Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

An experimental and theoretical study of the gas phase kinetics of atomic chlorine reactions with CH_3NH_2, $(CH_3)_2NH$, and $(CH_3)_3N$

Electronic Supplementary Information

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Table S1. Experimental polarizabilities, α, and the first ionisation potentials, I, used for calculating capture rates.[a]

	α /Å^3	I /eV
MA	3.75	8.90
DMA	5.45	8.24
TMA	7.08	7.85
Cl	2.18	12.97

[a] NIST Computational Chemistry Comparison and Benchmark Database. NIST Standard Reference Database Number 101, R. D. Johnson III, Release 16a, August 2013. http://cccbdb.nist.gov/

[a] Present address: Portnoy Environmental Inc. (PEI), 1414 Sam Houston Parkway N., Suite170, Houston, TX 77043, USA.

Table S2: Kinetic Data for the reaction $Cl(^2P_J) + CH_3NH_2 \rightarrow$ products (R1) [a]

T	P	# exp [b]	$[Cl_2CO]$	$[Cl]_0$	$[CH_3NH_2]_{max}$	k_{max}	$k_{R1} \pm 2\sigma$ [c]
298	25	6	393–1360	6.9	784	24500	3.14 ± 0.52
298	25	6	1440	1.2	448	13600	2.97 ± 0.25
297	26	5	355	4.2	406	11500	2.82 ± 0.45
297	26	5	395	2.6	522	16200	2.95 ± 0.35
297	26	5	181	1.8	572	18600	3.13 ± 0.38
297	25	11	1250	0.84–3.4	689	19800	2.92 ± 0.12
296	25	7	665	5.1	610	16800	2.78 ± 0.26
296	25	10	804	0.81–5.8	642	18700	2.93 ± 0.16
296	25	5	575	3.0	447	14600	3.13 ± 0.20
296	25	6	401	1.0	686	19500	2.86 ± 0.11
296	25	6	2120	6.9	704	17700	2.54 ± 0.04
296	25	4	590	2.4	678	20700	3.02 ± 0.07
296	25	5	1170	4.3	672	20700	3.08 ± 0.08
297 ± 1	25.5 ± 0.5	81					3.00 ± 0.13 [d]
296	200	6	797	6.1	530	15000	2.90 ± 0.15
351	25	7	953	4.4	559	16400	2.89 ± 0.13
403	100	5	852	3.1	688	19600	2.82 ± 0.09
419	25	6	615–1320	1.9–3.5	507	14500	2.89 ± 0.10

[a] Units are T (K); P (Torr); concentrations (10^{11} cm^{-3}); k (s^{-1}); k_{R1} (10^{-10} cm^3 $molecule^{-1}$ s^{-1}). [b] # exp ≡ number of pseudo–first–order $Cl(^2P_J)$ decay rates measured. [c] Uncertainties are 2σ, precision only. [d] Data at one temperature and pressure combined into a single linear fit.

Table S3: Kinetic Data for the reaction $Cl(^2P_J) + (CH_3)_2NH \rightarrow$ products (R2) [a]

T	P	# exp [b]	$[Cl_2CO]$	$[Cl]_0$	$[(CH_3)_2NH]_{max}$	k_{max}	$k_{R2} \pm 2\sigma$ [c]
296	25	4	424	2.1	393	16000	3.99 ± 0.06
296	25	6	1050	2.7	511	18600	3.58 ± 0.21
296	25	3	2020	6.5	434	15300	3.51 ± 0.09
296	25	13					3.57 ± 0.28 [d]
296	101	6	741–2320	2.2–7.1	634	20200	3.53 ± 0.12
296	99	8	1260	3.5	762	27500	3.72 ± 0.27
296	100	10	361–962	1.7–4.0	574	21800	3.83 ± 0.10
296	100 ± 1	24					3.74 ± 0.15 [d]
337	25	5	666	2.9	509	20900	4.11 ± 0.13
364	25	4	1080	1.2	282	11800	4.17 ± 0.13
435	25	7	419–922	1.2–3.9	443	17400	3.95 ± 0.12
435	100	4	848	3.7	378	14300	3.77 ± 0.02

[a] Units are T (K); P (Torr); concentrations (10^{11} cm^{-3}); k (s^{-1}); k_{R2} (10^{-10} cm^3 $molecule^{-1}$ s^{-1}). [b] # exp ≡ number of pseudo–first–order $Cl(^2P_J)$ decay rates measured. [c] Uncertainties are 2σ, precision only. [d] Data at one temperature and pressure combined into a single linear fit.

