Supporting Information for

Mechanism and Selectivity of Methyl and Phenyl Migrations in Hypervalent Silylated Iminoquinones

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I. X-ray Crystallography of Cl(Ph)Si(ON[Ph]O)

Table S1. Crystallographic details for Cl(Ph)Si(ON[Ph]O).

Empirical formula	$C_{40}H_{50}ClNO_2Si$
Formula weight	640.35
Temperature	120(2) K
Wavelength	0.71073 Å (Mo Kα)
Crystal system	Monoclinic
Space group	*C*2/*c*
a (Å)	37.394(2)
b (Å)	10.6766(6)
c (Å)	18.4173(10)
α (deg)	90
β (deg)	101.1022(17)
γ (deg)	90
Volume ($Å^3$)	7215.4(7)
Z	8
Density (calculated)	1.179 g cm^{-3}
Absorption coefficient (μ)	0.173 mm^{-1}
Crystal size	0.148 × 0.106 × 0.059 mm
Reflections collected	84580
Independent reflections	7409 [R_{int} = 0.0327]
Data / restraints / parameters	7409 / 0 / 591
Goodness-of-fit on F^2	1.051
Final *R* indices [$I > 2\sigma(I)$]	$R1$ = 0.0342, $wR2$ = 0.0938
R indices (all data)	$R1$ = 0.0414, $wR2$ = 0.1041
Largest diff. peak and hole	0.469 and –0.463 e^- $Å^{-3}$

Table S2. Selected bond distances (Å) and angles (º) in Cl(Ph)Si(ON[Ph]O).

Si-O1	1.6318(10)	O1-Si-O2	114.35(5)
Si-O2	1.6304(10)	O1-Si-C41	116.68(6)
Si-C41	1.8423(14)	O1-Si-Cl	101.13(4)
Si-Cl	2.0553(5)	O1-Si-N	73.02(4)
Si-N	2.7147(12)	O2-Si-C41	114.31(6)
O1-C12	1.3742(16)	O2-Si-Cl	99.68(4)
O2-C22	1.3706(16)	O2-Si-N	73.35(4)
N-C31	1.4277(17)	C41-Si-Cl	107.93(5)
N-C21	1.4457(17)	C41-Si-N	84.83(5)
N-C11	1.4505(17)	Cl-Si-N	167.21(3)
		C12-O1-Si	128.63(9)
		C22-O2-Si	132.83(9)
		C31-N-C21	118.06(11)
		C31-N-C11	117.55(11)
		C21-N-C11	112.06(10)

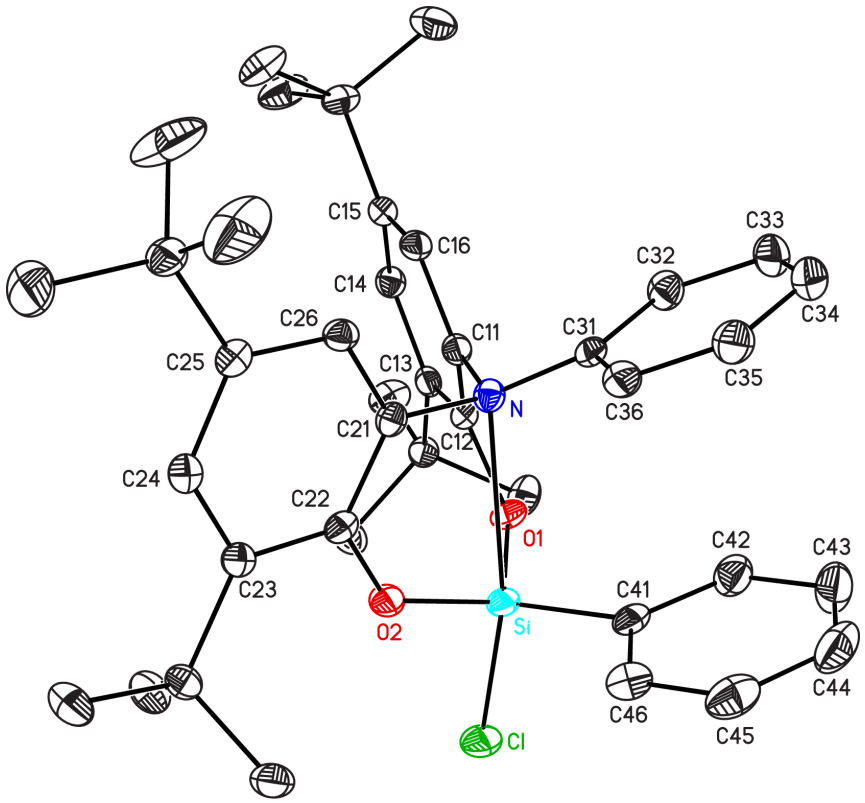


Figure S1. Thermal ellipsoid plot of the thermodynamic isomer of Cl(Ph)Si(ON[Ph]O), with hydrogen atoms and minor component of disordered *tert*-butyl group omitted for clarity.

II. Isomerization Reactions of Ph(Cl)Si(ON[R]O)

Figure S2. Concentration vs. time data for isomerization of Ph(Cl)Si(ON[Me]O) ($CDCl_3$, 20 ºC).

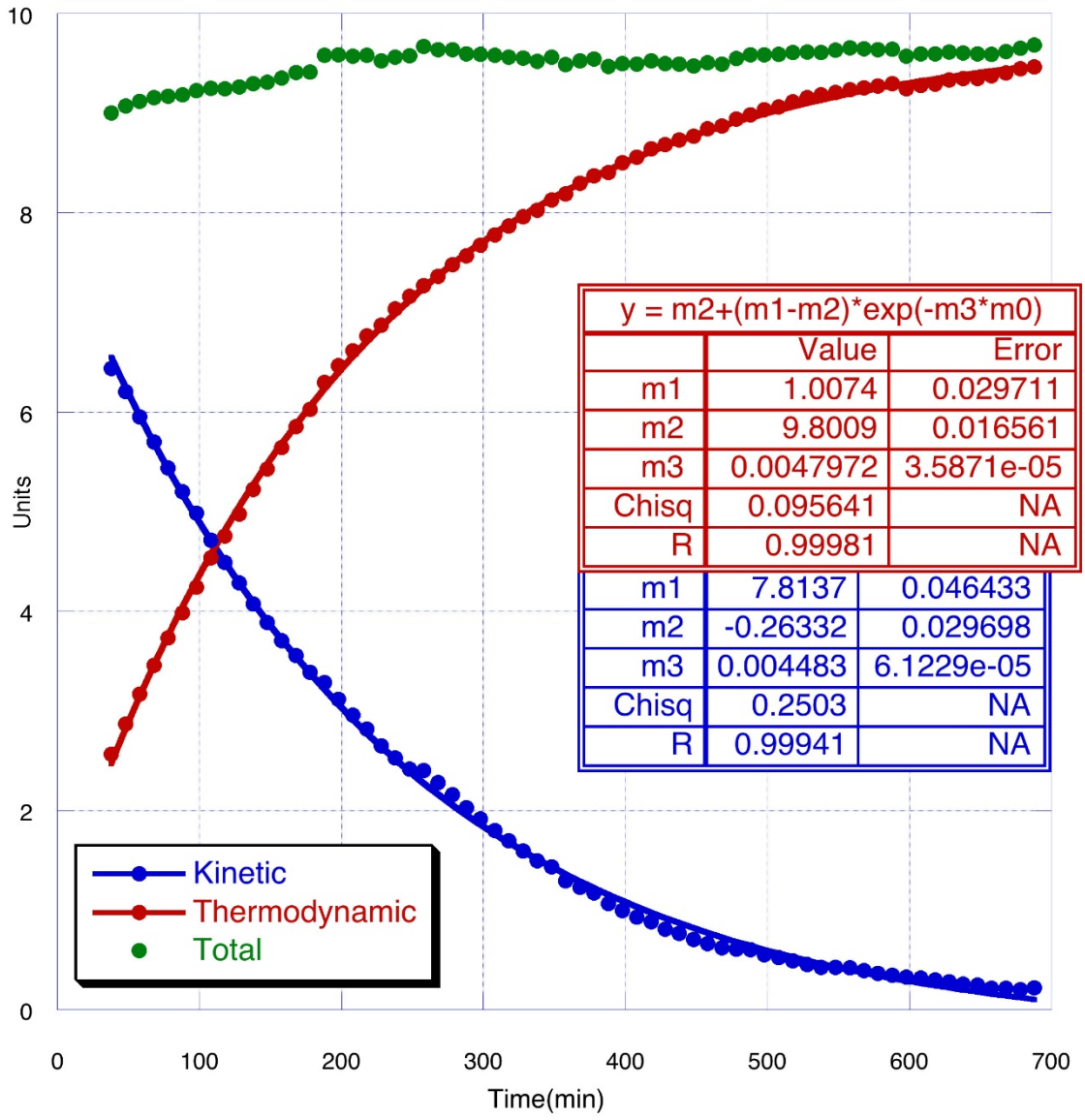
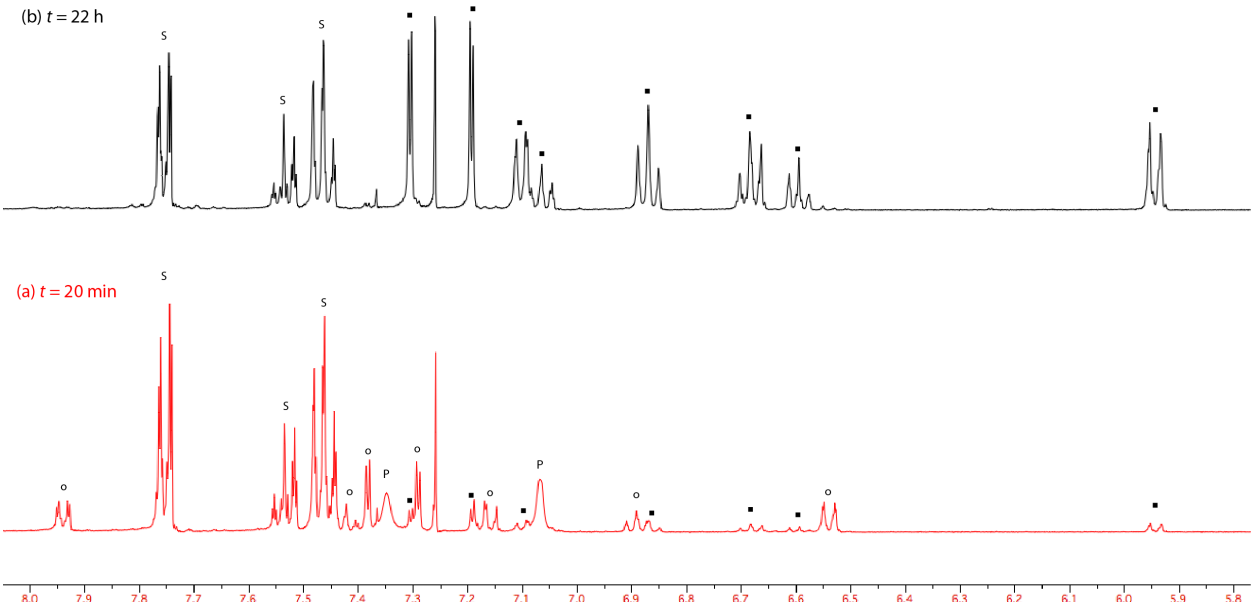
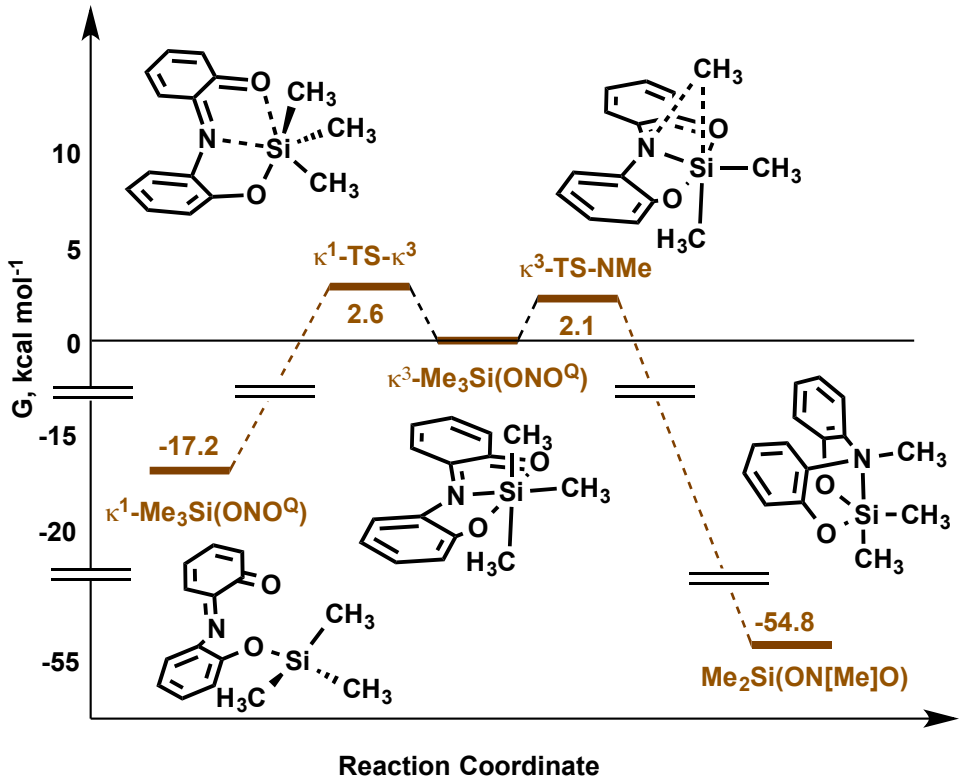


Figure S3. ^{1}H NMR spectra (400 MHz) of the reaction of Ph_2SiCl_2 with $Pb(ONO^{Q})_2$ ($CDCl_3$, 20 ºC). (a) t = 20 min. (b) t = 22 h. Key: o = Ph(Cl)Si(ON[Ph]O) (kinetic isomer); ■ = Cl(Ph)Si(ON[Ph]O) (thermodynamic isomer); S = Ph_2SiCl_2; P = $\{PbCl(ONO^{Q})\}_n$.



