Supporting Information

Stereoelectronic Substituent Effects on Silylene Insertion into Si–Cl Bond.

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Contents

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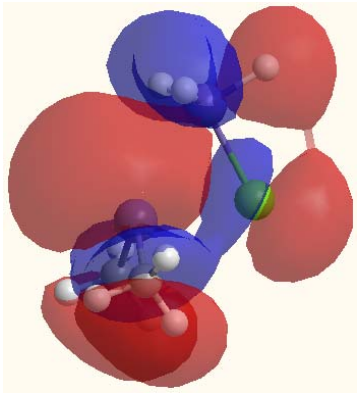
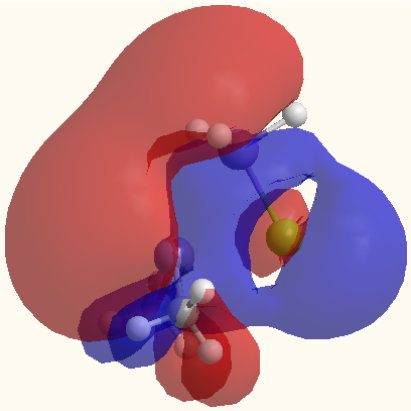
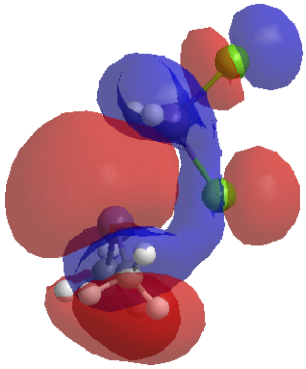
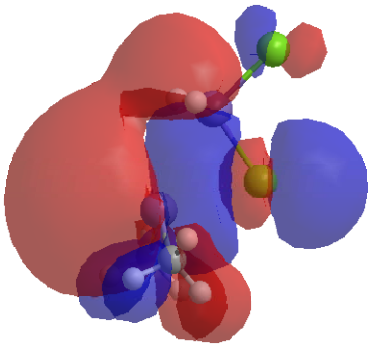
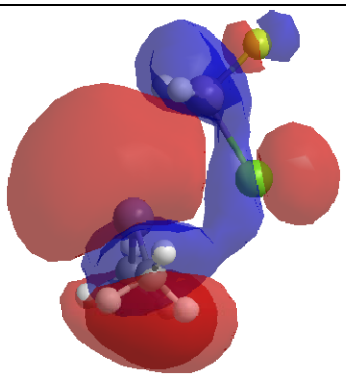
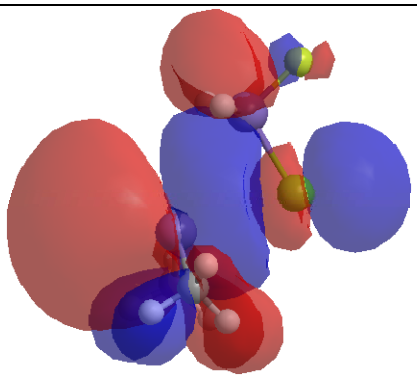
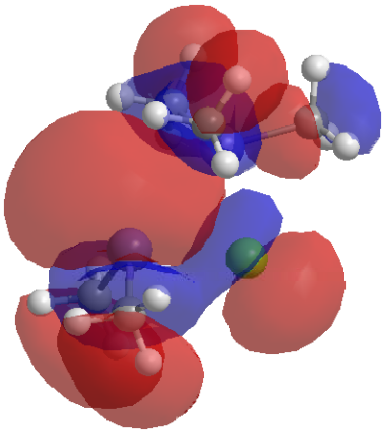
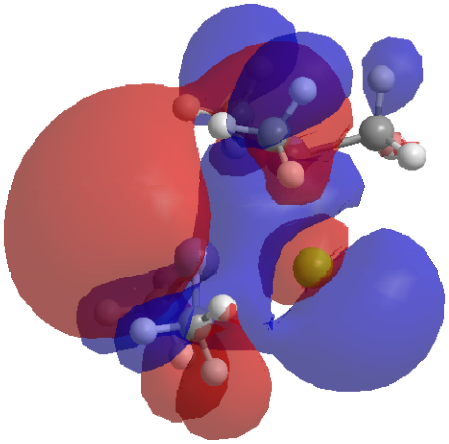
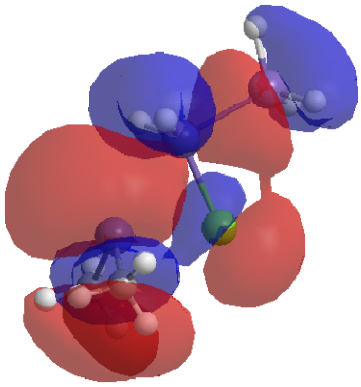
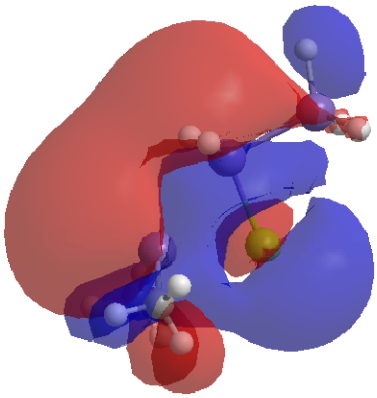
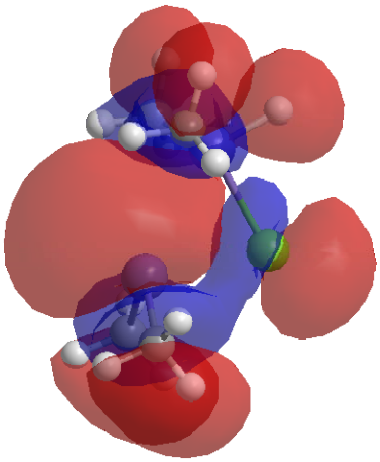
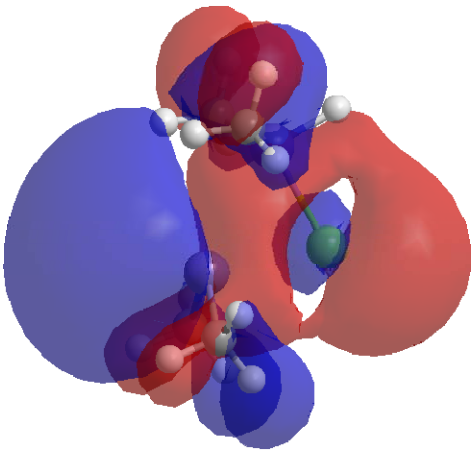
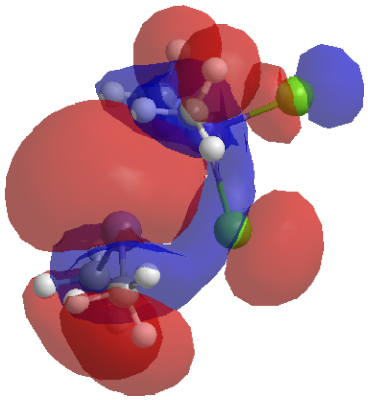
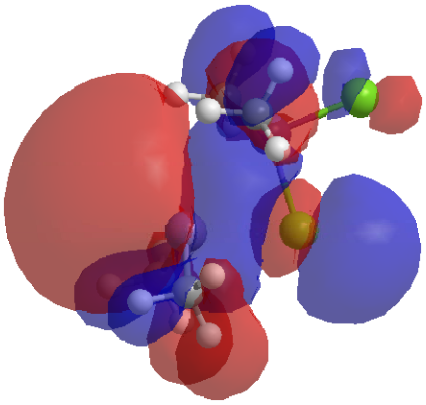
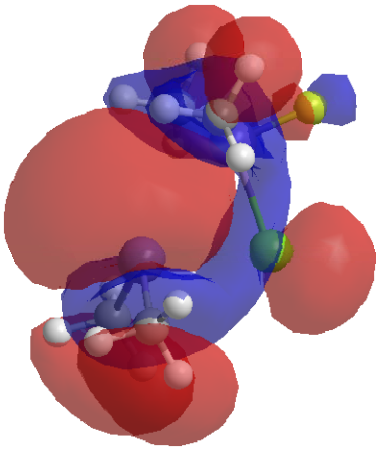
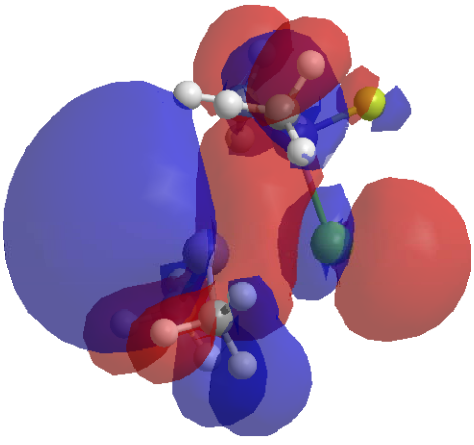
1. Computational details