Table S4: Kinetic Data for the reaction $Cl(^2P_J) + (CH_3)_3N \rightarrow$ products (R3) [a]

T	P	# exp [b]	$[Cl_2CO]$	$[Cl]_0$	$[(CH_3)_3N]_{max}$	k_{max}	$k_{R3} \pm 2\sigma$ [c]
274	26	5	453	1.7	518	18800	3.63 ± 0.01
294	28	4	427	2.8	710	24300	3.44 ± 0.10
294	24	8	277–1000	1.6–4.3	352	12000	3.46 ± 0.18
298	25	7	142–572	1.3–5.2	694	27300	3.89 ± 0.16
298	25	6	317	2.8	688	24500	3.51 ± 0.08
296 ± 2	26 ± 2	25					3.64 ± 0.15 [d]
298	201	5	609	5.4	788	30900	3.98 ± 0.14
298	399	5	648	5.7	596	21900	3.68 ± 0.17
360	26	4	288	2.6	416	14400	3.44 ± 0.07
418	200	4	360	3.2	564	21200	3.80 ± 0.14
421	27	6	294	2.3	522	18500	3.50 ± 0.09
421	26	12	124–607	1.1–5.0	584	22600	3.62 ± 0.27
421	26.5 ± 0.5	18					3.57 ± 0.20 [d]

[a] Units are T (K); P (Torr); concentrations (10^{11} cm^{-3}); k (s^{-1}); k_{R3} (10^{-10} cm^3 $molecule^{-1}$ s^{-1}). [b] # exp ≡ number of pseudo–first–order $Cl(^2P_J)$ decay rates measured. [c] Uncertainties are 2σ, precision only. [d] Data at one temperature and pressure combined into a single linear fit.

Table S5. Electronic energies of reactants, intermediates and products (/Hartree), and relative energies including Zero Point Energies and spin-orbit corrections, Δ (/kJ mol^{-1}), of stationary points on the potential energy surface of the CH_3NH_2 + Cl reaction.

Species	MP2/cc-pVTZ	CCSD(T)-F12a/aug-cc-pVTZ // MP2/cc-pVTZ
CH_3NH_2	-95.657700 (0.064934)[a]	-95.740211
Cl	-459.643363	-459.692305
PRE	-555.324596 (0.066683) Δ = -53.7 [b]	-555.4576578 Δ = -57.9
TSC	-555.298154 (0.062089) Δ = 3.7	-555.4333397 Δ = -6.1
POST-C	-555.320087 (0.060657) Δ = -57.7	-555.4531579 Δ = -61.9
CH_2NH_2	-95.000420 (0.050966)	-95.08056486
HCl	-460.309449 (0.006959)	-460.3630335
PROD-C	Δ = -38.0	Δ = -44.0
TSN	-555.300640 (0.059702) Δ = -9.1	-555.438471 Δ = -25.9
POST-N	-555.309277 (0.059676) Δ = -31.9	-555.44435 Δ = -41.4
CH_3NH	-94.985892 (0.049819)	-95.06878
PROD-N	Δ = -2.9	Δ = -16.1

[a]Zero point energy (ZPE) in parentheses. [b] Energy difference incl. ZPE and spin-orbit correction in kJ mol^{-1}.

Table S6. Electronic energies of reactants, intermediates and products (/Hartree), and relative energies including Zero Point Energies and spin-orbit corrections, Δ (/kJ mol^{-1}), of stationary points on the potential energy surface of the $(CH_3)_2NH$ + Cl reaction.