III. DFT Calculations for the Reactions of $Me_3Si(ONO^Q)$

Figure S4. Calculated reaction coordinate for migration of $Me_3Si(ONO^Q)$. Free energies in kcal mol^{-1}.



1. κ^1-$Me_3Si(ONO^Q)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1076.351321 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.02313800	-0.04878500	-0.38996500
C	0.20632300	1.01327400	0.49466400
H	-0.44711100	1.10314500	1.35588000
C	1.25215300	1.90593000	0.28500000
H	1.42476400	2.70640900	0.99828400
C	2.09637100	1.75750900	-0.82217000
H	2.94153200	2.42383200	-0.96246200
C	1.85915300	0.73779600	-1.73211500
H	2.53698700	0.58433900	-2.56487400
C	0.78700600	-0.17010300	-1.55874600
C	-2.39567800	-2.73613100	1.44835200
H	-1.85198400	-2.42819400	2.34773400

H	-3.30038200	-2.12284500	1.37947100
H	-2.70862000	-3.77734300	1.58729100
N	0.55714500	-1.25996600	-2.37605400
O	-1.06110700	-0.86217200	-0.13918800
C	0.27627700	-3.50566700	0.08878300
H	0.06490500	-4.52444400	0.43450000
H	0.79209200	-3.56687200	-0.87192800
H	0.94371800	-3.04119300	0.82274900
C	-2.31517400	-3.07194500	-1.60800800
H	-2.78990000	-4.04390400	-1.42899500
H	-3.10954500	-2.35199000	-1.83127600
H	-1.66455800	-3.17062600	-2.47917000
Si	-1.33110500	-2.55260000	-0.09676300
C	0.65567400	-2.65136600	-4.32100900
C	0.85305700	-2.69655800	-5.77630200
H	0.82691100	-3.68068100	-6.23250600
C	1.03600000	-1.56655000	-6.49784000
H	1.16694600	-1.62194100	-7.57545600
C	1.02614900	-0.25813700	-5.87274000
H	1.09933600	0.61975100	-6.50797000
C	0.89229900	-0.11494300	-4.53160800
H	0.83607400	0.87239400	-4.08810500
C	0.71852800	-1.27585600	-3.66551400
O	0.48394400	-3.67583300	-3.66592500

2. κ^1-TS-κ^3 $Me_3Si(ONO^Q)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1076.319777 a.u.

Imaginary frequencies = -124.48 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.11457300	-0.21928800	-0.06659600
C	0.09128200	0.91045700	0.81863500
H	-0.38290300	0.86227700	1.79284000
C	0.86235400	1.96372500	0.43460400
H	1.01666900	2.79871300	1.11259100
C	1.50366600	1.99287000	-0.85193600
H	2.14205300	2.83424200	-1.10239900
C	1.33334100	0.97786400	-1.74636300
H	1.85952200	1.00906900	-2.69026200
C	0.50713300	-0.15868300	-1.42423800
C	-1.98534500	-4.40157900	-0.41996300

H	-1.39572100	-5.32362400	-0.37803400
H	-2.27933700	-4.16024500	0.60990500
H	-2.90530200	-4.60799400	-0.97727200
N	0.22443000	-1.21162800	-2.16975100
O	-0.79629300	-1.20496400	0.29729300
C	0.70263100	-3.36941300	-0.34587100
H	1.05329200	-4.31000700	-0.78586500
H	1.50186200	-2.63138000	-0.44083100
H	0.53547400	-3.55012800	0.72048200
C	-2.50944800	-1.86094200	-1.68574800
H	-3.02509900	-2.37858200	-2.50335100
H	-3.20503400	-1.81067300	-0.84219000
H	-2.30086300	-0.83884800	-2.00941900
Si	-0.99370000	-2.94222900	-1.17050300
C	0.01396200	-2.91955100	-3.72542300
C	0.23576200	-3.47791800	-5.00974300
H	-0.11647200	-4.48680500	-5.19335700
C	0.86518800	-2.73581400	-5.98359600
H	1.02281700	-3.16755900	-6.96786400
C	1.29557000	-1.40785500	-5.73324300
H	1.75976800	-0.83446200	-6.52890900
C	1.11442000	-0.84143100	-4.49297500
H	1.41377300	0.18500900	-4.33243200
C	0.49207100	-1.57899800	-3.44300600
O	-0.60877200	-3.61335200	-2.81647800

3. κ^3-$Me_3Si(ONO^Q)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1076.323897 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.03863400	-0.06077600	-0.03149200
C	0.23441000	1.00313200	0.89918700
H	-0.18002800	0.89028300	1.89468200
C	0.92996800	2.12129800	0.51830500
H	1.07776600	2.92957100	1.22884200
C	1.46933800	2.25274400	-0.79609700
H	2.01443500	3.15349500	-1.05869500
C	1.30529000	1.25686100	-1.72380600
H	1.72246300	1.37724500	-2.71416200
C	0.58778900	0.06890500	-1.38096400
C	-1.83983600	-3.76796200	0.03870800
H	-1.28751000	-4.12738800	0.91333800
H	-2.79345500	-3.35632900	0.38588000

H	-2.07147300	-4.64348600	-0.58068500
N	0.31108400	-1.01309000	-2.11759000
O	-0.60610300	-1.12023000	0.29638900
C	0.94505500	-3.22955400	-0.53957600
H	0.88084200	-4.31795500	-0.64592500
H	1.78876700	-2.88969800	-1.14861900
H	1.17895400	-3.01617800	0.50849700
C	-2.40149500	-1.55703400	-1.73882800
H	-3.10941500	-2.32573400	-2.06760300
H	-2.89410300	-0.97235000	-0.95517100
H	-2.21974700	-0.89322100	-2.59011300
Si	-0.83480400	-2.49781800	-0.98819300
C	-0.01131200	-2.73914100	-3.62506000
C	0.15826200	-3.32459000	-4.91734500
H	-0.26985200	-4.30577500	-5.08920200
C	0.84418300	-2.64522800	-5.88918800
H	0.97096200	-3.09351500	-6.87051400
C	1.40120200	-1.35369800	-5.64475500
H	1.93763800	-0.84784700	-6.44088800
C	1.26493700	-0.75143100	-4.42140400
H	1.69420100	0.22765000	-4.25892000
C	0.55873000	-1.41391000	-3.36889500
O	-0.64903500	-3.35188900	-2.69894700

4. TS-NMe

Energy of optimized structure (sum of electronic and thermal free energies) = -1076.320516 a.u.

Imaginary frequencies = -174.11 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.24369100	0.10623100	-0.06974300
C	3.61259300	-0.21804200	-0.02380600
H	4.34518800	0.58130100	-0.04473100
C	3.98444700	-1.54986800	0.03329200
H	5.03783000	-1.81200800	0.04848800
C	3.01519300	-2.57724900	0.08127600
H	3.33457500	-3.61266300	0.13306800
C	1.66411000	-2.28167400	0.06913400
H	0.94619300	-3.08676700	0.12179200
C	1.25311800	-0.93247700	-0.03685200
C	0.02832100	3.41274300	0.19056600
H	0.77854800	3.62614400	0.95728200
H	0.27463400	4.01985000	-0.68904200

H	-0.94455400	3.74697500	0.56395400
N	0.00307300	-0.37928100	-0.07101700
O	1.79784000	1.34202400	-0.07852600
C	-0.01349900	0.95868900	2.05517900
H	-0.14036500	1.98430200	2.39303200
H	-0.85335900	0.31396600	2.29669800
H	0.95713000	0.53271100	2.29412200
C	-0.06482300	1.58222700	-2.21210700
H	-0.82318200	2.29666000	-2.55312100
H	0.89361800	1.89793400	-2.63910500
H	-0.31510100	0.60927700	-2.65003500
Si	-0.00356300	1.56474800	-0.29441900
C	-2.24053100	0.09993200	-0.05212700
C	-3.60802500	-0.23009500	-0.00148900
H	-4.34228200	0.56772500	0.02004700
C	-3.97664000	-1.56386000	-0.00396300
H	-5.02918600	-1.82931400	0.01013600
C	-3.00451200	-2.58924100	-0.02664400
H	-3.32089900	-3.62682300	-0.03789900
C	-1.65411400	-2.29001600	-0.03538600
H	-0.93457200	-3.09507700	-0.06083400
C	-1.24636400	-0.93606200	-0.06320800
O	-1.79949000	1.33742900	-0.02528800

5. $Me_2Si(ON[Me]O)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1076.411212 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.08851400	-0.02529900	0.00614100
O	-0.47590300	-1.59539700	0.25610400
O	-0.65830400	0.66643200	-1.33022800
N	-2.85542300	-0.10581200	0.19795600
C	-3.67081100	-0.05231800	1.41230300
H	-3.57749600	0.93695200	1.86928300
H	-3.29707200	-0.80020000	2.11651900
H	-4.73940800	-0.25585000	1.24162200
C	1.86586800	-0.24248000	-0.53303700
H	1.91725500	-0.79382100	-1.47687300
H	2.43487000	-0.80441300	0.21508100
H	2.35929200	0.72395900	-0.67862300
C	-0.01444900	1.01533200	1.55915200
H	-1.03926500	1.29164400	1.81265800
H	0.57189200	1.93272300	1.43829300

H	0.40797300	0.46193800	2.40507900
C	-2.79514700	-1.42368200	-0.38944500
C	-1.59185900	-2.14426800	-0.30118400
C	-1.52745200	-3.45635600	-0.78273900
H	-0.58871300	-3.99332300	-0.69610900
C	-2.64771600	-4.04107500	-1.36794700
H	-2.58591400	-5.05896200	-1.74175200
C	-3.83913700	-3.32122800	-1.48852900
H	-4.70821600	-3.77122900	-1.95816300
C	-3.90481000	-2.01818000	-0.99862000
H	-4.82394000	-1.44513100	-1.08431300
C	-2.98076900	0.98405600	-0.71450700
C	-1.83711500	1.34611900	-1.45775600
C	-1.89219600	2.40685600	-2.36144200
H	-0.99584700	2.65241700	-2.92145000
C	-3.06941600	3.13967700	-2.51493600
H	-3.09847700	3.96949100	-3.21457500
C	-4.19564400	2.81424100	-1.76063400
H	-5.11222700	3.38644800	-1.86630500
C	-4.14866200	1.73912000	-0.87102700
H	-5.02997500	1.48170000	-0.29227700

IV. DFT Calculations for the Reactions of Ph(Me)(Cl)Si(ONO^{Q})

6. κ^1-Ph(Me)(Cl)Si(ONO^{Q})

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.405707 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.39901400	1.09207100	-0.37113700
C	0.14017800	1.55082000	-1.65384500
H	-0.43535800	1.30152900	-2.53907700
C	1.29482600	2.25433000	-1.71708500
H	1.67786300	2.58905500	-2.67690700
C	2.06713600	2.55690800	-0.52639200
H	3.01818200	3.06669400	-0.64416000
C	1.64593900	2.18582200	0.70670200
H	2.26343600	2.37424000	1.57666100
C	0.41007500	1.43090500	0.87829000
N	-0.05224800	0.95539200	1.99569200
O	-1.47770700	0.50369800	-0.30023600
Si	-0.43231700	-2.06498400	2.96696700
C	0.42822200	0.34930000	4.27827500
C	0.79138100	0.71046600	5.57849800
H	0.82529100	-0.06638100	6.33469000
C	1.08186100	2.03512500	5.89394500
H	1.34324900	2.29776800	6.91411600
C	1.01652200	3.02242400	4.90500800
H	1.20767600	4.06164800	5.15152700
C	0.68786000	2.67007700	3.60325700
H	0.58740200	3.43633800	2.84252800
C	0.40251500	1.32997400	3.25039100
O	0.15952900	-0.96342700	4.06894500
C	-0.40727000	-3.67063600	3.92766800
C	0.29134400	-3.79676300	5.14197500
C	-1.09561400	-4.79775400	3.44009900
C	0.30483400	-5.00417300	5.84205200
H	0.82565800	-2.94147100	5.54371000
C	-1.08347000	-6.00657100	4.13709000
H	-1.64859600	-4.73973100	2.50584300
C	-0.38228100	-6.11138800	5.34033200
H	0.84955400	-5.08017700	6.77875500
H	-1.62162000	-6.86386000	3.74332100
H	-0.37308100	-7.05116100	5.88486800
C	-2.09955200	-1.66735000	2.24820500
H	-2.03104900	-0.82906800	1.55200000
H	-2.50549800	-2.53878000	1.72418100

H	-2.78900300	-1.41076500	3.06023300
Cl	0.98310000	-2.26317000	1.40641700

7. 1-κ[1]-TS-κ[3]

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.380526 a.u.