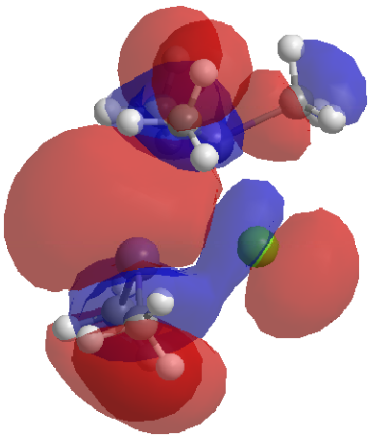
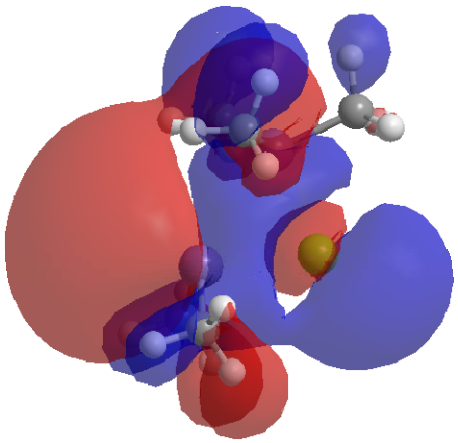
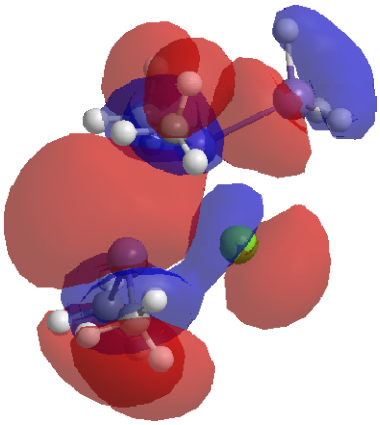
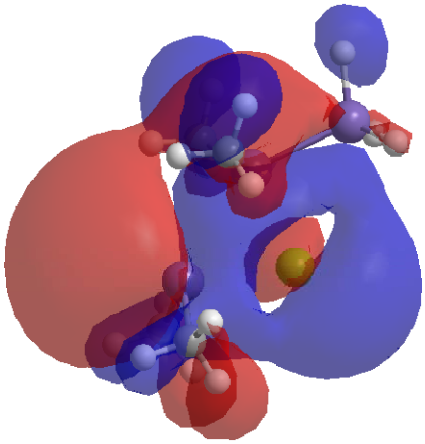
All calculations were performed on an SGI Altix 450 sever using Gaussian 03 package[S1] at B3LYP/6-31++G(d,p) level. All the structures obtained were verified, by examination of their Hessian matrix, as minima (all frequencies real) or transition states (one imaginary frequency). Zero-point vibrational energies were incorporated into total energies. At every transition state, the transition vector was animated with the GaussView program, and if necessary, the intrinsic reaction coordinates (IRC) were computed to connect the corresponding minima.