Species	MP2/cc-pVTZ	CCSD(T)-F12a/aug-cc-pVTZ // MP2/cc-pVTZ
$(CH_3)_2NH$	-134.8695333	-134.9860964
	(0.0936274)[a]	
Cl	-459.643363	-459.692305
PRE	-594.5434028	-594.7103488
	(0.0954794)	
	Δ = -71.7 [b]	Δ = -75.5
TSC	-594.5089551	-594.6786317
	(0.0903233)	
	Δ = 5.2	Δ = -5.8
POST-C	-594.5341658	-594.7016459
	(0.0894522)	
	Δ = -63.3	Δ = -68.5
CH_2NHCH_3	-134.2125047	-134.3274345
	(0.0798803)	
HCl	-460.309449	-460.3630335
	(0.006959)	
PROD-C	Δ = -38.1	Δ = -46.0
TSN	-594.5219298	-594.6985662
	(0.0912015)	
	Δ = -26.6	Δ = -55.8
POST-N	-594.5309378	-594.7011998
	(0.0880082)	
	Δ = -58.6	Δ = -71.1
$(CH_3)_2N$	-134.2055925	-134.3237353
	(0.0784431)	
PROD-N	Δ = -23.7	Δ = -40.1

[a]Zero point energy (ZPE) in parentheses. [b] Energy difference incl. ZPE and spin-orbit correction in kJ mol^{-1}.

Table S7. Electronic energies of reactants, intermediates and products (/Hartree), and relative energies including Zero Point Energies and spin-orbit corrections, Δ (/kJ mol^{-1}), of stationary points on the potential energy surface of the $(CH_3)_3N$ + Cl reaction.

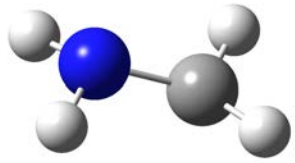
Species	MP2/cc-pVTZ	CCSD(T*)-F12a/aug-cc-pVTZ // MP2/cc-pVTZ
$(CH_3)_3N$	-174.0867604	-174.236782
	(0.12166688)[a]	
Cl	-459.643363	-459.692305
PRE	-633.7651449	-633.9654206
	(0.1238135)	
	Δ = -82.8 [b]	Δ = -86.3
TSC	-633.7525668	-633.9526191
	(0.1162385)	
	Δ = -69.7	Δ = -72.5
POST-C	-633.7527371	-633.9533776
	(0.1174582)	
	Δ = -66.9	Δ = -71.3
$(CH_3)NCH_2$	-173.4291449	-173.5782442
	(0.1082605)	
HCl	-460.309449	-460.3630335
	(0.006959)	
PROD-C	Δ = -35.7	Δ = -45.4

[a]Zero point energy (ZPE) in parentheses. [b] Energy difference incl. ZPE and spin-orbit correction in kJ mol^{-1}.

Table S8. Cartesian coordinates of reactants, intermediates and products in the reactions between the Cl atom and CH_3NH_2, $(CH_3)_2NH$ and $(CH_3)_3N$. Results from MP2/cc-pVTZ calculations.

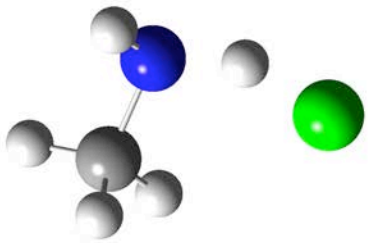
Species	Atom	X	Y	Z
HCl	H	0.000000	0.000000	-1.202463
	Cl	0.000000	0.000000	0.070733
CH_3NH_2	C	0.051730	0.703644	0.000000
	H	0.590539	1.059541	0.875164
	H	-0.937690	1.169764	0.000000
	H	0.590539	1.059541	-0.875164
	N	0.051730	-0.759486	0.000000
	H	-0.457937	-1.097154	0.805857
	H	-0.457937	-1.097154	-0.805857
CH_3NH_2*Cl Pre-reaction adduct	C	1.702966	-0.473362	0.000186
	H	2.754401	-0.182370	0.000348
	H	1.493879	-1.074800	-0.878548
	H	1.493647	-1.074939	0.878770
	N	0.808312	0.670333	0.000159
	H	0.821983	1.236048	-0.834408
	H	0.821763	1.235916	0.834819
	Cl	-1.368333	-0.117177	-0.000189
CH_3NH_2+Cl TSC	C	1.175375	0.616993	0.047145
	H	1.266134	1.274640	-0.812174
	H	1.259835	1.197357	0.967643
	H	0.097524	0.265994	0.030599
	N	2.048294	-0.515697	-0.079084
	H	2.265917	-0.929366	0.814138
	H	2.912843	-0.272870	-0.537739
	Cl	-1.717209	-0.095755	-0.011279
CH_2NH_2*HCl Post-reaction adduct	C	-1.434153	0.717006	-0.000001
	H	-1.526653	1.265808	0.924347
	H	-1.526666	1.265817	-0.924343
	H	0.431928	0.375470	0.000000
	N	-1.948370	-0.563547	-0.000002
	H	-1.794885	-1.102775	-0.835650
	H	-1.794919	-1.102759	0.835663
	Cl	1.673806	-0.062280	0.000000