Imaginary frequencies = -73.55 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.27129700	-0.93915100	-0.46308800
C	3.51448700	-1.31427300	-0.98445900
H	3.74168200	-2.36885800	-1.09234800
C	4.43483100	-0.33084300	-1.32171700
H	5.40455000	-0.61997400	-1.71462700
C	4.14252900	1.03153900	-1.12378300
H	4.89425000	1.78326300	-1.33850200
C	2.90694000	1.41715600	-0.63362800
H	2.71635000	2.46172200	-0.42780200
C	1.92586000	0.43955200	-0.33690200
N	0.65803800	0.61381800	0.17584700
O	1.39283700	-1.87056600	-0.07546700
Cl	0.74637700	-0.76598600	2.74178800
Si	-0.03925700	-1.48347300	0.81232300
C	-1.33364600	1.62615000	1.02563500
C	-2.13318700	2.84111100	1.14114500
H	-3.00740400	2.78768200	1.78065100
C	-1.80196200	3.96146600	0.45442000
H	-2.41369500	4.85474500	0.53677000
C	-0.66135400	3.98532900	-0.43474300
H	-0.48703700	4.87431100	-1.03199700
C	0.16633300	2.91535300	-0.56182800
H	0.97284200	2.94257700	-1.28153000
C	-0.08128500	1.69910400	0.18157300
O	-1.64868100	0.58587500	1.61483300
C	-1.42018900	-1.26619700	-0.49002000
C	-2.75670300	-1.56661300	-0.16731900
C	-1.13089200	-0.95376300	-1.82914300
C	-3.76200300	-1.54030300	-1.13446600
H	-3.02323500	-1.81560300	0.85557700
C	-2.13143000	-0.93404500	-2.80463300
H	-0.11193900	-0.72804600	-2.13018600
C	-3.45205300	-1.22299100	-2.45908200
H	-4.78676700	-1.76774600	-0.85397800

H	-1.87674100	-0.69439600	-3.83339600
H	-4.23231300	-1.20475100	-3.21459800
C	-0.48694900	-3.19711300	1.49491100
H	0.34529200	-3.62710000	2.05845200
H	-1.34930700	-3.14263800	2.16801200
H	-0.74859000	-3.87280200	0.67348100

8. 2-κ^1-TS-κ^3

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.391722 a.u.

Imaginary frequencies = -64.80 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-2.08777100	-1.31547800	0.17418100
C	-3.23892900	-2.00971000	0.58053100
H	-3.22481900	-3.09352500	0.57913900
C	-4.36413700	-1.29273900	0.94927600
H	-5.25972900	-1.82498800	1.25408500
C	-4.37892700	0.11932700	0.90359700
H	-5.28904600	0.65612100	1.14735400
C	-3.25103000	0.82079400	0.52823500
H	-3.30030300	1.89673600	0.44331300
C	-2.06484000	0.11813600	0.19102100
N	-0.84784400	0.60048100	-0.22277000
O	-1.00489500	-1.96609600	-0.22467200
Si	0.32981300	-1.05644200	-0.93504700
C	0.91341900	1.99027700	-0.96864900
C	1.46377400	3.32471700	-1.10347800
H	2.37924700	3.42670400	-1.67524600
C	0.85546500	4.38127900	-0.50443300
H	1.27908600	5.37674100	-0.59467700
C	-0.33448400	4.20847400	0.29372900
H	-0.74114900	5.06876800	0.81452600
C	-0.93335000	2.99318800	0.42938500
H	-1.78636200	2.88792400	1.08379300
C	-0.37395600	1.83486800	-0.21892900
O	1.46662700	0.99360700	-1.47307200
C	1.51381900	-0.85789200	0.55551700
C	2.90227000	-0.69071900	0.39949000
C	1.01138400	-0.92439500	1.86569500
C	3.74866500	-0.58647700	1.50256700
H	3.32918300	-0.64584200	-0.59680000
C	1.85589100	-0.82414300	2.97559000
H	-0.05110100	-1.06344400	2.03990200

C	3.22800200	-0.65157800	2.79792800
H	4.81670700	-0.45626300	1.35104100
H	1.43774300	-0.88369700	3.97672200
H	3.88675600	-0.57234200	3.65803200
C	-0.25639900	-0.70285400	-2.71194200
H	0.59388200	-0.67391100	-3.39436900
H	-0.90418000	-1.53099000	-3.01551000
H	-0.81041300	0.23411400	-2.80343600
Cl	1.41264500	-2.94387200	-1.63951400

9. 3-κ^1-TS-κ^3

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.380761 a.u.

Imaginary frequencies = -73.55 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.42517600	2.24343800	-0.27568900
C	-0.46229100	3.64195600	-0.32226700
H	0.45161000	4.18397300	-0.53770700
C	-1.65669900	4.29919800	-0.06238600
H	-1.68453400	5.38409500	-0.08475900
C	-2.82120000	3.58013200	0.26849900
H	-3.73078700	4.11205000	0.52530700
C	-2.80550100	2.19706700	0.29176200
H	-3.68873700	1.65958000	0.60866200
C	-1.61591000	1.49580400	-0.02682800
C	2.78244400	-0.26056500	-0.14485600
C	3.38967400	-1.53037700	-0.11842100
H	2.77301900	-2.42705400	-0.11023700
C	4.77789600	-1.67546100	-0.09249400
H	5.21851000	-2.66860200	-0.06818500
C	5.59886000	-0.54527800	-0.10003700
H	6.67972400	-0.65393100	-0.08283100
C	5.01954400	0.72428700	-0.13082600
H	5.65014600	1.60958000	-0.13844700
C	3.62876000	0.86221100	-0.15055500
H	3.19694600	1.85838300	-0.17281700
N	-1.38871200	0.13817400	-0.04375900
O	0.72656700	1.59377000	-0.46539900
Cl	0.66305100	-0.27610900	1.97877700
C	0.57709100	-0.94303200	-1.88499800
H	1.11142700	-0.31377300	-2.60751200
H	1.03806500	-1.93229500	-1.91125400

H	-0.46282900	-1.02815400	-2.19970700
Si	0.87739800	-0.10926600	-0.20197900
C	-1.68472900	-2.22843900	0.10186700
C	-2.62583300	-3.34193000	0.14375300
H	-2.20851500	-4.32350800	0.33961400
C	-3.94774200	-3.14593700	-0.08309200
H	-4.63564700	-3.98585700	-0.06553200
C	-4.46830200	-1.83360700	-0.39640800
H	-5.51714600	-1.73932700	-0.65763200
C	-3.67039400	-0.73369600	-0.40308000
H	-4.07782500	0.22229900	-0.70101600
C	-2.25808400	-0.84513000	-0.10950000
O	-0.46935800	-2.40188900	0.25692400

10. 1-κ^3-Ph(Me)(Cl)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = --1688.405391 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.13669000	-0.92601400	0.26187900
C	3.37323400	-1.58268900	0.06586700
H	3.63356600	-2.41510100	0.70872200
C	4.20724500	-1.13690900	-0.93309700
H	5.16059600	-1.63056200	-1.09247000
C	3.85682000	-0.03444900	-1.76761300
H	4.54942700	0.28676200	-2.53735500
C	2.66378500	0.62328600	-1.60717000
H	2.42630700	1.46231300	-2.24394700
C	1.76544100	0.19079800	-0.58950100
N	0.56153000	0.66579000	-0.22817700
O	1.29797400	-1.28244900	1.18471400
Cl	1.08347500	1.44496500	2.53703100
Si	-0.29065100	-0.40088200	1.27856900
C	-1.40488500	1.77730500	0.16280700
C	-2.36321000	2.78293400	-0.10599400
H	-3.24059300	2.85367000	0.52580700
C	-2.14642600	3.63715900	-1.16040500
H	-2.87321300	4.41332300	-1.37780900
C	-0.98737800	3.53068100	-1.98763000
H	-0.86404100	4.22125600	-2.81430000
C	-0.03638200	2.57108500	-1.75474100
H	0.82673600	2.50419300	-2.40004000
C	-0.21667900	1.66685200	-0.66738900

O	-1.53429400	0.93809800	1.13823900
C	-1.23999600	-1.55605300	0.03228100
C	-2.64504100	-1.62514000	0.12646300
C	-0.62569000	-2.39142500	-0.91528300
C	-3.39458700	-2.48370400	-0.68019000
H	-3.16678200	-1.00015500	0.84547900
C	-1.36759900	-3.25055000	-1.73093600
H	0.45391100	-2.39131100	-1.03388800
C	-2.75720800	-3.30011500	-1.61604200
H	-4.47604500	-2.51313000	-0.57709000
H	-0.85735800	-3.88266900	-2.45268200
H	-3.33651300	-3.96793900	-2.24731500
C	-0.80243700	-1.04066300	2.98299500
H	0.06982200	-1.14557700	3.63009100
H	-1.50024300	-0.35020400	3.46298600
H	-1.28988500	-2.01700100	2.89013900

11. 2-κ^3-Me(Cl)(Ph)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.394769 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-2.24058300	-0.66558200	0.40760200
C	-3.61527400	-1.00226800	0.29691600
H	-4.34783800	-0.35108700	0.75956400
C	-3.97317800	-2.13028100	-0.39871500
H	-5.02282600	-2.38980700	-0.49502400
C	-2.99667200	-2.97698500	-1.00558900
H	-3.32399800	-3.85649800	-1.54894500
C	-1.65885200	-2.69486300	-0.90970300
H	-0.94146400	-3.35113200	-1.37935600
C	-1.23604600	-1.53175500	-0.19818400
N	0.00128200	-1.07043800	0.05274200
O	-1.84699400	0.39069500	1.03794300
Si	-0.00060400	0.66756900	1.15331200
C	2.24229400	-0.66032300	0.40701300
C	3.61774100	-0.99380100	0.29596600
H	4.34891900	-0.34077600	0.75820400
C	3.97806700	-2.12121900	-0.39938200
H	5.02828600	-2.37833500	-0.49592300
C	3.00334700	-2.97048900	-1.00554400
H	3.33253400	-3.84958800	-1.54844600
C	1.66491300	-2.69140500	-0.90940200
H	0.94886500	-3.34974100	-1.37819100
C	1.23961600	-1.52894300	-0.19833700

O	1.84639500	0.39511800	1.03730300
C	-0.00210900	1.70184100	-0.51623200
C	1.19362400	2.11728600	-1.13747700
C	-1.19899200	2.11427700	-1.13724800
C	1.19697300	2.87653600	-2.31030900
H	2.14996400	1.86277500	-0.69656800
C	-1.20446600	2.87351300	-2.31008400
H	-2.15461000	1.85738700	-0.69615300
C	-0.00428400	3.25634600	-2.90868100
H	2.14452400	3.17489100	-2.75173600
H	-2.15284700	3.16948600	-2.75133000
H	-0.00511400	3.84717800	-3.82043100
C	0.00091200	-0.37996800	2.80439300
H	0.88570400	-0.13133200	3.39394000
H	-0.88417700	-0.13333500	3.39432900
H	0.00208400	-1.45957800	2.62119700
Cl	-0.00270000	2.58756300	2.37149000

12. 3-κ^3-Me(Ph)(Cl)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.405707 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.82818900	2.23296700	-0.07635300
C	-1.14377200	3.61250700	-0.03797200
H	-0.33729700	4.33530200	-0.07330400
C	-2.46268300	3.98791600	0.05122200
H	-2.71683800	5.04257300	0.08545800
C	-3.51579700	3.02557600	0.10564000
H	-4.54125500	3.36895400	0.18341400
C	-3.24861600	1.68157400	0.06424400
H	-4.06122600	0.97232700	0.11690800
C	-1.89480000	1.24502000	-0.03544700
C	2.53765100	-0.00837800	-0.13157800
C	3.24442400	-1.13730300	0.32050800
H	2.69721400	-2.02080500	0.63330500
C	4.63884100	-1.14512700	0.38751600
H	5.15715800	-2.03209500	0.74250600
C	5.36706500	-0.01629700	0.00488300
H	6.45221600	-0.01944900	0.05947300
C	4.68778800	1.11565400	-0.44773700
H	5.24283700	2.00082500	-0.74727000
C	3.29211500	1.11436500	-0.51766200
H	2.78648800	2.00728600	-0.87383000

N	-1.38223100	0.00691300	-0.09627800
O	0.39019200	1.80488600	-0.15311600
Cl	0.40502900	-0.04598400	2.18017000
C	0.47219000	0.04335100	-2.25759900
H	1.00996900	0.91256500	-2.64724200
H	0.93699200	-0.85370100	-2.67715300
H	-0.55789400	0.09316300	-2.62336500
Si	0.64613900	0.00074100	-0.32377000
C	-0.84988200	-2.22253500	-0.18003500
C	-1.17761100	-3.59906700	-0.20457600
H	-0.37683500	-4.32748500	-0.25218200
C	-2.50180800	-3.96554100	-0.16416100
H	-2.76539300	-5.01831400	-0.18033700
C	-3.54786900	-2.99648300	-0.10439900
H	-4.57841100	-3.33250900	-0.08030600
C	-3.26791700	-1.65440000	-0.07926400
H	-4.07664300	-0.93978900	-0.03952700
C	-1.90793200	-1.22784600	-0.11289700
O	0.37404500	-1.80258600	-0.22047500

13. 1-TS-NPh

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.385628 a.u.

