4756731243575313	0.0134114665228324	0.680123711848837
0.2599560237377745	0.3726929144387238	0.2337544234079105	0.2613180088341862	0.2308302692658970	0.0368679229895060
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2,4-Dimethylpent-2-ylum (FAU)

Si O Al H C
1.000000000000000
17.4005000000000010 0.000000000000000 0.0000000000000000
8.7151432699999988 15.01622842999999544 0.0000000000000000
17.5186242368413545 10.0514156217992259 28.3978170584678011

Selective dynamics

Direct

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0.3298514779381916 0.63011244776017437 0.9465224137643790
0.3289826775905473 0.4521010401032360 0.1247462577667689
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0.8650058219026521 0.2698612910706212 0.2698612910706212
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Table with columns of numerical data, likely coordinates or identifiers. Includes a section for '1,4-Dimethylpent-2-ylium ST (MFI)' with sub-sections for 'Si O Al H C' and 'Selective dynamics Direct'.


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			0.7299751058744406	0.3778770116554995	0.1904321925696650
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			0.7418311540983795	0.3775174873497672	0.6918007466459931
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			0.2508301134677378	0.1270111912606763	0.5603152885261756
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			0.9170292402323345	0.7790506519198206	0.937348319957480
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Hex-2-ylum ST (TON)
Si O Al H C
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0.0034000834353423
0.0000000000000000
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0.0000000000000000
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Si O Al H C
95 191 1 13 6
Selective dynamics
Direct

0.1017065456592488	0.7786363648684608	0.1854902256193427	1.0000000000000000		
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0.4196640896788779	0.7199823378868698	0.1811065689956771	Si	Al	H
0.5985192297995653	0.272820987275618	0.1835835602466849	95	191	C
0.6035991888673673	0.2775287096865481	0.9314701400712241	15	7	
0.1006365488917234	0.2120221739428042	0.3097836161830958	Selective dynamics		
0.9118834279903795	0.774057921644973	0.6892146096044445	Direct		
0.9187991494527631	0.7740705316345236	0.4339349227122445	0.2935693263382382	0.0347519655735536	0.0443420829508311
0.1037014608858499	0.2157667162358449	0.8107647889282783	0.7028073590476868	0.9455246738749447	0.9335102875361537
0.9186076009583262	0.2174364625405170	0.8108239671845932	0.7018275040135181	0.94691720870469670	0.1826745610885135
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