CH_2NH_2



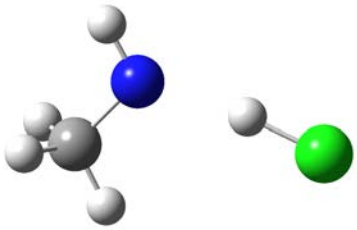
C	-0.725678	-0.000001	0.083561
H	-1.235530	0.925418	-0.125777
H	-1.235521	-0.925393	-0.125812
N	0.655111	0.000000	-0.102293
H	1.119706	0.827807	0.233124
H	1.119633	-0.827830	0.233152

CH_3NH_2+Cl TSN



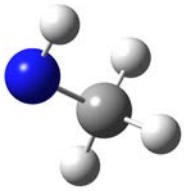
C	-1.783693	-0.476203	0.016820
H	-2.837900	-0.201747	0.086711
H	-1.523066	-1.034698	0.916113
H	-1.629930	-1.102309	-0.855156
N	-1.014506	0.737338	-0.120418
H	-1.018824	1.267640	0.748623
H	0.123141	0.543912	-0.420679
Cl	1.452369	-0.104526	0.015670

CH_3NH*HCl Post-reaction adduct



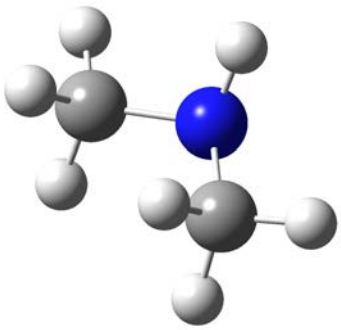
C	-2.123473	-0.473268	-0.000001
H	-2.775471	-0.457511	-0.877595
H	-2.775429	-0.457534	0.877625
H	-1.545614	-1.392039	-0.000024
N	-1.243095	0.664007	0.000001
H	-1.804331	1.514459	-0.000006
H	0.513374	0.344812	0.000002
Cl	1.754704	-0.080037	0.000000

CH_3NH



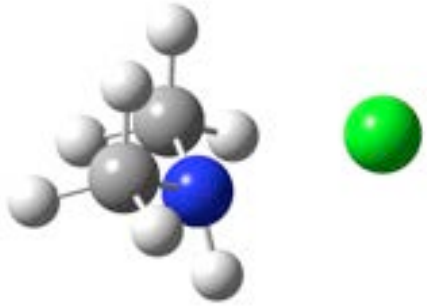
C	-0.629099	-0.012896	0.000005
H	-0.963037	-0.577039	0.876298
H	-0.963050	-0.577099	-0.876251
H	-1.122094	0.954681	-0.000070
N	0.803534	0.152298	0.000005
H	1.198036	-0.789257	-0.000046

$(CH_3)_2NH$



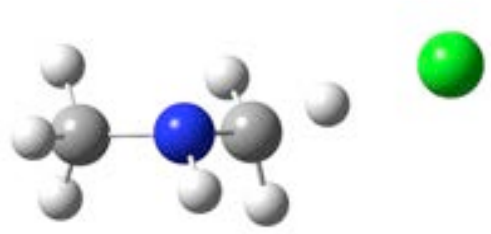
C	-1.199934	-0.225626	0.020344
H	-1.231970	-0.774751	0.970986
H	-1.256576	-0.957553	-0.784743
H	-2.082345	0.407197	-0.043691
N	0.000000	0.577311	-0.152494
H	0.000000	1.316543	0.538224
C	1.199934	-0.225626	0.020344
H	1.256576	-0.957553	-0.784743
H	2.082345	0.407197	-0.043690
H	1.231970	-0.774751	0.970986