Imaginary frequencies = -239.33 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.18110500	-0.09663400	0.08419100
C	0.41345000	-0.01565300	-1.29788900
H	0.06184400	-0.81248000	-1.94331300
C	1.09813700	1.08324800	-1.79158400
H	1.29768700	1.15415000	-2.85614300
C	1.53828400	2.11594200	-0.93612600
H	2.07193300	2.96413300	-1.35088400
C	1.29731200	2.06425800	0.42626400
H	1.63951400	2.87115700	1.05696600
C	0.63446000	0.93924500	0.95760100
N	0.28255900	0.63134000	2.25333100
O	-0.49695300	-1.07845100	0.65239700
Cl	1.36654700	-2.27495100	2.55393400
Si	-0.50916600	-1.10809800	2.43981900
C	0.19215500	0.37710800	4.52730700
C	0.42688600	0.74809100	5.85993900

H	0.08426500	0.10179600	6.66003500
C	1.10094600	1.93340600	6.10935500
H	1.30125700	2.22824100	7.13460700
C	1.52629400	2.76851300	5.05479300
H	2.04877000	3.69195700	5.27959900
C	1.28369200	2.42821500	3.73441100
H	1.60997800	3.09105800	2.94685100
C	0.63450800	1.20923500	3.45486800
O	-0.48156200	-0.70702200	4.18027300
C	-2.06583400	0.77795300	2.24194100
C	-2.64118000	1.24118000	3.41541600
C	-2.58951600	1.07374000	0.99439300
C	-3.84017300	1.96314800	3.33303200
H	-2.20311000	1.05502200	4.38948000
C	-3.78904300	1.79609600	0.92379900
H	-2.10707600	0.76443100	0.07320700
C	-4.41349600	2.23816200	2.09080200
H	-4.31339500	2.31078800	4.24711000
H	-4.22056300	2.01497500	-0.04888900
H	-5.33512300	2.80902700	2.03151900
C	-1.84378600	-2.43151900	2.58322700
H	-1.74359400	-3.14784100	1.76382500
H	-1.73811400	-2.96299400	3.53243500
H	-2.84664000	-1.99913500	2.54104200

14. 2-TS-NMe

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.381085 a.u.

Imaginary frequencies = -212.16 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-2.20898800	-0.69172900	0.36082600
C	-3.57812900	-0.96382800	0.25204700
H	-4.29422700	-0.28833300	0.70620700
C	-3.97612400	-2.08633200	-0.46080100
H	-5.03447800	-2.29680000	-0.57753800
C	-3.03044300	-2.95757200	-1.03801700
H	-3.36980600	-3.82294600	-1.59700100
C	-1.67040900	-2.72628500	-0.90136200
H	-0.96330400	-3.40580100	-1.35478600
C	-1.24486300	-1.57662800	-0.20782400
N	0.01847300	-1.12095900	0.09837000
O	-1.72193200	0.34266100	1.04207200

Si	0.02633700	0.62642600	0.84472500
C	2.25007300	-0.72233300	0.36496900
C	3.61545200	-1.01798300	0.27410600
H	4.33947700	-0.33505900	0.70389500
C	3.99934400	-2.17853000	-0.38406200
H	5.05488800	-2.41044700	-0.48449300
C	3.04302100	-3.06555100	-0.91755800
H	3.37132700	-3.96819500	-1.42145700
C	1.68602300	-2.80578400	-0.80168400
H	0.97051200	-3.50967200	-1.20161000
C	1.27552300	-1.61135800	-0.17822600
O	1.77523400	0.34424100	1.00506100
C	-0.00314900	1.75407300	-0.68292500
C	1.16993600	2.06535000	-1.39769600
C	-1.20804700	2.31838100	-1.14704100
C	1.14197800	2.89068600	-2.52389300
H	2.12451900	1.66712000	-1.07028900
C	-1.24188000	3.14664800	-2.27027200
H	-2.13401500	2.11589000	-0.61861900
C	-0.06560300	3.43377000	-2.96516100
H	2.06459500	3.11163900	-3.05358600
H	-2.18691500	3.56854700	-2.60130700
H	-0.08947000	4.07769900	-3.83979000
C	0.01094600	-1.25023500	2.52672200
H	-0.03462100	-0.49729700	3.30694100
H	-0.88333600	-1.85232300	2.41286200
H	0.95224700	-1.78294000	2.44956100
Cl	0.04075800	2.07137100	2.47495500

15. 2-TS-NPh

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.376357 a.u.

Imaginary frequencies = -204.75 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-2.19945400	-0.69928700	0.49157700
C	-3.55585700	-0.99946800	0.29369400
H	-4.30697200	-0.46630400	0.86539700
C	-3.89095100	-1.98371000	-0.62315400
H	-4.93503100	-2.23913100	-0.77418500
C	-2.90020400	-2.65647300	-1.36938400
H	-3.19249000	-3.41941200	-2.08268300
C	-1.55841300	-2.35420700	-1.20733700
H	-0.82023900	-2.87421800	-1.80047200

C	-1.18990100	-1.38535700	-0.25218700
N	0.04601200	-0.89479200	0.10318600
O	-1.78063100	0.24748500	1.31718400
Si	-0.01410100	0.33209400	1.57208700
C	2.26112400	-0.47793800	0.49731600
C	3.64246400	-0.65618900	0.30804300
H	4.33813900	-0.04299200	0.86940700
C	4.07012900	-1.62713100	-0.58208400
H	5.13378100	-1.79001000	-0.72398000
C	3.14810000	-2.40953600	-1.31225300
H	3.51387200	-3.16352600	-2.00072700
C	1.78458800	-2.22802000	-1.16375900
H	1.09961900	-2.83738800	-1.73467500
C	1.32104400	-1.27189700	-0.23559000
O	1.75412700	0.43907400	1.30159800
C	-0.06766200	1.39301400	-0.72406000
C	1.11073200	1.73366400	-1.36065600
C	-1.30261500	1.85673500	-1.15194200
C	1.06014800	2.62699700	-2.44145400
H	2.07368900	1.33276500	-1.06020500
C	-1.34173400	2.74808500	-2.23424400
H	-2.22984400	1.56861100	-0.67181600
C	-0.16456800	3.13351600	-2.87658300
H	1.98327300	2.91200700	-2.93866700
H	-2.30173900	3.13462400	-2.56585300
H	-0.20264400	3.81669600	-3.71970700
C	0.05598000	-0.77212200	3.11262600
H	0.93591300	-0.54281100	3.71960100
H	-0.83505900	-0.63390600	3.73078800
H	0.10827900	-1.83209600	2.83738600
Cl	-0.11605200	2.31616600	2.43277600

16. 3-TS-NMe

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.385909 a.u.

Imaginary frequencies = -280.25 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.352211	-0.255592	0.153217
C	0.637209	-0.218194	-1.217041
H	0.385918	-1.070747	-1.837786
C	1.247675	0.915321	-1.735745
H	1.491478	0.954166	-2.792752

C	1.552930	2.018987	-0.915007
H	2.029822	2.892781	-1.345743
C	1.249206	2.007483	0.438072
H	1.485134	2.870632	1.042608
C	0.663348	0.853006	0.991327
C	-1.556784	-2.673902	2.648517
C	-1.549229	-3.695274	1.678226
H	-0.850199	-3.643941	0.850455
C	-2.424184	-4.779599	1.757280
H	-2.391881	-5.554923	0.996732
C	-3.340063	-4.867322	2.807859
H	-4.023990	-5.709189	2.869048
C	-3.369408	-3.865041	3.778208
H	-4.077649	-3.922801	4.600210
C	-2.486337	-2.785413	3.699118
H	-2.520151	-2.019951	4.466598
N	0.254053	0.573488	2.281449
O	-0.269934	-1.266347	0.746888
Cl	1.619390	-2.133687	2.859473
C	-2.081426	0.490981	2.084677
H	-2.769525	-0.346660	2.162636
H	-2.145062	1.210106	2.893412
H	-1.984958	0.910234	1.089714
Si	-0.338821	-1.222808	2.528805
C	-0.051001	0.478578	4.544795
C	-0.010871	0.962233	5.857855
H	-0.394086	0.348064	6.664853
C	0.535212	2.218057	6.084165
H	0.590891	2.601440	7.098109
C	1.015888	3.005999	5.019773
H	1.437822	3.984147	5.223939
C	0.954788	2.551739	3.710910
H	1.322811	3.179942	2.913369
C	0.438414	1.265427	3.463552
O	-0.587268	-0.688403	4.208800

17. 1-NPh-Cl(Me)Si(ON[Ph]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.471097 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.18826100	0.07230800	0.10252100
N	-2.53385700	0.33710600	-0.96120400
Cl	1.79284500	-0.33384700	1.39169100
O	-0.59703800	-1.39243700	0.09894100
O	-0.66307300	1.25466900	0.90912000
C	-1.62317400	-1.90093400	-0.65640400
C	-2.61878200	-1.07431900	-1.20450800
C	-3.66125100	-1.66029900	-1.93294000
C	-3.71006300	-3.04035900	-2.12068300
H	-4.52311500	-3.47922700	-2.68981100
C	-2.71781200	-3.85209400	-1.56446100
C	-1.67703500	-3.28508400	-0.83158300
H	-0.89668400	-3.89643000	-0.39124600
C	-1.98665200	1.19676700	1.26544000
C	-2.95622200	0.75000400	0.35391800
C	-4.29690000	0.70598200	0.74990100
C	-4.67275800	1.11907600	2.02706000
H	-5.71601000	1.08287400	2.32325000
C	-3.70087700	1.58179400	2.91884700
C	-2.35926400	1.61965400	2.54310600
H	-1.58999000	1.96418900	3.22571500
H	-5.04015300	0.34927700	0.04372400
H	-3.98560000	1.90772200	3.91443200
H	-2.75164700	-4.92839900	-1.70084400
H	-4.42742100	-1.02007000	-2.35833600
C	-2.64849000	1.25944900	-2.03881300
C	-2.31045900	0.87274100	-3.34987800
C	-3.03639700	2.59107800	-1.81137200
C	-2.37246800	1.79239000	-4.39560900
H	-2.00280500	-0.14674000	-3.55129300
C	-3.08854700	3.50112500	-2.86731600
H	-3.29791700	2.91639600	-0.81195200
C	-2.76188900	3.11359200	-4.16706300
H	-2.10893800	1.46666500	-5.39780700
H	-3.39314100	4.52375600	-2.66373100
H	-2.80829000	3.82547800	-4.98487600
C	0.90834300	0.64341200	-1.50495600
H	0.13200600	0.84697800	-2.24598700
H	1.48165900	1.56120100	-1.34374100
H	1.58635200	-0.11791100	-1.90103700