2. Kohn-Sham HOMO and LUMO and their energy levels for the insertion via transition state A

Chlorosilane	HOMO	LUMO
2a		
	-5.713 eV	-1.731 eV
2b		
	-6.061 eV	-1.965 eV

2c		
	-5.934 eV	-1.979 eV
2d		
	-5.394 eV	-1.211 eV
2e		
	-5.684 eV	-1.803 eV

3a		
	-5.537 eV	-1.330 eV
3b		
	-5.881 eV	-1.573 eV
3c		
	-5.787 eV	-1.492 eV

3d		
	-5.394 eV	-1.211 eV
3e		
	-5.518 eV	-1.467 eV

3. Activation parameters for the insertion of silylene 1 into YMe_2Si-Cl (3a-3e)

Table S1. Activation Parameters of the Insertion of Silylene **1** into **3a-3e** Calculated at the B3LYP/6-31++G(d,p) + ZPE level

Y	TS	$\Delta G^{\neq a}$	$\Delta H^{\neq a}$	$\Delta S^{\neq b}$
H(**3a**)	**A**	18.4	6.7	−39.2
	B	19.6	7.3	−41.3
Cl(**3b**)	**A**	17.4	5.6	−39.6
	B	21.4	9.2	−40.9
F(**3c**)	**A**	16.3	4.0	−41.3
	B	20.7	8.7	−40.2
Me(**3d**)	**A = B**	21.6	8.9	−42.6
SiH_3(**3e**)	**A**	20.9	8.6	−41.3
	B	18.6	5.5	−43.9

a. kcal mol^{-1}, at 298 K.

b. cal mol^{-1} K^{-1}, at 298 K.