$(CH_3)_2NH$*Cl Pre-reaction adduct



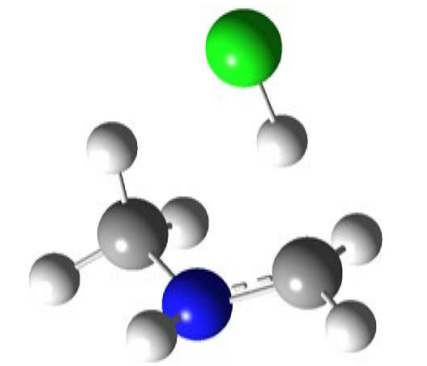
C	1.188107	1.231454	0.145511
H	2.266925	1.317551	-0.011947
H	0.979287	1.240967	1.212243
H	0.679913	2.073664	-0.312799
N	0.666380	0.000000	-0.409335
H	0.590055	0.000000	-1.416328
Cl	-1.609661	0.000000	0.044738
C	1.188106	-1.231455	0.145511
H	0.979284	-1.240968	1.212243
H	0.679911	-2.073664	-0.312800
H	2.266924	-1.317553	-0.011946

$(CH_3)_2NH$+Cl TSC



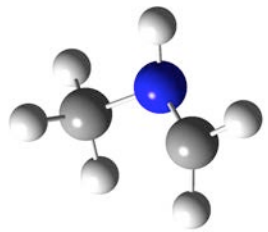
C	0.473323	0.668568	0.154546
H	0.631770	1.262271	-0.742810
H	0.467001	1.316466	1.037088
H	-0.604318	0.291190	0.075391
N	1.364022	-0.446189	0.179792
H	1.362712	-0.883823	1.090083
C	2.723574	-0.114958	-0.226683
H	3.343662	-1.005753	-0.164397
H	2.712607	0.212230	-1.264831
H	3.188020	0.675566	0.373945
Cl	-2.342999	-0.121558	-0.072364

CH_3NHCH_2*HCl Post-reaction adduct



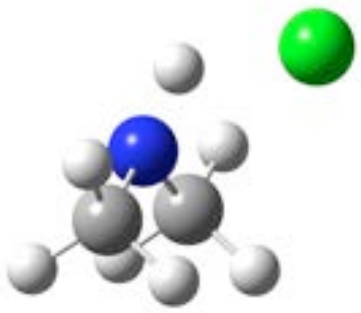
C	0.815778	1.225271	-0.251267
H	0.975669	1.250067	-1.320396
H	0.665045	2.164599	0.259883
H	-0.847319	0.511057	-0.167971
N	1.526501	0.271466	0.430888
H	1.375813	0.254220	1.427150
C	1.725791	-1.029568	-0.178963
H	2.455110	-1.592640	0.396423
H	0.798515	-1.601464	-0.244642
H	2.117965	-0.885602	-1.183205
Cl	-1.969160	-0.186748	0.023407

CH_3NHCH_2



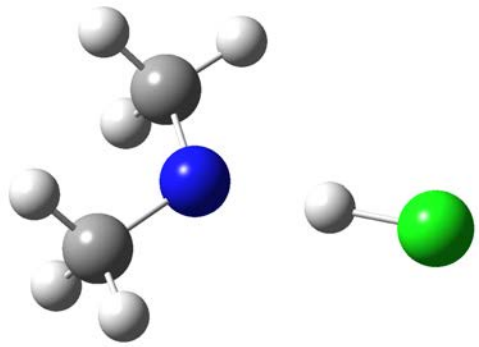
C	-1.179119	-0.188323	0.035508
H	-1.986185	0.467966	-0.280014
H	-1.358291	-0.502457	1.067435
H	-1.199770	-1.074383	-0.596156
N	0.093827	0.480858	-0.142957
C	1.241203	-0.255861	0.088499
H	1.220456	-1.281238	-0.246133
H	2.175133	0.280836	0.062128
H	0.119360	1.408373	0.249401

$(CH_3)_2NH+Cl$ TSN



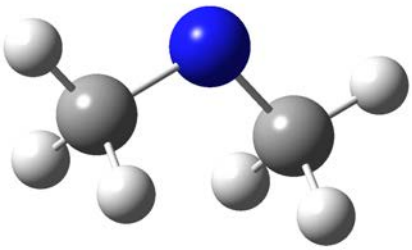
C	0.099792	1.233007	1.228113
H	-0.080670	2.305122	1.327128
H	1.177047	1.062077	1.228523
H	-0.347476	0.704092	2.062089
N	-0.499079	0.786896	0.000000
H	-0.898208	-0.204644	0.000000
Cl	0.099792	-1.661311	0.000000
C	0.099792	1.233007	-1.228113
H	1.177047	1.062077	-1.228523
H	-0.347476	0.704092	-2.062089
H	-0.080670	2.305122	-1.327128