18. 2-NMe-Ph(Cl)Si(ON[Me]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.46047 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.16588100	-0.06202700	0.13164600
N	-2.40337200	0.29044900	-0.92363000
O	-0.59673400	-1.53529200	0.06064400
C	-2.69535700	1.22321000	-2.02338300
O	-0.61121600	1.10412800	1.02968700
C	-1.65219900	-1.99189300	-0.68914800
C	-2.60592600	-1.09845000	-1.20679800
C	-3.64463200	-1.60598500	-1.99376000
C	-3.74623400	-2.97718100	-2.23829800
H	-4.55888700	-3.35618600	-2.84983700
C	-2.80765800	-3.85423200	-1.69225800
C	-1.75533200	-3.36239900	-0.91873000
H	-1.00235800	-4.02276600	-0.50179900
C	-1.95494700	1.17624600	1.29692400
C	-2.89850300	0.74590500	0.35321600
C	-4.25844300	0.81440600	0.67108800
C	-4.67469100	1.32082000	1.90206500
H	-5.73263300	1.36923300	2.13911800
C	-3.72387300	1.76594800	2.82485400
C	-2.36382500	1.69263100	2.52813700
H	-1.61156300	2.02065700	3.23748200
H	-3.77002500	1.33593300	-2.22157100
H	-4.98826100	0.46779700	-0.05445300
H	-2.29045100	2.20406700	-1.76434000
H	-4.04012500	2.16478500	3.78382500
H	-2.88432700	-4.92140200	-1.87550500
H	-2.20039600	0.87080600	-2.93024900
H	-4.37507000	-0.92506800	-2.41858200
C	1.73954600	-0.40246900	1.06454700
C	2.21752400	0.49399200	2.03714300
C	2.49028400	-1.56312400	0.80055600
C	3.40924000	0.24204800	2.71920200
H	1.65086400	1.39088000	2.26743800
C	3.67984400	-1.81761000	1.48302000
H	2.14113500	-2.27921700	0.06175500
C	4.14220800	-0.91341300	2.44238400
H	3.76273000	0.94528600	3.46763800
H	4.24429000	-2.72040600	1.26874000
H	5.06871800	-1.11069900	2.97382900
Cl	0.72856100	0.63916700	-1.76369300

19. 2-NPh-Me(Cl)Si(ON[Ph]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1688.47011 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.25184000	-0.08328600	0.16080400
N	-2.54498000	0.30996700	-0.99037600
O	-0.63823800	-1.47704500	0.09038900
O	-0.59045000	1.17494600	0.85314800
C	-1.67181700	-1.94990800	-0.67838500
C	-2.64314500	-1.09716700	-1.23247000
C	-3.68659800	-1.66192000	-1.97811700
C	-3.76268600	-3.03912300	-2.17473500
H	-4.57800000	-3.45686700	-2.75654700
C	-2.79608100	-3.87530200	-1.61007400
C	-1.75423600	-3.33173800	-0.86166500
H	-0.99099500	-3.96058500	-0.41576400
C	-1.91378700	1.16540500	1.22055100
C	-2.91336000	0.73480000	0.33375600
C	-4.24541500	0.72697000	0.76326900
C	-4.58452000	1.16263000	2.04294700
H	-5.62169400	1.15437700	2.36184800
C	-3.58289500	1.61410500	2.90690200
C	-2.24996300	1.61326400	2.50045200
H	-1.45738200	1.94617700	3.16208000
H	-5.01204600	0.38206200	0.07634200
H	-3.83703000	1.96000400	3.90405600
H	-2.85012500	-4.94999500	-1.75234600
H	-4.43385500	-1.00361300	-2.40929900
C	-2.64809100	1.23661400	-2.06266800
C	-2.30415000	0.85462800	-3.37310700
C	-3.04246700	2.56636100	-1.83470800
C	-2.37098200	1.77360600	-4.41732300
H	-1.97726800	-0.15891800	-3.57152800
C	-3.09667800	3.47831900	-2.88951200
H	-3.30690300	2.89034600	-0.83559200
C	-2.76811400	3.09343700	-4.18900600
H	-2.10077800	1.45124600	-5.41900800
H	-3.40562900	4.49954100	-2.68462200
H	-2.81683200	3.80563700	-5.00659800
C	1.73572100	-0.43781600	1.21029800
H	2.36396100	-1.20681100	0.75302000
H	2.33598300	0.46649500	1.34371600
H	1.41743200	-0.78874200	2.19681900
Cl	0.90463300	0.49017500	-1.73488800

20. 3-NMe - ClPhSi(ON[Me]O)

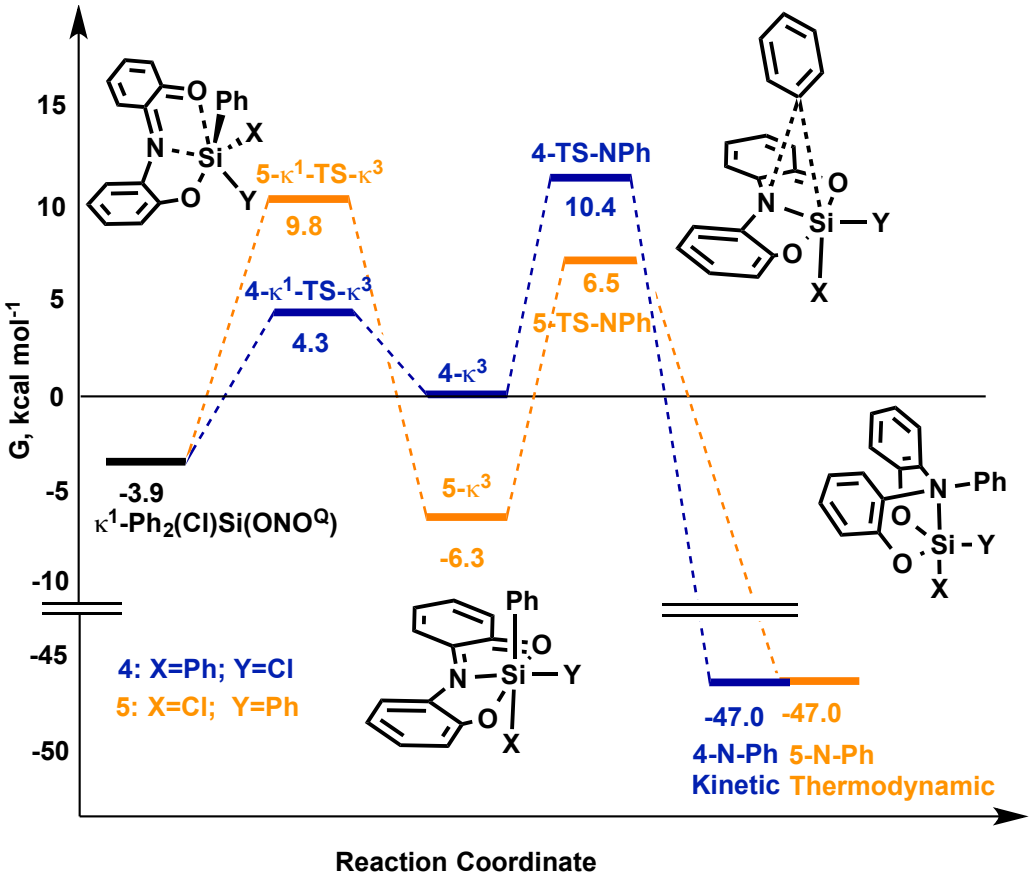
Energy of optimized structure (sum of electronic and thermal free energies) = -1688.462717 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	-0.79928900	-0.38477600	1.02414700
N	0.77762900	0.14790200	-0.84936000
Cl	-1.78668700	-0.86186600	2.85746200
O	-0.04653700	1.00425300	1.58209300
C	0.23340800	0.16873300	-2.22806600
O	0.09954500	-1.79511200	0.92421500
C	0.78913600	1.82544900	0.87369400
C	1.25403400	1.43453800	-0.38860800
C	2.08837000	2.29153200	-1.10914800
C	2.46868500	3.51912200	-0.56386500
H	3.11780900	4.18112100	-1.12755200
C	2.01186400	3.89090100	0.70299900
C	1.16804700	3.04841900	1.42664600
H	0.79353500	3.32456000	2.40634000
C	1.28808700	-1.93350200	0.26123400
C	1.70571200	-0.95005000	-0.64262900
C	2.92974200	-1.09172700	-1.29944000
C	3.72572300	-2.21212700	-1.05946800
H	4.67703300	-2.31815800	-1.57041900
C	3.29340800	-3.19419500	-0.16322400
C	2.07582200	-3.06012900	0.50222400
H	1.72860200	-3.80729700	1.20755000
C	-2.20676700	-0.18685500	-0.17205200
C	-2.70858000	-1.29359000	-0.87961200
C	-3.78242300	-1.14978100	-1.75949300
C	-4.37048200	0.10309300	-1.94663200
C	-3.88352100	1.21144400	-1.25029700
C	-2.81023900	1.06783700	-0.36917100
H	1.01483200	0.33739500	-2.97721200
H	3.26058000	-0.32809600	-1.99578400
H	-0.24500400	-0.79058200	-2.43011100
H	-2.44553000	1.93963000	0.16732500
H	3.90975000	-4.06802800	0.02392600
H	2.30728400	4.84441400	1.12953900
H	-0.51449900	0.95912000	-2.30180400
H	2.43662700	2.00810100	-2.09682200
H	-5.20584300	0.21511300	-2.63146600
H	-4.15903900	-2.01443100	-2.29796200
H	-4.33902800	2.18706600	-1.39196300
H	-2.26099900	-2.27446900	-0.74397500

V. DFT Calculations for the Reactions of $Ph_2ClSi(ONO^Q)$

Figure S5. Calculated reaction coordinate for migration of $Ph_2(Cl)Si(ONO^Q)$. Free energies are in kcal mol^{-1}.



21. κ^1-$Ph_2(Cl)Si(ONO^Q)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.088906 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.05025600	2.30404000	-0.35640000
C	-0.35756500	3.59402500	-0.69630200
H	-1.38126800	3.74109700	-1.02351700
C	0.53064300	4.66466000	-0.60364200
H	0.19226100	5.66522500	-0.85321400
C	1.84314400	4.44976200	-0.17338600
H	2.53028100	5.28307400	-0.06861400
C	2.26751500	3.16240200	0.13395100
H	3.27206900	2.99398400	0.50688500
C	1.39182900	2.05873000	0.03278800

N	1.73165700	0.77683900	0.44250200
O	-0.85949800	1.29889500	-0.50128900
Si	-1.40174700	-0.03889600	0.32972000
C	3.14550800	-1.09896000	0.92112600
C	4.36250900	-1.82758000	0.54575600
H	4.54788800	-2.76185100	1.06541200
C	5.21317800	-1.33771200	-0.38522600
H	6.11681200	-1.88368300	-0.64097500
C	4.94199200	-0.09400900	-1.08413300
H	5.63254900	0.22147300	-1.86010100
C	3.84201300	0.64920000	-0.81486700
H	3.63382700	1.54742400	-1.38397600
C	2.86301800	0.20310200	0.17126100
O	2.41418000	-1.48628800	1.82837300
C	-3.23418900	-0.09289500	-0.04386200
C	-3.98349100	1.09185900	-0.17249700
C	-3.90498900	-1.32125700	-0.18525400
C	-5.35402400	1.05034300	-0.42779100
H	-3.49132200	2.05552100	-0.07685400
C	-5.27724500	-1.36581300	-0.43888600
H	-3.35219600	-2.25302400	-0.10353000
C	-6.00335900	-0.17983800	-0.56014500
H	-5.91489200	1.97526800	-0.52600000
H	-5.77675800	-2.32423400	-0.54611100
H	-7.07040100	-0.21284600	-0.76035200
Cl	-1.18687700	0.26711900	2.39934700
C	-0.54159500	-1.60551900	-0.19657000
C	-0.51210900	-2.75036800	0.61849500
C	0.01138600	-1.68914200	-1.48776900
C	0.04904100	-3.94257000	0.15759300
H	-0.91867500	-2.71251100	1.62515500
C	0.57861100	-2.87803400	-1.94741600
H	0.00756000	-0.81741800	-2.13637700
C	0.59589100	-4.00751500	-1.12529900
H	0.06547000	-4.81655000	0.80200000
H	1.00587300	-2.92358300	-2.94495000
H	1.03542500	-4.93404100	-1.48320000

22. 4-κ[1]-TS-κ[3]

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.075984 a.u.

