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Supporting information

Theoretical study on the reaction mechanism of Si_2Cl_6 and HCl catalyzed by amine catalysts

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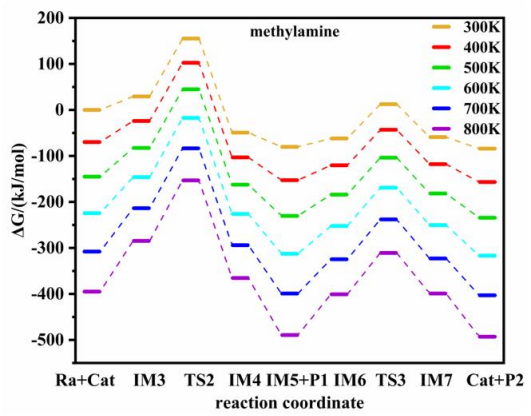
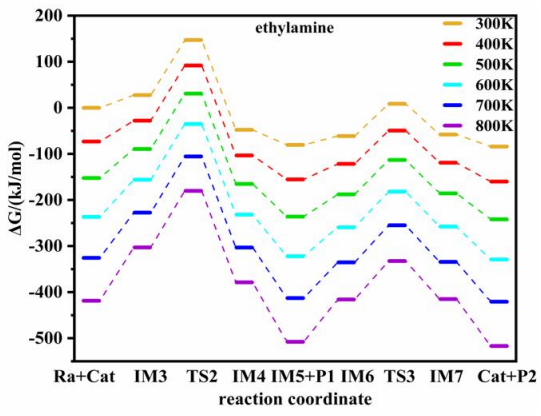
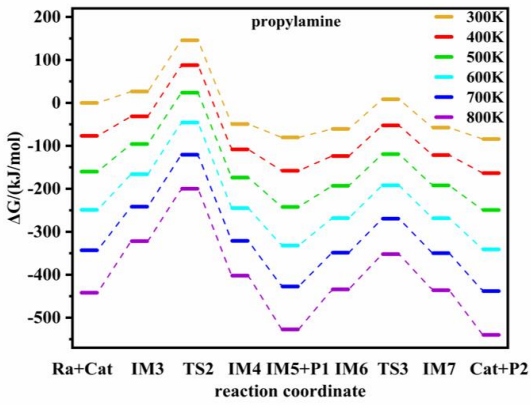
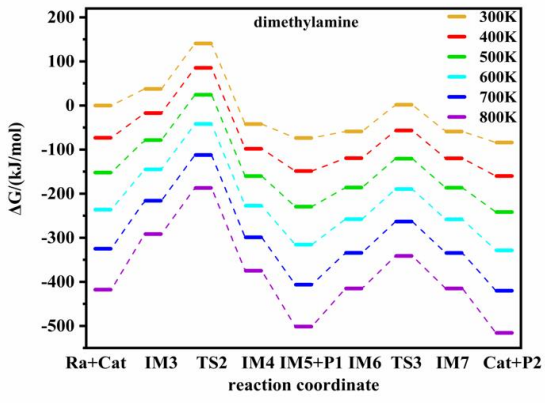
Table S1. Experimental and calculated values of reaction Gibbs free energy change.

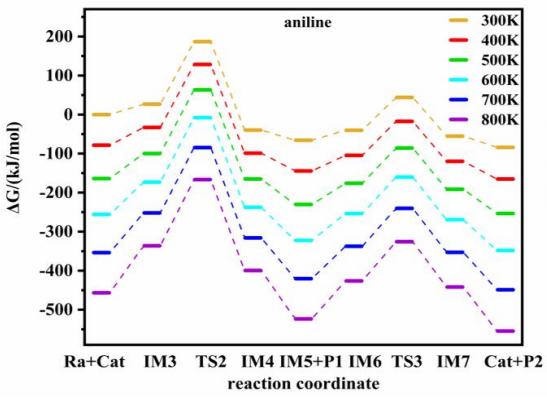
	Experiment[1-4]	Calculation
$\Delta_r G$/ (kJ/mol)	-79.69	-78.88