$(CH_3)_2N*HCl$ Post-reaction adduct



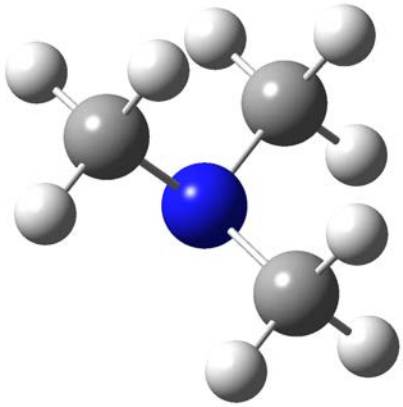
C	1.665436	1.197055	0.000001
H	2.314997	1.222989	-0.880489
H	2.315063	1.222955	0.880442
H	1.025223	2.073589	0.000038
N	0.873019	0.000002	0.000001
H	-0.822555	0.000003	0.000002
Cl	-2.152015	0.000002	0.000000
C	1.665424	-1.197059	-0.000001
H	2.314997	-1.222995	0.880480
H	1.025203	-2.073587	-0.000026
H	2.315039	-1.222971	-0.880451

$(CH_3)_2N$



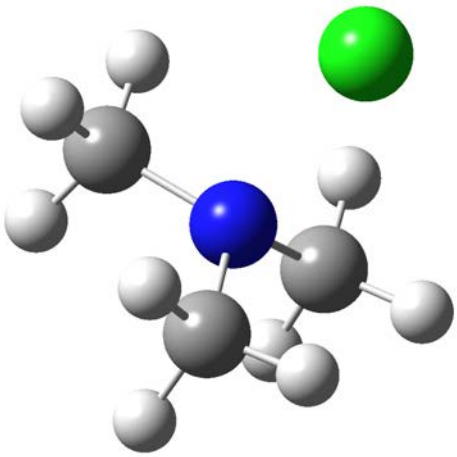
C	-1.190467	-0.175933	-0.000013
H	-2.092275	0.450755	-0.000480
H	-1.209125	-0.835262	0.890742
H	-1.208740	-0.836191	-0.890077
N	0.000000	0.650371	-0.000033
C	1.190467	-0.175934	-0.000017
H	1.208648	-0.836363	-0.889955
H	2.092275	0.450755	-0.000685
H	1.209217	-0.835089	0.890864

$(CH_3)_3N$



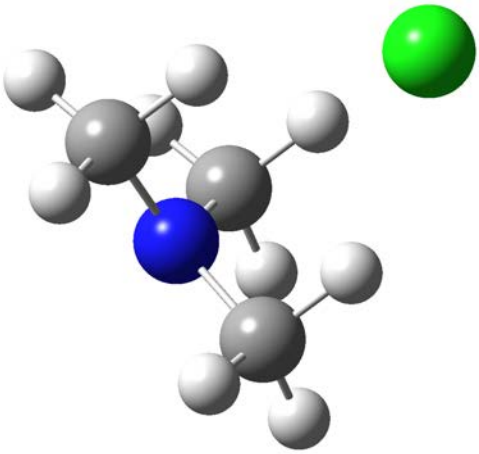
C	-0.658798	1.203275	0.065529
H	-0.689481	1.259320	1.165880
H	-1.681646	1.232959	-0.306033
H	-0.132752	2.080984	-0.306035
N	-0.000001	0.000000	-0.405852
C	-0.712668	-1.172173	0.065530
H	-0.226951	-2.072827	-0.306035
H	-0.745860	-1.226769	1.165880
H	-1.735810	-1.155459	-0.306034
C	1.371467	-0.031102	0.065530
H	1.435343	-0.032550	1.165880
H	1.868561	-0.925526	-0.306035
H	1.908596	0.839868	-0.306036