4. A plot of $\Delta G^{\neq}_{A\text{-}B}(Y)$ for the insertions of 3a - 3e vs. those of 2a - 2e.

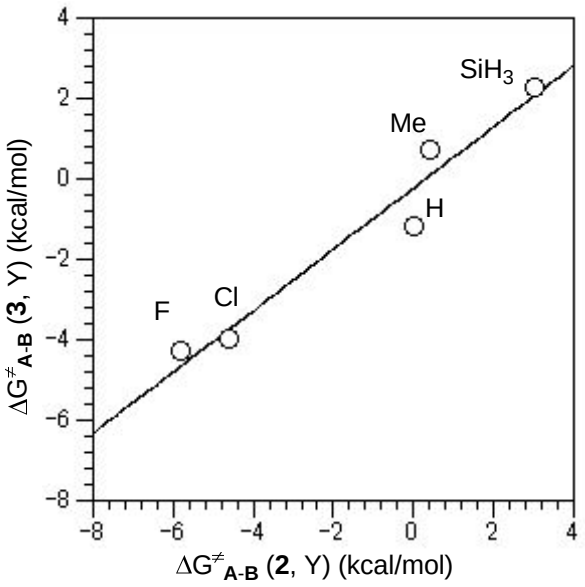


Figure S1. A plot of $\Delta G^{\neq}_{A\text{-}B}(Y)$ for the insertions of **3a-3e** vs. those of **2a - 2e**. The linear relationship obeys the following equation: $\Delta G^{\neq}_{A\text{-}B}(\mathbf{3}, Y) = 0.764\Delta G^{\neq}_{A\text{-}B}(\mathbf{2}, Y) - 2.29$ (correlation coefficient = 0.976).

5. Imaginary frequency and Cartesian coordinates of calculated transition structures

Table S2. Imaginary frequency

2a	**A=B**	181i	**3a**	**A**	173i
				B	-194i
2b	**A**	85i	**3b**	**A**	125i
	B	156i		**B**	-170i
2c	**A**	27i	**3c**	**A**	113i
	B	149i		**B**	-169i
2d	**A**	200i	**3d**	**A=B**	187i
	B	176i			
2e	**A**	197i	**3d**	**A**	177i
	B	154i		**B**	-172i

Table S3. Cartesian coordinates of calculated transition structures (Å)

2a-A(B)

Si	-0.88523100	0.00134600	-0.59639400
Si	1.89294200	0.00178800	-0.73134300
H	1.80947500	-1.25821300	-1.49945200
H	1.80911000	1.26554300	-1.49322100
Cl	0.86955400	-0.00323300	1.24549200
C	-1.91008100	1.49965800	-0.00111800
H	-1.35148300	2.43800300	-0.07434700
H	-2.78916000	1.59169900	-0.65549000
H	-2.27527600	1.38357600	1.02620200
C	-1.91075500	-1.49918000	-0.00789400
H	-2.79005900	-1.58768200	-0.66244800
H	-1.35268500	-2.43747400	-0.08563400
H	-2.27561300	-1.38768000	1.02005400
H	3.25032700	0.00045200	-0.10663200

2b-A

Si	-1.71407800	0.00000000	-0.62959500
C	-2.72020900	1.49473900	0.00492000
H	-2.16463000	2.43441400	-0.07328100
H	-3.60798800	1.58994000	-0.63832700
H	-3.07653300	1.37569900	1.03448800
C	-2.72021000	-1.49473800	0.00492200
H	-3.60798200	-1.58994600	-0.63833200
H	-2.16462800	-2.43441300	-0.07327000
H	-3.07654200	-1.37569400	1.03448600
Si	1.13916300	-0.00000100	-0.66444400
Cl	0.15045200	0.00000100	1.24681000
H	0.99713300	1.28607900	-1.35627100
H	0.99713300	-1.28608100	-1.35626900
Cl	3.16692200	0.00000000	-0.06302900

2b-B

Si	-1.23478800	0.54605800	-0.46111200
Si	1.39614800	-0.72491000	-0.48883100
H	1.05419400	-0.98313600	-1.89608300
Cl	-0.08694600	-1.44808700	0.90862400
C	-1.82324700	1.58460100	1.02966100
H	-0.98763100	2.02679700	1.58037200
H	-2.42864300	2.41488700	0.63545900

H	-2.45628200	1.02383800	1.72725700
C	-2.82277400	-0.39021000	-0.97232700
H	-3.48346300	0.33065900	-1.47728600
H	-2.62189700	-1.19685700	-1.68427800
H	-3.37818400	-0.79765200	-0.11926900
H	2.47314000	-1.66287600	-0.09536100
Cl	2.28964400	1.10584700	-0.06836500