Imaginary frequencies = -52.72 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.75877000	-0.65402100	2.09468200
C	1.22309900	-0.94219400	3.43818900
H	1.39617300	-1.98270800	3.68859300
C	1.45617000	0.06905900	4.31344500
H	1.82121000	-0.14654100	5.31276300
C	1.26923700	1.44832800	3.92965400
H	1.54491700	2.22571200	4.63426000
C	0.78663800	1.79210100	2.70406200
H	0.71860000	2.83494500	2.43249100
C	0.45606700	0.77005400	1.74310100
N	-0.06335800	0.92657300	0.53808100
O	0.59803700	-1.55171800	1.24723200
Si	-0.10327600	-0.67992000	-0.91063400
C	-0.82587200	1.84050800	-1.44943600
C	-1.31623200	2.87879100	-2.25434800
H	-1.48081900	2.69185900	-3.30922200
C	-1.60260500	4.10427800	-1.67373700
H	-1.99339800	4.90810500	-2.28957900
C	-1.42792700	4.31271800	-0.28948800
H	-1.70860200	5.26238000	0.15234200
C	-0.92297500	3.30787200	0.51370500
H	-0.85496000	3.46791600	1.57979000
C	-0.56971200	2.06008600	-0.05881900
O	-0.59776000	0.63344100	-1.95856500
C	1.80796000	-0.61036600	-1.01368600
C	2.61507400	-1.74583400	-0.81292400
C	2.45100700	0.58928400	-1.36015300
C	4.00151500	-1.68264800	-0.94411300
H	2.15555100	-2.69452700	-0.55675800
C	3.84094400	0.65715900	-1.49776700
H	1.87460600	1.49204300	-1.53608800
C	4.62198300	-0.47823800	-1.28702000
H	4.59841500	-2.57573900	-0.78086300
H	4.30827100	1.59890200	-1.77209800
H	5.70198000	-0.42849700	-1.39212600
C	-1.73876200	-1.32300300	-0.14509000
C	-1.86746300	-2.62983600	0.36405000
C	-2.88736300	-0.51293600	-0.13963300

C	-3.08088500	-3.09907400	0.86509500
H	-1.01033600	-3.29394500	0.36461400
C	-4.10758200	-0.98005600	0.35804400
H	-2.85395100	0.49769300	-0.53237800
C	-4.20851000	-2.27403800	0.86678900
H	-3.14643300	-4.11202900	1.25264100
H	-4.97705800	-0.32863300	0.34449900
H	-5.15474100	-2.63862600	1.25622100
Cl	-0.20280800	-2.22277500	-2.57433900

23. 5-κ^1-TS-κ^3

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.067114 a.u.

Imaginary frequencies = -61.60 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-1.67345500	-1.78307200	-1.23023600
C	-2.55518600	-2.88578500	-1.59780400
H	-2.10156800	-3.71169700	-2.13459400
C	-3.86589900	-2.87439700	-1.25397900
H	-4.50896600	-3.70749400	-1.52105500
C	-4.43018000	-1.78422000	-0.48891500
H	-5.46131100	-1.85997400	-0.15972700
C	-3.69258300	-0.69536200	-0.14762200
H	-4.12579800	0.07225300	0.47855400
C	-2.29967200	-0.59993200	-0.52656300
N	-1.49111200	0.40746000	-0.29059300
O	-0.46833600	-1.79890900	-1.50644800
Si	0.80868100	0.31682600	-0.31553700
C	-0.64818300	2.38483400	0.60444000
C	-0.76580000	3.68515900	1.10687000
H	0.12342600	4.19248000	1.46348000
C	-2.00931000	4.30307200	1.10804500
H	-2.10081700	5.31671600	1.48535600
C	-3.14244200	3.64810600	0.59098000
H	-4.09427900	4.16615100	0.54754800
C	-3.04445800	2.35224300	0.11471400
H	-3.90843600	1.88287600	-0.33593800
C	-1.80098500	1.67504700	0.15410400
O	0.55091900	1.79292900	0.53996100
C	2.71537000	0.34995600	-0.45529400
C	3.46155200	0.87285100	0.61870000
C	3.43144700	-0.19354000	-1.53625200
C	4.85780700	0.86880100	0.60651900

H	2.94689500	1.30056700	1.47499200
C	4.82843600	-0.21786200	-1.54646300
H	2.89461000	-0.59590800	-2.39048100
C	5.54664600	0.31792200	-0.47615800
H	5.40705600	1.29370000	1.44246400
H	5.35470800	-0.64836500	-2.39417500
H	6.63297100	0.30816700	-0.48604700
Cl	0.45187300	0.87705100	-2.39759700
C	0.62430000	-1.07524500	0.97998900
C	1.35138600	-2.27289900	0.84975900
C	-0.12766400	-0.89473800	2.15331500
C	1.31060800	-3.25745700	1.83686900
H	1.96001900	-2.44053900	-0.03369500
C	-0.15995300	-1.87079000	3.15302400
H	-0.69476300	0.01894900	2.30520800
C	0.55374800	-3.05910800	2.99436400
H	1.87373800	-4.17718900	1.70499100
H	-0.74301000	-1.70040400	4.05390100
H	0.52608400	-3.82162900	3.76749600

24. 4-κ^3-Ph(Cl)(Ph)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.082775 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.19699300	0.01155200	0.10057100
C	3.57015100	-0.33185900	0.18616000
H	4.30729900	0.46233900	0.17553000
C	3.92066400	-1.65652600	0.28522100
H	4.96923400	-1.92817500	0.35438400
C	2.93909200	-2.69284800	0.31376200
H	3.26145600	-3.72297400	0.41631700
C	1.60203000	-2.40285700	0.22477100
H	0.87535900	-3.20045700	0.27651800
C	1.19067600	-1.04275800	0.10386500
N	-0.04208000	-0.51704500	-0.00008700
O	1.80044300	1.23894600	0.00206000
Si	-0.03791500	1.51892300	-0.00015600
C	-2.27904300	0.02053300	-0.10042200
C	-3.65358900	-0.31742100	-0.18582300
H	-4.38757300	0.47970000	-0.17501100
C	-4.00936800	-1.64065900	-0.28503200
H	-5.05901100	-1.90814400	-0.35413600
C	-3.03192500	-2.68088500	-0.31377200
H	-3.35841300	-3.70971000	-0.41636400

C	-1.69371800	-2.39624400	-0.22486700
H	-0.97023900	-3.19673100	-0.27669700
C	-1.27692100	-1.03779900	-0.10395300
O	-1.87757800	1.24628600	-0.00189400
C	0.00057200	1.48702900	1.97842700
C	1.08743500	2.07696800	2.65675000
C	-0.99999900	0.91583900	2.78266000
C	1.16925200	2.09564100	4.04967400
H	1.88200000	2.54521900	2.08587300
C	-0.92751800	0.92810100	4.17978100
H	-1.87215000	0.45030100	2.33688000
C	0.15963200	1.51800800	4.82216900
H	2.02314900	2.56542100	4.53110000
H	-1.72722200	0.47727000	4.76176600
H	0.21906600	1.53044800	5.90689900
Cl	-0.03350300	3.77008900	-0.00014000
C	-0.07697700	1.48714100	-1.97860300
C	-1.16148500	2.08153400	-2.65678000
C	0.92118000	0.91189100	-2.78290200
C	-1.24345400	2.10037400	-4.04969100
H	-1.95394900	2.55320600	-2.08579200
C	0.84853700	0.92427900	-4.18001200
H	1.79154200	0.44296900	-2.33714300
C	-0.23634100	1.51849800	-4.82228700
H	-2.09548400	2.57361600	-4.53103500
H	1.64632600	0.47016500	-4.76207300
H	-0.29591800	1.53102900	-5.90700800

25. 5-κ^3-Ph_2(Cl)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.092751 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.82282800	2.19214300	-0.61599100
C	1.07119900	3.57720300	-0.75742100
H	0.23194200	4.25116000	-0.88155600
C	2.37211800	4.02113200	-0.73332600
H	2.57640000	5.08156700	-0.84130600
C	3.46975000	3.12442200	-0.56301600
H	4.47776400	3.52277200	-0.53847200
C	3.26652900	1.77558200	-0.42542300
H	4.11001900	1.11669600	-0.28260900
C	1.93428200	1.27001500	-0.45358300
N	1.47864900	0.01185600	-0.35720300
O	-0.37363500	1.69716400	-0.63094300

Si	-0.55427000	-0.08848000	-0.30133100
C	1.05019500	-2.23341300	-0.20027900
C	1.43756800	-3.58990400	-0.10770400
H	0.67022200	-4.35301700	-0.05570100
C	2.77888400	-3.89448500	-0.09651800
H	3.08975800	-4.93228500	-0.03112100
C	3.78079500	-2.88169800	-0.17685100
H	4.82558100	-3.17116700	-0.17535100
C	3.44117800	-1.55558700	-0.26106500
H	4.21650000	-0.80732900	-0.33614900
C	2.06289900	-1.19342500	-0.26835500
O	-0.19368800	-1.86730300	-0.22612900
Cl	-0.07668300	-0.32667400	-2.77034500
C	-2.41515100	-0.22285100	-0.65985800
C	-3.13609900	0.79389700	-1.31139900
C	-3.13801900	-1.34294600	-0.21022600
C	-4.51540500	0.69723400	-1.50608800
H	-2.61320000	1.67000400	-1.68107900
C	-4.51694700	-1.44859300	-0.40776300
H	-2.62003400	-2.14895700	0.30102900
C	-5.21189200	-0.42644600	-1.05597900
H	-5.04591000	1.49882900	-2.01336200
H	-5.04715800	-2.32872500	-0.05360300
H	-6.28469400	-0.50431500	-1.20935100
C	-0.55414400	0.17496600	1.63584700
C	-1.28042200	1.26431000	2.15872800
C	0.07399100	-0.67097600	2.56477700
C	-1.37229700	1.49631400	3.53224500
H	-1.79230800	1.94079200	1.48080800
C	-0.01025300	-0.44657600	3.94199800
H	0.64640100	-1.53150100	2.23106500
C	-0.73391100	0.64075700	4.43205500
H	-1.94384200	2.34511800	3.89830000
H	0.48924500	-1.12399900	4.62944700
H	-0.80132100	0.81822100	5.50168100

26. 4-TS-NPh

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.066107 a.u.

Imaginary frequencies = -183.33 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-0.03059100	2.23825900	0.26608800
C	0.00558600	3.62322600	0.49802300

H	-0.24541300	4.30370800	-0.30753300
C	0.34571400	4.07314100	1.76301900
H	0.35799900	5.13936000	1.96506200
C	0.67918100	3.17015900	2.79721400
H	0.93753100	3.55380000	3.77820400
C	0.68292100	1.80415000	2.57908800
H	0.94067200	1.13445300	3.38640200
C	0.30572300	1.31684200	1.30941100
N	0.23124900	0.03826500	0.82288000
O	-0.31876600	1.70995600	-0.91198200
Si	-0.53110800	-0.06071700	-0.93048500
C	0.12353300	-2.21386900	0.45936100
C	0.27072100	-3.56592700	0.79702800
H	0.04773200	-4.32753000	0.05843600
C	0.68892400	-3.88634300	2.08035500
H	0.79056700	-4.92920100	2.36343700
C	0.99129000	-2.88196000	3.02315700
H	1.32044900	-3.16218400	4.01785300
C	0.87862200	-1.54047000	2.69615400
H	1.13019100	-0.78934100	3.43071200
C	0.41839800	-1.19175700	1.41119700
O	-0.23505000	-1.80328100	-0.75151700
Cl	-0.42665200	-0.15253700	-3.09049700
C	2.00025200	0.02139900	-0.88778500
C	2.62973600	-1.17263900	-1.20861500
C	2.67571400	1.22293400	-0.82463100
C	3.99590000	-1.13676600	-1.52519900
H	2.10218200	-2.11750800	-1.24222000
C	4.04198600	1.24656800	-1.14501600
H	2.19415800	2.15047300	-0.52912500
C	4.69991800	0.06747700	-1.49436900
H	4.49791400	-2.06111800	-1.79832900
H	4.57987700	2.18989300	-1.10979500
H	5.75903200	0.08534300	-1.73301300
C	-2.41340200	-0.08537400	-0.60476100
C	-3.17462200	1.10079300	-0.57154800
C	-3.10965100	-1.29385200	-0.40040800
C	-4.55129700	1.08378000	-0.33826400
H	-2.69010300	2.05644800	-0.74032100
C	-4.48616000	-1.31810600	-0.16609500
H	-2.57334500	-2.23586900	-0.43419500
C	-5.21317300	-0.12741700	-0.13147400
H	-5.10630100	2.01786400	-0.32086600
H	-4.98993800	-2.26875600	-0.01341400
H	-6.28415900	-0.14341000	0.05019000

27. 5-TS-NPh

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.0724 a.u.