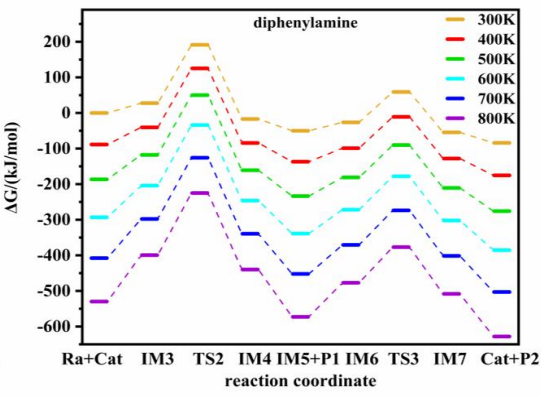












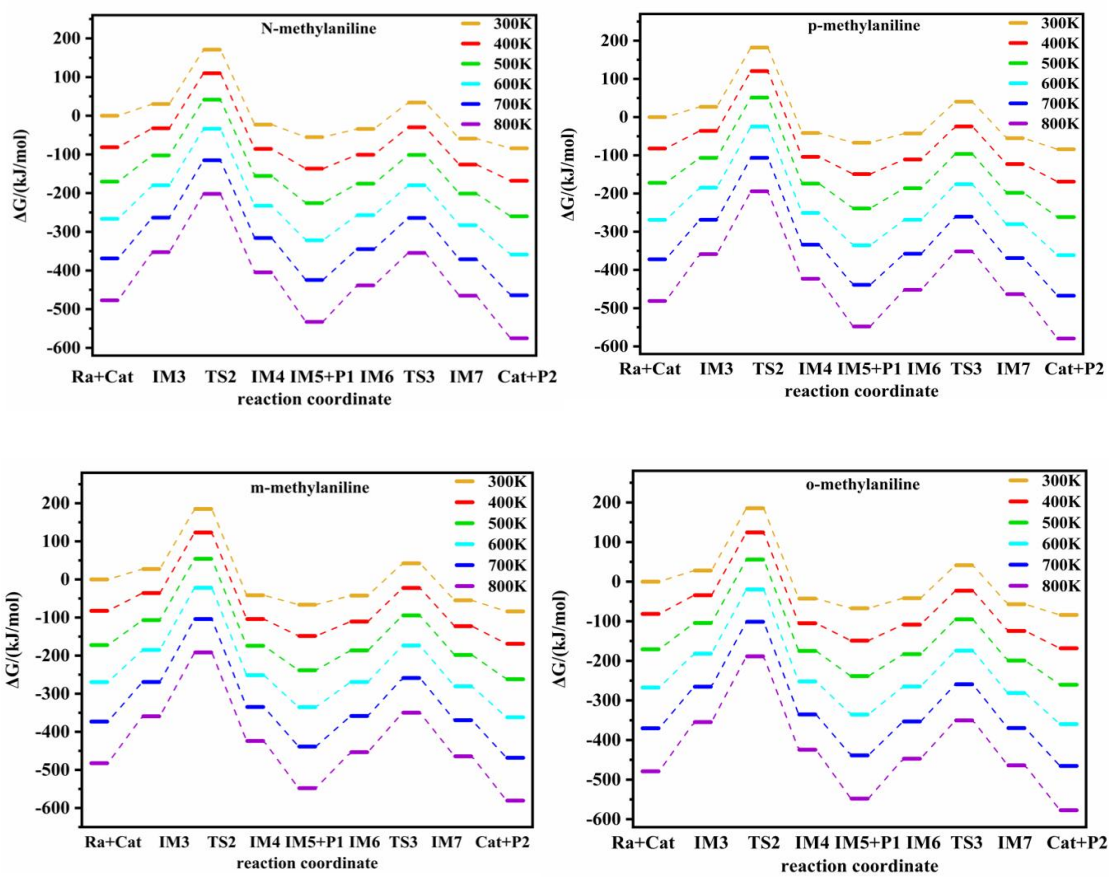


Figure S1. Gibbs free energy change at 300 - 800 K during the reaction of Si_2Cl_6 with HCl Catalyzed by amine catalysts (methylamine, ethylamine, propylamine, dimethylamine, aniline, diphenylamine, N-methyl aniline, p-methyl aniline, m-methyl aniline, o-methyl aniline).