2c-A

0 1

Si	1.45245100	0.02802700	-0.68533900
Si	-1.64592500	0.02750200	-0.62800400
H	-1.43273500	1.32789600	-1.27255200
H	-1.43774200	-1.20915000	-1.38910100
Cl	-0.61363400	-0.05854500	1.21966800
C	2.42322300	-1.47640300	-0.00447900
H	1.89786600	-2.42322700	-0.16385800
H	3.36557400	-1.53236400	-0.57211800
H	2.69113100	-1.38920200	1.05481400
C	2.41148900	1.48070200	0.11407200
H	3.34806000	1.59535100	-0.45437000
H	1.87420700	2.43121700	0.03791000
H	2.68948000	1.30899300	1.16034500
F	-3.20707800	0.00917300	-0.15624100

2c-B

0 1

Si	-1.08613300	0.43758200	-0.44281900
Si	1.74435900	-0.07911900	-0.48881500
H	1.51217000	-0.45921200	-1.89133900
Cl	0.54870500	-1.23697200	0.88636000
C	-1.91291800	1.25865200	1.06979800
H	-1.20599900	1.86208500	1.64705100
H	-2.68844900	1.94175600	0.69120200
H	-2.40750900	0.54492400	1.73884300
C	-2.38889000	-0.85084700	-0.98811500
H	-3.21216300	-0.30438300	-1.47277200
H	-1.99454500	-1.55906000	-1.72345000
H	-2.82052400	-1.41000100	-0.14969400
H	3.07325700	-0.58234100	-0.07310800
F	1.89016100	1.50327300	-0.14245200

2d-A

Si	1.27241400	0.00009300	-0.59329400

Si	-1.48083100	0.00012300	-0.75030000
H	-1.36989400	1.26277200	-1.51648000
H	-1.36991100	-1.26226200	-1.51691600
Cl	-0.41426500	-0.00022200	1.25309500
C	2.30383500	-1.50251700	-0.01838400
H	1.74207000	-2.43921800	-0.08978100
H	3.17519800	-1.59300500	-0.68277100
H	2.67900900	-1.39233000	1.00606000
C	2.30379400	1.50255200	-0.01791500
H	3.17510800	1.59332000	-0.68232800
H	1.74197600	2.43924900	-0.08894900
H	2.67904100	1.39202600	1.00646600
C	-3.22608200	0.00000600	-0.01167800
H	-3.94615800	0.00017300	-0.84101600
H	-3.41769800	-0.88765200	0.60046400
H	-3.41767500	0.88743400	0.60080400

2d-B

Si	-0.98320100	0.47733500	-0.41982600
Si	1.69180000	-0.30746100	-0.47399200
H	1.44031400	-0.72889500	-1.87010200
Cl	0.22528200	-1.23255600	0.96274400
C	-1.87753500	1.39515400	0.99950900
H	-1.17886100	1.93067900	1.64990800
H	-2.54725400	2.14429300	0.55303900
H	-2.49239600	0.72782300	1.61526700
C	-2.33961000	-0.66102800	-1.13667000
H	-3.04167900	-0.03640500	-1.70770700
H	-1.93063500	-1.40461500	-1.82802200
H	-2.91499000	-1.17900900	-0.36028800
H	2.78453800	-1.20798500	0.00703800
C	2.33477800	1.43247800	-0.14737000
H	3.42350700	1.43675700	-0.28442500
H	1.86901100	2.16586100	-0.80864400
H	2.13245900	1.72709300	0.88794400

2e-A

Si	1.72198400	0.00012700	-0.58465600
Si	-1.05027900	0.00019100	-0.81939600
H	-0.91464400	1.25278200	-1.60059600
H	-0.91466400	-1.25202700	-1.60119900
Cl	-0.05906600	-0.00028900	1.21574800
C	2.73092900	-1.50035300	0.03107900
H	2.17653200	-2.43913100	-0.06439300

H	3.63042900	-1.58681300	-0.59552000
H	3.06228500	-1.38863600	1.07039200
C	2.73090800	1.50035800	0.03172400
H	3.63037800	1.58713200	-0.59487600
H	2.17647900	2.43916200	-0.06330000
H	3.06231500	1.38818000	1.07097100
Si	-3.26953500	-0.00000600	0.02918200
H	-3.54613200	1.20796500	0.85409500
H	-4.21414900	0.00024500	-1.12548200
H	-3.54611700	-1.20834700	0.85355600

2e-B

Si	1.06838300	0.61021000	0.37427200
Si	-1.26004500	-0.95143800	0.44955900
H	-0.92444700	-1.25705700	1.86004600
Cl	0.46761000	-1.48640200	-0.87802500
C	1.71762300	1.63216800	-1.10236300
H	0.92414900	1.88369900	-1.81240100
H	2.12046100	2.57794000	-0.71232000
H	2.52744700	1.12468700	-1.64008500
C	2.66020000	-0.00881200	1.22771200
H	3.11466000	0.84340300	1.75322300
H	2.45609000	-0.78112600	1.97571700
H	3.40111100	-0.39131300	0.51571800
H	-2.06366400	-2.12212800	-0.02904600
Si	-2.48941000	1.00817600	0.05810900
H	-3.94039100	0.72564100	-0.14701800
H	-2.32331000	1.90903700	1.22653200
H	-1.97340400	1.67864900	-1.16319800