$(CH_3)_3N$*Cl Pre-reaction adduct N



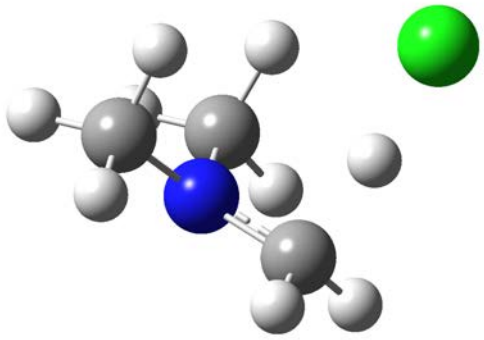
C	0.933460	0.763384	1.177278
H	2.023163	0.827999	1.277415
H	0.515423	0.280619	2.056138
H	0.515822	1.762851	1.094688
N	0.569843	-0.000050	0.000004
C	0.935233	-1.400695	0.072141
H	0.518195	-1.920955	-0.785555
H	2.025120	-1.518398	0.078196
H	0.518208	-1.830088	0.978754
C	0.933434	0.638385	-1.249487
H	2.023134	0.692363	-1.355763
H	0.515368	0.067881	-2.074083
H	0.515802	1.641051	-1.270014
Cl	-1.763053	-0.000554	0.000036

$(CH_3)_3N$*Cl Pre-reaction adduct 3H



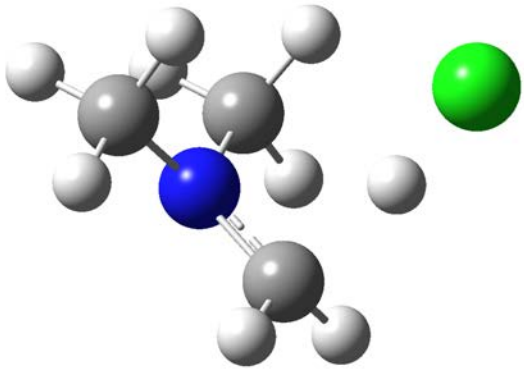
C	-0.946075	1.138356	0.808761
H	0.175503	1.139217	0.809423
H	-1.322717	1.002577	1.816982
H	-1.322644	2.045753	0.348726
N	-1.244260	0.000010	-0.000035
C	-0.946105	-1.269595	0.581432
H	-1.322693	-2.074856	-0.040293
H	0.175471	-1.270595	0.581927
H	-1.322753	-1.324893	1.597249
C	-0.945961	0.131253	-1.390239
H	0.175631	0.131336	-1.391204
H	-1.322521	-0.720829	-1.946084
H	-1.322506	1.072312	-1.776798
Cl	1.949876	-0.000010	0.000035

$(CH_3)_3N$+Cl TSC



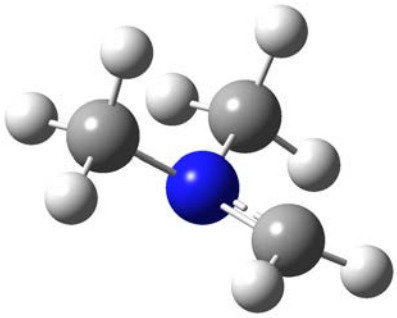
C	-0.953596	-1.093874	1.223668
H	0.120493	-1.271776	1.324849
H	-1.479472	-2.045198	1.199090
H	-1.298620	-0.511679	2.073292
N	-1.224441	-0.362896	0.000000
C	-0.953596	-1.093874	-1.223668
H	-1.298620	-0.511679	-2.073292
H	0.120493	-1.271776	-1.324849
H	-1.479472	-2.045198	-1.199090
C	-0.953596	0.981926	0.000000
H	0.469739	1.005210	0.000000
H	-1.213502	1.492897	-0.920192
H	-1.213502	1.492897	0.920192
Cl	1.941663	0.790677	0.000000

$(CH_3)_2NCH_2$*Cl Post-reaction adduct



C	1.366119	1.222291	-0.528317
H	0.501533	1.329155	-1.189103
H	2.273842	1.205073	-1.127677
H	1.401694	2.072937	0.146770
N	1.278938	-0.000001	0.246721
C	1.366077	-1.222333	-0.528260
H	1.401626	-2.072948	0.146867
H	0.501487	-1.329199	-1.189040
H	2.273800	-1.205171	-1.127622
C	0.463081	0.000039	1.345940
H	-1.028919	0.000027	0.607884
H	0.438396	-0.925006	1.906772
H	0.438436	0.925107	1.906733
Cl	-2.136831	0.000003	-0.208518

$(CH_3)_2NCH_2$



C	-1.211557	-0.655552	0.042247
H	-1.319936	-0.863875	1.113356
H	-1.201039	-1.600945	-0.497190
H	-2.072049	-0.077645	-0.286121
N	0.000000	0.081369	-0.246154
C	1.211557	-0.655552	0.042247
H	2.072049	-0.077645	-0.286120
H	1.319936	-0.863875	1.113356
H	1.201040	-1.600944	-0.497191
C	0.000000	1.415078	0.101170
H	0.930037	1.945751	-0.025496
H	-0.930037	1.945751	-0.025496

Table S9. Calculated wave numbers (cm^{-1}) of the saddle points to H-abstraction in CH_3NH_2, $(CH_3)_2NH$ and $(CH_3)_3N$ by Cl atoms. Results from MP2/cc-pVTZ calculations.