Imaginary frequencies = -244.81 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.89764200	-2.16798100	-0.74690000
C	1.24920300	-3.51828900	-0.89633600
H	0.48344900	-4.24299500	-1.14817400
C	2.57608200	-3.87919000	-0.72326900
H	2.86742500	-4.91735800	-0.84734900
C	3.55669000	-2.92272900	-0.38355100
H	4.58705900	-3.23522300	-0.25363400
C	3.22312400	-1.59011700	-0.21095700
H	3.99150200	-0.87986100	0.05574000
C	1.88691700	-1.19250800	-0.41818100
N	1.29255300	0.04703000	-0.33044500
O	-0.34361800	-1.72339000	-0.84825200
Si	-0.56252500	0.04361000	-0.82601200
C	0.80943700	2.28094300	-0.42849500
C	1.10447400	3.65103600	-0.38128600
H	0.31032500	4.37247100	-0.53612500
C	2.41439000	4.03817000	-0.14228800
H	2.66181500	5.09464200	-0.11420400
C	3.43146500	3.08467700	0.07223500
H	4.44647900	3.41678100	0.26104200
C	3.15235400	1.72799400	0.04900600
H	3.94628500	1.01855400	0.22914200
C	1.83646000	1.31105300	-0.23158900
O	-0.41306500	1.80377300	-0.59948100
Cl	-0.29915400	0.20349000	-3.01479900
C	-0.07581900	-0.11761100	1.56055800
C	-0.21976400	1.04446900	2.30353100
C	-0.02907600	-1.37065300	2.14789800
C	-0.41283500	0.93269500	3.68723800
H	-0.20320800	2.02910200	1.85063500
C	-0.22416300	-1.47061300	3.53245600
H	0.15104800	-2.27509300	1.57628400
C	-0.41740800	-0.32125100	4.29985900
H	-0.55344600	1.83426500	4.27680000
H	-0.21226700	-2.45061200	4.00098300
H	-0.55360400	-0.40122000	5.37399200
C	-2.43973200	-0.00555200	-0.57761700
C	-3.10372500	-1.18325000	-0.18871400

C	-3.22583700	1.14326000	-0.79194500
C	-4.49003900	-1.21643200	-0.02555500
H	-2.53062600	-2.08581300	-0.00849400
C	-4.61243700	1.11352700	-0.63404200
H	-2.75018500	2.07193300	-1.08721600
C	-5.25024600	-0.06732600	-0.24890900
H	-4.97517300	-2.14053000	0.27674700
H	-5.19419500	2.01399000	-0.81136300
H	-6.32907800	-0.09112300	-0.12294900

28. 4-NPh-Ph(Cl)Si(ON[Ph]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.157688 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.07090900	0.09112400	0.02091600
O	-0.52723500	-1.40626700	0.42479700
O	-0.68997700	0.77602300	-1.27551700
N	-2.98290100	-0.06523700	0.15201800
C	-2.80954600	-1.39389700	-0.36967400
C	-1.57087800	-2.03611100	-0.21246700
C	-1.38252600	-3.33704000	-0.68291900
H	-0.41609800	-3.80947500	-0.54374000
C	-2.42660000	-3.99611400	-1.33000700
H	-2.27433300	-5.00630200	-1.69714900
C	-3.65647700	-3.35902100	-1.51581700
H	-4.46642800	-3.86892700	-2.02716900
C	-3.84224000	-2.06385800	-1.03487200
H	-4.79438400	-1.55828800	-1.16241000
C	-3.07139600	0.97652900	-0.82392300
C	-1.90669300	1.36934100	-1.50752800
C	-1.96034900	2.35846000	-2.49121400
H	-1.04381300	2.63179300	-3.00309000
C	-3.17187300	2.97700900	-2.79244400
H	-3.20470700	3.74911000	-3.55460200
C	-4.33532900	2.60472400	-2.11412100
H	-5.28240600	3.08104400	-2.34631300
C	-4.28179500	1.60642600	-1.14378000
H	-5.18001500	1.30699200	-0.61355400
C	-3.55263500	0.10007800	1.44273900
C	-3.71507500	1.38561200	1.99273100
C	-3.91785700	-1.01203500	2.22067800
C	-4.23863700	1.54509400	3.27325100
H	-3.42326800	2.25800700	1.42058000

C	-4.43315600	-0.83719200	3.50566800
H	-3.80019700	-2.01334400	1.82477000
C	-4.60352000	0.43816800	4.04357600
H	-4.35331700	2.54887200	3.67272000
H	-4.70709000	-1.71459300	4.08484500
H	-5.00897300	0.56859900	5.04189200
Cl	-0.07686400	1.32570600	1.69358000
C	1.84784200	-0.10803200	-0.46284600
C	2.57402900	-1.24514200	-0.06453000
C	2.50376700	0.87646300	-1.22508200
C	3.91764700	-1.39049800	-0.41242100
H	2.08523700	-2.02291300	0.51436600
C	3.84576700	0.72962400	-1.57499200
H	1.96277900	1.75900900	-1.55443200
C	4.55434800	-0.40324800	-1.16707000
H	4.46506100	-2.27413800	-0.09821400
H	4.33754800	1.49596200	-2.16666600
H	5.59949500	-0.51710500	-1.43954800

29. 5-NPh-Cl(Ph)Si(ON[Ph]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1880.157627 a.u.

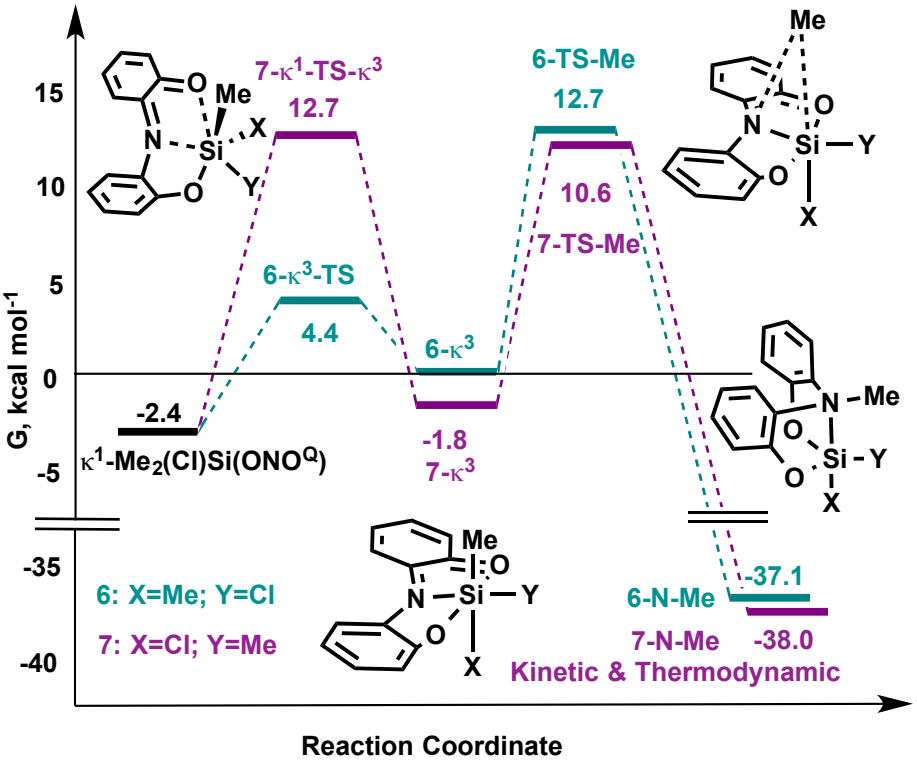
Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	-0.05817000	-0.07540800	0.18117000
O	-0.62323400	-1.63120700	0.33743100
O	-0.66098400	0.73925100	-1.13215000
N	-2.98719900	-0.14853100	0.16119300
C	-2.89174200	-1.44380200	-0.46310500
C	-1.68924200	-2.15893800	-0.35038900
C	-1.56294700	-3.42814400	-0.91775700
H	-0.62337100	-3.95937400	-0.81130800
C	-2.63532800	-3.98012900	-1.61653800
H	-2.53294500	-4.96563400	-2.06000700
C	-3.82956600	-3.26780400	-1.75760200
H	-4.66028100	-3.69469400	-2.30996300
C	-3.95334700	-2.00471600	-1.18068100
H	-4.87721200	-1.44273700	-1.27521400
C	-3.04762500	0.95832100	-0.74793000
C	-1.85753000	1.36984200	-1.37111000
C	-1.86503400	2.41751100	-2.29352800
H	-0.93027400	2.70649800	-2.76184700
C	-3.05901300	3.07264200	-2.58912800
H	-3.05826700	3.88999300	-3.30332100
C	-4.24796200	2.68081100	-1.96812000

H	-5.17950900	3.18828400	-2.19680300
C	-4.23931200	1.62495900	-1.05859400
H	-5.15656300	1.31182500	-0.57055300
C	-3.59928000	-0.05100800	1.44403600
C	-3.72443900	1.19944400	2.07622000
C	-4.03885800	-1.19686100	2.12678700
C	-4.28979400	1.29442000	3.34524400
H	-3.36991100	2.09372600	1.57787200
C	-4.59552000	-1.08769500	3.40221100
H	-3.94975800	-2.17228100	1.66444300
C	-4.73243300	0.15440400	4.02092200
H	-4.37604200	2.27204000	3.81087400
H	-4.92927700	-1.98921900	3.90818800
H	-5.17152000	0.23414200	5.01032400
Cl	1.93635600	-0.34300200	-0.41028900
C	-0.08812200	0.84792700	1.78127600
C	-0.23671600	0.16562100	3.00209900
C	0.06982800	2.24613800	1.80101800
C	-0.21710900	0.86199300	4.21061300
H	-0.37574300	-0.91116400	3.00677500
C	0.08208200	2.94180500	3.00991700
H	0.18349700	2.79712100	0.87126100
C	-0.05768300	2.24942400	4.21510600
H	-0.33131300	0.32366000	5.14659100
H	0.20207500	4.02098500	3.01201400
H	-0.04444900	2.79109900	5.15633200

VI. DFT Calculations for the Reactions of $Me_2(Cl)Si(ONO^Q)$

Figure S6. Calculated reaction coordinate for migration of $Me_2(Cl)Si(ONO^Q)$. Free energies are given in kcal mol^{-1}.



30. κ^1-$Me_2(Cl)Si(ONO^Q)$

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.717533a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	0.20733600	-0.01386400	-0.24892700
C	0.36757100	1.09810100	0.58282500
H	-0.23462200	1.15245600	1.48340500
C	1.28712800	2.09526200	0.26909900
H	1.41006500	2.94064900	0.93867900
C	2.06118800	1.99598400	-0.89215400
H	2.80421700	2.75184400	-1.12435500
C	1.88744100	0.91309500	-1.74292600
H	2.51719500	0.80455600	-2.61908700
C	0.94997100	-0.10771500	-1.45716200
N	0.83548800	-1.26641300	-2.20847000
O	-0.71495700	-0.92875300	0.13863700

Si	-1.24466100	-2.49472200	-0.12069000
C	1.01486500	-2.69850700	-4.12141800
C	0.99155000	-2.77992000	-5.58413700
H	1.07539500	-3.77171700	-6.01584800
C	0.88033300	-1.66698200	-6.34660700
H	0.86984000	-1.74673000	-7.42989800
C	0.74335100	-0.34977000	-5.75364800
H	0.59155700	0.49948500	-6.41242300
C	0.76285600	-0.17016200	-4.41082800
H	0.60481700	0.81442800	-3.98735000
C	0.88544400	-1.30738100	-3.50627500
O	1.18232900	-3.69901900	-3.42434600
C	-2.48170200	-2.75865100	1.25255400
Cl	-2.36056500	-2.53159300	-1.91865300
H	-1.97429200	-2.73934400	2.22308900
H	-3.24981900	-1.98026800	1.25218600
H	-2.97474800	-3.72969700	1.14582200
C	0.09059800	-3.78847500	-0.17800600
H	0.78150800	-3.63812800	0.65923100
H	-0.35898300	-4.78155900	-0.07036300
H	0.64568400	-3.73975500	-1.11655100

31. 6-κ^1-TS-κ^3

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.706582 a.u.

Imaginary frequencies = -72.62 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	-2.24393200	-0.87374900	0.14754500
C	-3.68921400	-0.97149300	0.20308900
H	-4.11256300	-1.95496000	0.37344800
C	-4.45924400	0.13234800	0.01660200
H	-5.54157500	0.05174200	0.04308800
C	-3.87079000	1.42072500	-0.25811800
H	-4.52627100	2.25756900	-0.47420900
C	-2.52077000	1.59800600	-0.27997200
H	-2.11379400	2.56205800	-0.54753200
C	-1.64008200	0.48412000	-0.03755500
N	-0.31727800	0.48973300	0.01168100
O	-1.50805800	-1.87386400	0.26558400
Si	0.79957900	-1.35254300	-0.00498100
C	1.91844000	1.07815700	-0.12317600
C	2.97710500	2.00285700	-0.16740000
H	3.98744500	1.63415200	-0.30227100

C	2.70420000	3.34959500	-0.01314600
H	3.51981000	4.06561200	-0.03458100
C	1.38450600	3.80904100	0.20599200
H	1.20414100	4.86471600	0.37598600
C	0.32838000	2.92252500	0.22885800
H	-0.66315500	3.28638300	0.45600300
C	0.56595400	1.53670200	0.02543100
O	2.14637100	-0.21875600	-0.22047500
C	0.27043500	-1.70949400	-1.79804100
H	-0.47523300	-1.00611800	-2.17559300
H	1.16510200	-1.64518900	-2.42344200
H	-0.12711000	-2.72180500	-1.88157600
C	0.64299100	-1.49711500	1.88511200
H	0.29492300	-2.49349500	2.16081300
H	1.63920400	-1.35647600	2.31492600
H	-0.03771800	-0.75832000	2.31496100
Cl	2.20583900	-3.19004700	-0.04613300

32. 7-κ^1-TS-κ^3

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.693426 a.u.