3a-A

Si	-1.11673300	0.00000300	-0.62001100
C	-2.28466700	1.49739600	-0.38665900
H	-1.73679800	2.43960000	-0.28490300
H	-2.91484300	1.58191400	-1.28369700
H	-2.95132500	1.38278000	0.47647300
C	-2.28466300	-1.49739500	-0.38667300
H	-2.91483600	-1.58190800	-1.28371300
H	-1.73679200	-2.43959800	-0.28492400
H	-2.95132300	-1.38278800	0.47645800
Si	1.60003700	0.00000200	0.11264800
Cl	-0.09321200	-0.00000500	1.63908700
C	1.91092100	-1.62679000	-0.78648100
H	1.54650300	-1.60011900	-1.81572600

H	2.99003500	-1.82864100	-0.77823400
H	1.41858200	-2.45652200	-0.26858700
C	1.91092400	1.62679100	-0.78648200
H	2.99003900	1.82863900	-0.77823900
H	1.54650300	1.60012200	-1.81572700
H	1.41859000	2.45652600	-0.26858700
H	2.59891900	0.00000300	1.22577500

3a-B

0 1

Si	1.36839400	0.37704400	-0.40570000
C	2.50967900	-0.96070500	-1.15483400
H	1.98029900	-1.60511500	-1.86388800
H	3.31277100	-0.45482300	-1.70959600
H	2.98060300	-1.59004600	-0.39018700
C	2.41327400	1.09880200	1.02488900
H	3.20686000	1.72225600	0.58888600
H	1.82402000	1.73944400	1.68856700
H	2.89649900	0.31927500	1.62620000
Si	-1.38838700	0.11829500	-0.50689300
Cl	-0.08119000	-1.10868500	0.93700000
C	-1.64876400	1.94711000	-0.12067200
H	-1.10348300	2.57564800	-0.82858900
H	-2.71926400	2.18529100	-0.15607600
H	-1.28817600	2.18519100	0.88562700
H	-1.18717900	-0.27770900	-1.92171000
C	-2.98562500	-0.76398200	0.01666100
H	-3.81202900	-0.38544300	-0.60002800
H	-2.92327900	-1.84637700	-0.13513200
H	-3.23889700	-0.58204500	1.06697400

3b-A

Si	-1.81953800	0.00000000	0.46661400
C	-2.87826700	-1.49819300	-0.07003900
H	-2.32039200	-2.43905400	-0.03078100
H	-3.71593200	-1.58854200	0.63663700
H	-3.30608500	-1.38343300	-1.07288300
C	-2.87826600	1.49819400	-0.07004000
H	-3.71593200	1.58854300	0.63663600
H	-2.32039000	2.43905500	-0.03078100
H	-3.30608400	1.38343400	-1.07288400
Si	0.99592000	0.00000000	0.40994600
Cl	-0.20770800	0.00000000	-1.45340700
C	1.06073900	1.64757600	1.31127100

H	0.43114700	1.62931300	2.20317200
H	2.09799300	1.86586700	1.58604200
H	0.71184400	2.45192100	0.65603700
C	1.06073900	-1.64757500	1.31127200
H	2.09799300	-1.86586600	1.58604300
H	0.43114700	-1.62931300	2.20317300
H	0.71184500	-2.45192100	0.65603800
Cl	2.88675700	0.00000000	-0.61265600

3b-B

Si	1.62388300	0.24767600	0.48696600
C	2.47228100	1.58145000	-0.58477200
H	1.75840900	2.32353400	-0.95466400
H	3.19425900	2.11241400	0.05297100
H	3.02763300	1.16447500	-1.43317000
C	2.98377800	-1.08837100	0.67060100
H	3.73985700	-0.70480100	1.37126200
H	2.59741100	-2.02231300	1.09084200
H	3.49431800	-1.31044400	-0.27415600
Si	-1.18844300	-0.27162900	0.15967100
Cl	0.30526900	-0.90284600	-1.37662900
C	-1.17593800	-1.20603100	1.79179000
H	-0.80806100	-0.57174300	2.59967800
H	-2.19224500	-1.55076100	2.01999800
H	-0.52266500	-2.08187600	1.72076000
C	-2.69775700	-0.84672500	-0.81582900
H	-3.60947300	-0.60643900	-0.25672600
H	-2.76213100	-0.36194900	-1.79406900
H	-2.66544900	-1.93143900	-0.97084100
Cl	-1.53128100	1.79900900	0.28277300