CH_3NH_2		$(CH_3)_2NH$		$(CH_3)_3N$
TSC	TSN	TSC	TSN	TSC
-318	-450	-327	-447	-309
67	130	50	138	82
125	175	74	161	98
232	612	204	162	177
695	715	240	233	202
970	948	394	405	329
1088	1035	753	510	410
1164	1060	970	945	443
1321	1264	1032	1043	518
1327	1401	1084	1089	557
1415	1426	1136	1098	858
1490	1473	1180	1203	1021
1659	1502	1258	1246	1064
2179	1520	1289	1422	1079
3078	3056	1361	1440	1108
3186	3128	1455	1449	1135
3576	3198	1479	1476	1141
3680	3523	1509	1495	1155
		1513	1498	1194
		1536	1522	1354
		1998	2689	1434
		3022	3060	1440
		3046	3061	1465
		3127	3134	1491
		3168	3134	1498
		3176	3210	1511
		3592	3210	1514
				1560
				3053
				3055
				3133
				3152
				3153
				3195
				3197
				3245

Table S10. Calculated rate coefficients (/10^{-10} cm^3 $molecule^{-1}$ s^{-1}) and branching ratios for the Cl atom reaction with CH_3NH_2, $(CH_3)_2NH$ and $(CH_3)_3N$.

	CH_3NH_2		$(CH_3)_2NH$		$(CH_3)_3N$
T/K	k_{tot}	k_C/k_{tot}	k_{tot}	k_C/k_{tot}	k_{tot}
200	4.11	0.06	4.43	0.00	4.53
210	4.12	0.06	4.45	0.00	4.55
220	4.12	0.06	4.47	0.00	4.57
230	4.13	0.07	4.49	0.00	4.59
240	4.13	0.07	4.51	0.00	4.61
250	4.14	0.07	4.53	0.00	4.63
260	4.14	0.08	4.55	0.00	4.66
270	4.15	0.08	4.58	0.00	4.68
280	4.15	0.08	4.60	0.00	4.70
290	4.16	0.09	4.62	0.00	4.72
300	4.16	0.09	4.64	0.00	4.74
310	4.16	0.09	4.66	0.00	4.76
320	4.17	0.10	4.68	0.00	4.78
330	4.17	0.10	4.70	0.00	4.80
340	4.17	0.10	4.71	0.00	4.82
350	4.17	0.11	4.73	0.00	4.84
360	4.18	0.11	4.75	0.00	4.86
370	4.18	0.11	4.77	0.00	4.88
380	4.18	0.12	4.79	0.00	4.90
390	4.18	0.12	4.80	0.00	4.92
400	4.18	0.13	4.82	0.00	4.94
410	4.18	0.13	4.84	0.00	4.96
420	4.18	0.13	4.85	0.00	4.97
430	4.18	0.14	4.87	0.00	4.99
440	4.18	0.14	4.88	0.00	5.01
450	4.18	0.15	4.90	0.00	5.03
460	4.18	0.15	4.91	0.00	5.04
470	4.17	0.16	4.93	0.00	5.06
480	4.17	0.16	4.94	0.00	5.08
490	4.17	0.17	4.96	0.00	5.09
500	4.17	0.17	4.97	0.00	5.11
510	4.17	0.17	4.98	0.00	5.12
520	4.17	0.18	5.00	0.00	5.14
530	4.17	0.18	5.01	0.00	5.15
540	4.16	0.19	5.02	0.00	5.17
550	4.16	0.19	5.03	0.00	5.18
560	4.16	0.20	5.05	0.00	5.19
570	4.16	0.20	5.06	0.00	5.21
580	4.16	0.21	5.07	0.00	5.22
590	4.15	0.21	5.08	0.00	5.24
600	4.15	0.22	5.09	0.00	5.25