Imaginary frequencies = -95.97 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.39060800	-0.42026000	0.08588200
C	3.80858900	-0.08621000	0.16444100
H	4.49328500	-0.91038000	0.33211900
C	4.23446400	1.19005600	-0.00062300
H	5.29443900	1.42210900	0.04098400
C	3.30377700	2.26092800	-0.27971500
H	3.69731700	3.24938600	-0.49280600
C	1.96219600	2.04742200	-0.31205700
H	1.29687400	2.85564800	-0.58222900
C	1.41888100	0.72607900	-0.08119800
N	0.14819400	0.39364900	-0.04143000
O	1.99602400	-1.58983600	0.17308000
Si	-0.65933700	-1.74740300	-0.31401300
C	-2.16316200	0.49505500	-0.29778700
C	-3.39244700	1.16585700	-0.33388100
H	-4.28688900	0.60626200	-0.58355800
C	-3.44073900	2.51676300	-0.02148600
H	-4.39485300	3.03431100	-0.03623500
C	-2.27626000	3.21514900	0.35231900

H	-2.34146200	4.25624000	0.64927300
C	-1.05126800	2.57315700	0.36597500
H	-0.17570200	3.10367100	0.71465500
C	-0.96001600	1.20781500	-0.00484600
O	-2.10758800	-0.81625800	-0.53772100
C	-1.38389700	-3.50417800	-0.34715100
Cl	-0.42239700	-1.73493100	1.87800000
H	-1.77117600	-3.73604000	-1.34601600
H	-0.60592600	-4.24018000	-0.11502300
H	-2.18987600	-3.63189100	0.38007800
C	0.23476900	-1.75283200	-1.99500400
H	0.87888200	-2.63285600	-2.06578800
H	-0.56031900	-1.86633200	-2.74257600
H	0.81905300	-0.86807700	-2.24475200

33. 6-κ^3-Me(Cl)(Me)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.713665 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.24287900	0.06709900	0.01264200
C	3.61659700	-0.29948100	0.01972500
H	4.36124800	0.48773200	0.04004200
C	3.95613300	-1.62840600	-0.00391000
H	5.00328100	-1.91446800	-0.00087700
C	2.96248800	-2.65395300	-0.03924700
H	3.27510700	-3.69186000	-0.06816300
C	1.62743700	-2.34484300	-0.04156400
H	0.89875000	-3.14071500	-0.08052700
C	1.22099600	-0.97607400	-0.00783800
N	-0.01122800	-0.43963500	0.00041600
O	1.86908400	1.30044700	0.02530700
Si	0.01128500	1.62230200	-0.00063000
C	-2.25399800	0.11550700	-0.01243700
C	-3.63533600	-0.22182300	-0.01938600
H	-4.36310400	0.58102000	-0.04007300
C	-4.00299600	-1.54317300	0.00468600
H	-5.05598200	-1.80692400	0.00166800
C	-3.03141100	-2.58966800	0.04038800
H	-3.36605400	-3.62068500	0.06952800
C	-1.69014100	-2.30903600	0.04278900
H	-0.97846500	-3.12006100	0.08211600
C	-1.25458600	-0.94930700	0.00869200
O	-1.85373900	1.34033700	-0.02592500

C	0.03634000	1.63089700	-1.94129300
H	0.93025700	2.14898200	-2.29532800
H	0.03266800	0.62308300	-2.36961400
H	-0.83805900	2.16539000	-2.31873500
C	-0.01415500	1.63405300	1.94000300
H	0.86822200	2.15588100	2.31654500
H	-0.90014200	2.16591500	2.29361100
H	-0.02519700	0.62684400	2.36963000
Cl	0.03420500	3.92037200	-0.00238700

34. 7-κ^3-Me_2(Cl)Si(ONO^Q)

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.716534 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.23600200	0.14766800	-0.05562600
C	3.61266900	-0.18341900	-0.06654300
H	4.34326800	0.61644400	-0.09057800
C	3.97538700	-1.50862700	-0.04401000
H	5.02754900	-1.77513100	-0.05085800
C	3.00243200	-2.55280900	-0.01558100
H	3.33530400	-3.58462900	-0.00598200
C	1.66084200	-2.26989200	-0.00285500
H	0.94491500	-3.07808900	0.01217500
C	1.23746200	-0.90847900	-0.01878500
N	0.00355700	-0.38000900	-0.00858800
O	1.81734000	1.37075000	-0.07887900
Si	0.00902400	1.64917600	-0.21550900
C	-2.22563400	0.16463000	-0.00539000
C	-3.60454500	-0.15657000	0.01342600
H	-4.32988900	0.64777300	-0.01892700
C	-3.97606300	-1.47784800	0.08037800
H	-5.03002100	-1.73657800	0.09902600
C	-3.01003700	-2.52749600	0.13209300
H	-3.34971700	-3.55532900	0.19311100
C	-1.66655700	-2.25439700	0.10978400
H	-0.95569900	-3.06549100	0.16140100
C	-1.23412700	-0.89810600	0.03127500
O	-1.79916200	1.38414800	-0.05894500
Cl	0.02425800	1.31992700	2.36244200
C	0.02533500	3.51123000	0.11905300
H	0.88798100	3.78921600	0.72792500
H	0.07355600	4.06488100	-0.82596700
H	-0.87716700	3.81754000	0.65273100
C	-0.01252200	1.53024100	-2.14637800

H	-0.86656900	2.10109300	-2.52395900
H	0.89870100	1.98482500	-2.54704300
H	-0.08621300	0.51399000	-2.54428200

35. 6-TS-NMe

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.693463 a.u.

Imaginary frequencies = -227.64 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.23115300	-0.01329100	0.01538500
C	3.59889800	-0.31399700	-0.02983100
H	4.32057100	0.49397200	-0.07188800
C	3.98742600	-1.64580600	0.00329600
H	5.04410500	-1.89385800	-0.00529700
C	3.03428700	-2.68308900	0.04821200
H	3.36599200	-3.71538400	0.07838600
C	1.67623900	-2.40402100	0.05191500
H	0.96425100	-3.21607600	0.08505000
C	1.25953000	-1.05857200	0.05262200
N	-0.00117500	-0.50226100	0.03013600
O	1.75420300	1.22590700	-0.03791000
Si	0.00207800	1.38014900	0.28328500
C	-2.23276200	-0.01238000	0.03797900
C	-3.60116500	-0.31161400	0.00338600
H	-4.32288500	0.49717500	-0.01558000
C	-3.98989000	-1.64374500	0.01307900
H	-5.04672200	-1.89130800	0.01161500
C	-3.03682800	-2.68216500	0.01923100
H	-3.36877900	-3.71481600	0.02274000
C	-1.67875500	-2.40351900	0.01503100
H	-0.96688200	-3.21627800	0.00529800
C	-1.26152100	-1.05859400	0.05021200
O	-1.75539300	1.22691900	-0.00473100
Cl	-0.00668800	3.45600900	-0.37924200
C	-0.00953100	0.60696300	-2.12295900
H	0.89297400	0.04620000	-2.33812300
H	-0.94276100	0.09336900	-2.32498200
H	0.01592200	1.65279000	-2.41236200
C	0.02911500	1.58785400	2.16277700
H	0.86934700	2.21844300	2.46584800
H	-0.89336100	2.05683400	2.51566700
H	0.13339300	0.62377000	2.67292100

36. 7-TS-NMe

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.696767 a.u.

Imaginary frequencies = -272.22 cm^{-1}

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
C	2.23499800	-0.08442300	0.14902700
C	3.59957900	0.22574500	0.09435900
H	4.33103100	-0.56698000	0.20386700
C	3.97185700	1.54607400	-0.11631900
H	5.02517900	1.80042800	-0.18031200
C	3.00584000	2.56283100	-0.24974200
H	3.32305000	3.58580500	-0.42128900
C	1.65166300	2.27602000	-0.16445400
H	0.93198800	3.07396200	-0.27248300
C	1.25180800	0.93890100	0.02084200
N	-0.00548300	0.37945200	0.15308300
O	1.76662300	-1.30461600	0.37832500
Si	0.00478400	-1.52692000	0.16338700
C	-2.24077900	-0.10448000	0.10394000
C	-3.60712400	0.19441300	0.03094500
H	-4.33269800	-0.60831100	0.09860400
C	-3.98855700	1.51837800	-0.13584800
H	-5.04298500	1.76493900	-0.21116700
C	-3.03116400	2.55007200	-0.20102900
H	-3.35638300	3.57738000	-0.32503900
C	-1.67611300	2.27260000	-0.10212800
H	-0.96398700	3.08390100	-0.13593500
C	-1.26556800	0.93145900	0.02293700
O	-1.76549000	-1.32543200	0.31312900
C	-0.01758200	-0.37478100	2.37191500
H	0.84867900	0.25593400	2.53498500
H	-0.97960900	0.10090500	2.52632700
H	0.06955000	-1.37417700	2.78941900
C	-0.00448500	-3.30066200	0.80953200
H	0.92743700	-3.80222500	0.53783900
H	-0.11579300	-3.35682200	1.89628400
H	-0.83970800	-3.84572900	0.36226600
Cl	0.04884400	-1.81416300	-2.00575700

37. 6-NMe-Me(Cl)Si(ON[Me]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.772845 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	0.08786600	-0.03765000	-0.04294000
O	-0.39773500	-1.63326300	-0.04378000
O	-0.53375900	0.88422100	-1.28089400
N	-2.68816400	-0.07354800	0.14570300
C	-2.77160400	-1.40155100	-0.41498200
C	-1.59253900	-2.15915000	-0.45888700
C	-1.60994100	-3.47444500	-0.92937100
H	-0.68300100	-4.03765600	-0.94868900
C	-2.80879800	-4.03211300	-1.36986800
H	-2.81931500	-5.05372600	-1.73717600
C	-3.98813100	-3.28202200	-1.34807800
H	-4.91942100	-3.71477000	-1.69913900
C	-3.96451300	-1.97225100	-0.87010500
H	-4.87614900	-1.38279600	-0.84684800
C	-2.89458700	1.00133200	-0.78173700
C	-1.76330800	1.45667400	-1.47994900
C	-1.86244600	2.50292400	-2.39639500
H	-0.96957300	2.82875900	-2.91940700
C	-3.09579700	3.11941700	-2.60896200
H	-3.17015600	3.93702000	-3.31920600
C	-4.22327100	2.69636000	-1.90283400
H	-5.18146200	3.18179300	-2.05843300
C	-4.12006400	1.64082200	-0.99474400
H	-4.99686600	1.31373400	-0.44522100
C	-3.39136400	0.05352300	1.43331100
H	-3.20377300	1.04697600	1.84444600
H	-4.47544300	-0.10146200	1.35055700
H	-2.99093100	-0.69130000	2.12444000
C	1.91251800	-0.11265400	-0.38629700
H	2.35970800	0.88421500	-0.34569300
H	2.41828300	-0.74652300	0.34752000
H	2.08946700	-0.53184300	-1.38163000
Cl	-0.08501300	0.87366400	1.84296100

38. 7-NMe-Cl(Me)Si(ON[Me]O)

Energy of optimized structure (sum of electronic and thermal free energies) = -1496.774289 a.u.

Cartesian coordinates of optimized structure:

Atom Type	Coordinates (Å) X	Y	Z
Si	-0.08882100	-0.00933200	0.09557000
O	-0.39410000	-1.65747200	-0.03029500
O	-0.50537400	0.90084800	-1.25581000
N	-2.59328500	-0.07388200	0.14454400
C	-2.74286000	-1.40287600	-0.42547600
C	-1.58105400	-2.18283500	-0.46013200
C	-1.62189200	-3.49511100	-0.93483800
H	-0.70885600	-4.08026800	-0.95118500
C	-2.83278100	-4.01861700	-1.38577500
H	-2.86673100	-5.03780000	-1.75819400
C	-3.99480900	-3.24091400	-1.37093300
H	-4.93220300	-3.65107100	-1.73208500
C	-3.94839600	-1.93261100	-0.88884000
H	-4.84632000	-1.32279500	-0.87528800
C	-2.85445600	1.00305700	-0.78487400
C	-1.73003900	1.46815600	-1.48215100
C	-1.84559800	2.50277200	-2.40935900
H	-0.95988400	2.84248900	-2.93523900
C	-3.09430700	3.08539200	-2.62963700
H	-3.18657000	3.89341800	-3.34866300
C	-4.21636100	2.64453700	-1.92455900
H	-5.18357700	3.10764700	-2.09020700
C	-4.09620500	1.60238200	-1.00220000
H	-4.96782600	1.26453900	-0.45134600
C	-3.29763400	0.04761200	1.44184600
Cl	2.00525200	-0.12192900	-0.31534300
H	-3.11815500	1.03948400	1.85904100
H	-4.37783300	-0.10712600	1.34350700
H	-2.90524900	-0.70770700	2.12539700
C	-0.15519500	0.81119700	1.77118600
H	-0.78503700	1.70451400	1.73399500
H	-0.57152800	0.13183900	2.51944700
H	0.84528900	1.10712500	2.09161200