3c-A

Si	1.49258200	0.00000000	-0.57339300
C	2.59823800	-1.49350200	-0.11666600
H	2.04621100	-2.43867600	-0.11655800
H	3.38088500	-1.57577300	-0.88509100
H	3.10037400	-1.37794600	0.85099100
C	2.59823800	1.49350200	-0.11666400
H	3.38088500	1.57577500	-0.88508900
H	2.04621200	2.43867700	-0.11655400
H	3.10037500	1.37794500	0.85099300
Si	-1.34000200	0.00000000	-0.19079200
Cl	0.05283900	0.00000000	1.51886100
C	-1.49336400	1.64492400	-1.07517500

H	-1.07602500	1.59464000	-2.08309600
H	-2.55396700	1.91742700	-1.12417800
H	-0.96859900	2.43406900	-0.52806000
C	-1.49336300	-1.64492400	-1.07517400
H	-2.55396600	-1.91742600	-1.12418000
H	-1.07602300	-1.59464100	-2.08309500
H	-0.96860000	-2.43406900	-0.52805800
F	-2.68340500	0.00000000	0.77244500

3c-B

Si	1.50425100	0.16701500	-0.50795000
C	2.49045000	-1.46676900	-0.58058700
H	1.86057900	-2.31188700	-0.87446800
H	3.26544000	-1.35507800	-1.35322200
H	2.99803100	-1.70785200	0.36083700
C	2.70363200	1.35212000	0.39774400
H	3.50499100	1.62183900	-0.30567900
H	2.21843600	2.28268600	0.70843700
H	3.17687300	0.89053900	1.27259900
Si	-1.31033000	0.07407500	-0.23156300
Cl	0.02438700	-0.40297000	1.50004200
C	-1.44413100	1.89642200	-0.66456800
H	-1.09243700	2.05974000	-1.68620900
H	-2.48626900	2.22823100	-0.57817900
H	-0.82979800	2.50760300	0.00318600
C	-2.90884000	-0.48198700	0.58923100
H	-3.74284000	-0.35336200	-0.11131300
H	-2.87012500	-1.53709700	0.87651800
H	-3.12188900	0.10974600	1.48628900
F	-1.22857100	-0.97317600	-1.48858300

3d-A(B)

Si	-1.46410500	0.00000000	-0.51869600
C	-2.58815400	1.49820400	-0.12472700
H	-2.03388200	2.44213500	-0.11360900
H	-3.34789800	1.57495400	-0.91555000
H	-3.11411900	1.38915900	0.83154900
C	-2.58815700	-1.49820300	-0.12472400
H	-3.34790000	-1.57495400	-0.91554800
H	-2.03388700	-2.44213500	-0.11360200
H	-3.11412400	-1.38915400	0.83155100
Si	1.32953700	0.00000000	-0.24702000
Cl	-0.15692400	0.00000000	1.55179400
C	1.44609100	-1.62345700	-1.20462400

H	0.95007200	-1.55022400	-2.17522600
H	2.50209100	-1.88781800	-1.34777600
H	0.97615600	-2.43949400	-0.64551900
C	1.44608900	1.62345800	-1.20462100
H	2.50209000	1.88781900	-1.34777400
H	0.95007000	1.55022700	-2.17522300
H	0.97615600	2.43949400	-0.64551300
C	2.82606200	0.00000000	0.92551900
H	2.84281500	-0.88544800	1.56991400
H	3.74961300	0.00000000	0.33100300
H	2.84281500	0.88544700	1.56991300

3e-A

Si	-1.85313700	0.00000000	0.41100500
C	-2.90689000	-1.49698900	-0.14416500
H	-2.35631100	-2.44085500	-0.08023100
H	-3.76967800	-1.57661000	0.53279100
H	-3.29540200	-1.38509800	-1.16364200
C	-2.90689000	1.49698900	-0.14416600
H	-3.76967800	1.57661000	0.53279100
H	-2.35631100	2.44085500	-0.08023100
H	-3.29540200	1.38509800	-1.16364200
Si	0.97160300	0.00000000	0.50534000
Cl	-0.24296800	0.00000000	-1.47161600
C	0.95766500	1.62007700	1.48382300
H	0.29765100	1.54842800	2.35181500
H	1.97737000	1.85864900	1.81339200
H	0.61207400	2.44836200	0.85684600
C	0.95766500	-1.62007700	1.48382300
H	1.97737000	-1.85864800	1.81339200
H	0.29765100	-1.54842800	2.35181500
H	0.61207400	-2.44836200	0.85684600
Si	3.03025000	0.00000000	-0.69079000
H	3.16642300	1.20622000	-1.55359200
H	4.17486400	0.00000000	0.26905600
H	3.16642400	-1.20622000	-1.55359200