Table S2. Gibbs free energy (hartree) and relative free energy (Grel ,kJ/mol) at each step of the reaction catalyzed by an amine catalyst.

Species	ammonia		methylamine		ethylamine		propylamine	
	G	Grel	G	Grel	G	Grel	G	Grel
Ra+Cat	-3397.152681	0.00	-3436.425768	0.00	-3475.715741	0.00	-3515.002893	0.00
IM3	-3397.146687	15.74	-3436.414918	28.49	-3475.706025	25.51	-3514.994151	22.95
TS2	-3397.086265	174.38	-3436.367802	152.19	-3475.661848	141.50	-3514.949987	138.90
IM4	-3397.176178	-61.69	-3436.447082	-55.96	-3475.736410	-54.27	-3515.025695	-59.87
IM5+P1	-3397.180823	-73.89	-3436.454978	-76.69	-3475.745727	-78.73	-3515.033356	-79.98
IM6	-2187.104478	-58.45	-2226.379067	-62.39	-2265.669297	-63.06	-2304.956616	-63.50
TS3	-2187.068426	36.21	-2226.349268	15.85	-2265.641299	10.44	-2304.929070	8.82
IM7	-2187.106229	-63.04	-2226.377693	-58.78	-2265.668569	-61.15	-2304.956146	-62.27
Cat+P2	-2187.112262	-78.88	-2226.385349	-78.88	-2265.675322	-78.88	-2304.962474	-78.88

Species	dimethylamine		aniline		diphenylamine		N-methyl aniline	
	G	Grel	G	Grel	G	Grel	G	Grel
Ra+Cat	-3475.703437	0.00	-3628.106302	0.00	-3859.057866	0.00	-3667.382817	0.00
IM3	-3475.689186	37.42	-3628.098756	19.81	-3859.050332	19.78	-3667.374580	21.63

TS2	-3475.651755	135.69	-3628.037869	179.67	-3858.986965	186.15	-3667.320446	163.76
IM4	-3475.722004	-48.75	-3628.124819	-48.62	-3859.068163	-27.03	-3667.396018	-34.66
IM5+P1	-3475.730649	-71.45	-3628.131304	-65.64	-3859.077004	-50.25	-3667.404448	-56.79
IM6	-2265.655546	-59.27	-2418.053113	-45.36	-2648.998471	-29.06	-2457.326873	-38.12
TS3	-2265.631433	4.04	-2418.018994	44.22	-2648.964459	60.24	-2457.299057	34.91
IM7	-2265.655484	-59.10	-2418.059008	-60.83	-2649.010922	-61.75	-2457.337378	-65.70
Cat+P2	-2265.663018	-78.88	-2418.065883	-78.88	-2649.017447	-78.88	-2457.342398	-78.88

Species	p-methyl aniline		m-methyl aniline		o-methyl aniline	
	G	Grel	G	Grel	G	Grel
Ra+Cat	-3667.398198	0.00	-3667.399628	0.00	-3667.397509	0.00
IM3	-3667.390450	20.34	-3667.392163	19.60	-3667.389355	21.41
TS2	-3667.331846	174.21	-3667.332019	177.51	-3667.329329	179.01
IM4	-3667.417198	-49.88	-3667.418091	-48.47	-3667.417330	-52.04
IM5+P1	-3667.423786	-67.18	-3667.424985	-66.57	-3667.423296	-67.70
IM6	-2457.346379	-48.95	-2457.347728	-48.74	-2457.344425	-45.63
TS3	-2457.312280	40.57	-2457.312862	42.80	-2457.311239	41.50
IM7	-2457.350356	-59.39	-2457.351792	-59.41	-2457.350979	-62.84
Cat+P2	-2457.357779	-78.88	-2457.359209	-78.88	-2457.35709	-78.88

Table S3. the values of reaction rate constants, activation energies (kJ/mol) and pre-exponential factors (s^{-1}) in the temperature range of 300 - 800 K.