3e-B

Si	1.52041700	0.35459500	0.38287200
C	2.52719700	1.44455700	-0.82062300
H	1.88535000	2.07455800	-1.44358200
H	3.16590100	2.11273900	-0.22599000
H	3.18031700	0.85152700	-1.47219500
C	2.81439600	-0.88159500	1.05719500

H	3.47872400	-0.33994500	1.74527300
H	2.35505800	-1.69850300	1.62244100
H	3.43636300	-1.31005400	0.26209800
Si	-1.19822600	-0.31784200	0.14485500
Cl	0.46337100	-1.10155800	-1.27814000
C	-1.17310400	-1.25197000	1.78952000
H	-0.71950500	-0.66406400	2.59050300
H	-2.20261500	-1.51209800	2.06578600
H	-0.61321000	-2.18827100	1.69025100
C	-2.58468500	-1.11458000	-0.88933300
H	-3.54930500	-0.90247000	-0.40937300
H	-2.62401500	-0.71200000	-1.90682200
H	-2.47035500	-2.20202100	-0.95899900
Si	-1.58731000	1.99868400	0.22890900
H	-3.01555100	2.35822700	-0.03302100
H	-1.21497900	2.49073200	1.58093300
H	-0.76063200	2.69353300	-0.79238000

6. Dependence of activation parameters of the insertion of silylene 1 into 2a-2e on the theoretical methods

Table S4. Activation Parameters for the Insertion of **1** into **2a-2e** at Various Calculation Methods[a]

		B3LYP		MP2		BMK	
Y	TS	$\Delta G^{\neq b}$	$\Delta S^{\neq c}$	$\Delta G^{\neq b}$	$\Delta S^{\neq c}$	$\Delta G^{\neq b}$	$\Delta S^{\neq c}$
H(**2a**)	**A=B**	15.3	-39.6	10.5	-13.1	4.2	-11.1
Cl(**2b**)	**A**	11.1	-37.9	7.2	-16.4	---	---
	B	15.7	-36.9	10.1	-12.7	5.2	-10.7
F(**2c**)	**A**	9.8	-37.2	4.3	-2.1	---	---
	B	15.6	-38.3	9.9	-11.4	4.8	-10.4
Me(**2d**)	**A**	17.5	-40.6	12.8	-16.8	6.2	-11.4
	B	17.1	-39.9	11.2	-11.4	4.9	-7.4
SiH_3(**2e**)	**A**	17.2	-39.6	12.8	-15.8	6.6	-12.4
	B	14.2	-40.9	7.9	-14.4	0.7	-8.7

a. at 6-31++G(d,p) +ZPE. b. kcal mol^{-1}, at 298 K. c. cal mol^{-1} K^{-1}, at 298 K.

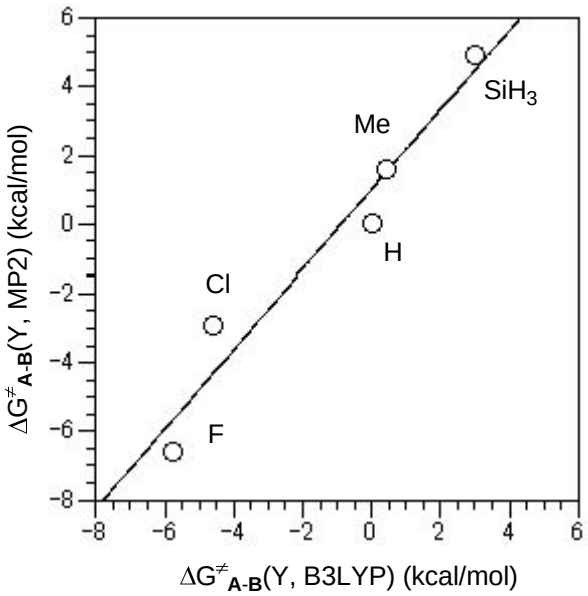


Figure S2. A plot of $\Delta G^{\neq}_{A\text{-}B}(Y)$ calculated at MP2/6-31++G(d,p) +ZPE level vs. $\Delta G^{\neq}_{A\text{-}B}(Y)$ calculated at B3LYP/6-31++G(d,p) +ZPE level. The least square linear line is: $\Delta G^{\neq}_{A\text{-}B}(Y, MP2) = 1.16\Delta G^{\neq}_{A\text{-}B}(Y, B3LYP) + 1.02$, correlation coefficient = 0.973.

7. Reference

S1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; N. Rega; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision D.01*; Gaussian, Inc., Wallingford CT, 2004.