Catalyst	300K			400K			500K		
	Ea	A	k	Ea	A	k	Ea	A	k
ammonia	159.64	2.69×10^{12}	4.30×10^{-16}	158.88	2.14×10^{12}	3.83×10^{-9}	158.31	1.89×10^{12}	5.47×10^{-5}
methylamine	128.45	1.80×10^{13}	7.75×10^{-10}	128.42	1.52×10^{13}	2.57×10^{-4}	128.39	1.33×10^{13}	5.12×10^{-1}
ethylamine	123.96	3.60×10^{13}	9.36×10^{-9}	123.96	3.00×10^{13}	1.95×10^{-3}	123.93	2.60×10^{13}	2.93
propylamine	122.54	2.46×10^{13}	1.13×10^{-8}	122.53	2.24×10^{13}	2.23×10^{-3}	122.50	2.07×10^{13}	3.30
dimethylamine	108.94	6.94×10^{13}	7.46×10^{-6}	109.11	5.79×10^{13}	3.26×10^{-1}	109.23	4.96×10^{13}	1.92×10^{2}
aniline	157.72	2.42×10^{12}	8.34×10^{-16}	157.20	2.22×10^{12}	6.55×10^{-9}	156.75	2.11×10^{12}	8.87×10^{-5}
diphenylamine	159.49	1.07×10^{12}	1.81×10^{-16}	159.06	1.11×10^{12}	1.87×10^{-9}	158.70	1.16×10^{12}	3.06×10^{-5}
N-methyl aniline	136.40	1.27×10^{12}	2.25×10^{-12}	136.08	1.33×10^{12}	2.24×10^{-6}	135.81	1.39×10^{12}	8.99×10^{-3}
p-methyl aniline	153.44	3.30×10^{12}	6.34×10^{-15}	152.91	2.89×10^{12}	3.11×10^{-8}	152.44	2.65×10^{12}	3.14×10^{-4}
m-methyl aniline	155.31	2.52×10^{12}	2.29×10^{-15}	154.89	2.29×10^{12}	1.36×10^{-8}	154.49	2.15×10^{12}	1.55×10^{-4}
o-methyl aniline	155.36	2.83×10^{12}	2.51×10^{-15}	154.90	2.66×10^{12}	1.57×10^{-8}	154.47	2.56×10^{12}	1.87×10^{-4}

Catalyst	600K			700K			800K		
	Ea	A	k	Ea	A	k	Ea	A	k
ammonia	157.90	1.77×10^{12}	3.18×10^{-2}	157.64	1.73×10^{12}	2.98	157.48	1.72×10^{12}	8.94×10
methylamine	128.38	1.20×10^{13}	7.96×10	128.41	1.10×10^{13}	2.88×10^{3}	128.46	1.03×10^{13}	4.22×10^{4}
ethylamine	123.92	2.31×10^{13}	3.76×10^{2}	123.93	2.11×10^{13}	1.19×10^{4}	123.97	1.95×10^{13}	1.57×10^{5}
propylamine	122.48	1.94×10^{13}	4.23×10^{2}	122.47	1.85×10^{13}	1.34×10^{4}	122.49	1.78×10^{13}	1.79×10^{5}
dimethylamine	109.34	4.36×10^{13}	1.32×10^{4}	109.44	3.91×10^{13}	2.66×10^{5}	109.56	3.56×10^{13}	2.50×10^{6}
aniline	156.40	2.07×10^{12}	5.01×10^{-2}	156.15	2.08×10^{12}	4.63	155.97	2.11×10^{12}	1.38×10^{2}
diphenylamine	158.41	1.23×10^{12}	1.99×10^{-2}	158.21	1.31×10^{12}	2.05	158.07	1.40×10^{12}	6.68×10

N-methyl aniline	135.59	1.46×10^{12}	2.28	135.43	1.54×10^{12}	1.20×10^{2}	135.32	1.62×10^{12}	2.37×10^{3}
p-methyl aniline	152.07	2.53×10^{12}	1.46×10^{-1}	151.80	2.47×10^{12}	1.16×10	151.61	2.45×10^{12}	3.09×10^{2}
m-methyl aniline	154.18	2.07×10^{12}	7.81×10^{-2}	153.95	2.04×10^{12}	6.62	153.80	2.04×10^{12}	1.85×10^{2}
o-methyl aniline	154.12	2.53×10^{12}	9.68×10^{-2}	153.87	2.55×10^{12}	8.40	153.70	2.60×10^{12}	2.40×10^{2}

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