Supporting Information

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Cycloaddition reactions of silacyclopropylidenoids to ethylene

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**Table S1**: Cartesian coordinates of the optimized structure and energy values for **1F** by B3LYP/6-311+G(d,p).

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| Li   | -1.2670763858 | 0.0718659876 | -0.0066783967 |
| Si   | 0.984872737 | -0.788050492 | -0.0016007598 |
| C    | 2.6874688772 | -0.451187283 | -0.7641040981 |
| H    | 2.845785709 | 0.5065375548 | -1.2527984863 |
| H    | 3.217833873 | -1.2623205049 | -1.2566050507 |
| C    | 2.6836752142 | -0.4522597247 | 0.7698120684 |
| H    | 3.2116251937 | -1.2641691579 | 1.2637387344 |
| H    | 2.8395275987 | 0.5046809001 | 1.2606973116 |
| F    | 0.2312768207 | 0.9371615853 | -0.0024311028 |

Zero-point correction= 0.056221 (Hartree/Particle)
Thermal correction to Energy= 0.062641
Thermal correction to Enthalpy= 0.063585
Thermal correction to Gibbs Free Energy= 0.026519

Sum of electronic and zero-point Energies= -475.537802
Sum of electronic and thermal Energies= -475.531382
Sum of electronic and thermal Enthalpies= -475.530437
Sum of electronic and thermal Free Energies= -475.567504

**Table S2**: Cartesian coordinates of the optimized structure and energy values for **1Cl** by B3LYP/6-311+G(d,p).

| Atom | X (Å) | Y (Å) | Z (Å) |
|------|-------|-------|-------|
| Li   | -1.304826172 | -0.0764702087 | -0.0068099243 |
| Si   | 1.0318694811 | -0.7412827495 | -0.0015465561 |
| C    | 2.7498540495 | -0.4739095481 | -0.76115254 |
| H    | 2.9539840227 | 0.4704748837 | -1.2564194869 |
| H    | 3.2269201485 | -1.3168726192 | -1.2554713983 |
| C    | 2.7459984839 | -0.4749712981 | 0.7670951839 |
| H    | 3.2205722684 | -1.3186211157 | 1.2626401479 |
| H    | 2.9476238215 | 0.4687239506 | 1.2646961406 |
| Cl   | 0.1245148964 | 1.5494487051 | -0.0022075668 |

Zero-point correction= 0.055493 (Hartree/Particle)
Thermal correction to Energy= 0.062300
Thermal correction to Enthalpy= 0.063244
Thermal correction to Gibbs Free Energy= 0.024456

Sum of electronic and zero-point Energies= -835.890021
Sum of electronic and thermal Energies= -835.883214
Sum of electronic and thermal Enthalpies= -835.882270
Sum of electronic and thermal Free Energies= -835.921058
**Table S3:** Cartesian coordinates of the optimized structure and energy values for 1Br by B3LYP/6-31+G(d,p).

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Li      | -1.310566 | -0.091613  | -0.006843  |
| Si      | -0.706573 | 0.454296   | 0.125672   |
| C       | 0.483038  | -0.766657  | -1.001486  |
| H       | -1.255438 | -0.002139  | 0.760620   |
| Br      | 0.003545  | 0.006843   | 1.754655   |

**Table S4:** Cartesian coordinates of the optimized structure and energy values for 5F by B3LYP/6-31+G(d,p).

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 3.313897  | -1.191716  | 1.015223   |
| Si      | -0.617158 | 0.072559   | 0.054134   |
| C       | -2.866564 | 1.015223   | -0.108266  |
| H       | -3.01655  | 0.185831   | -3.526856  |
| C       | 0.175674  | 0.485921   | -2.923617  |
| Li      | -0.716241 | -0.002139  | 0.099435   |

**Zero-point correction** = 0.055193 (Hartree/Particle)

**Thermal correction to Energy** = 0.062158

**Thermal correction to Enthalpy** = 0.063102

**Thermal correction to Gibbs Free Energy** = 0.022934

**Sum of electronic and zero-point Energies** = -2949.812600

**Sum of electronic and thermal Energies** = -2949.805635

**Sum of electronic and thermal Enthalpies** = -2949.804691

**Sum of electronic and thermal Free Energies** = -2949.844859

**Zero-point correction** = 0.108506 (Hartree/Particle)

**Thermal correction to Energy** = 0.119612

**Thermal correction to Enthalpy** = 0.120557

**Thermal correction to Gibbs Free Energy** = 0.068979

**Sum of electronic and zero-point Energies** = -554.115941

**Sum of electronic and thermal Energies** = -554.104834

**Sum of electronic and thermal Enthalpies** = -554.103890

**Sum of electronic and thermal Free Energies** = -554.155467
Table S5: Cartesian coordinates of the optimized structure and energy values for 6F by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 1.3427615449 | -0.8938833353 | -0.4115559462 |
| C    | 2.4456680368 | 0.0718542004  | 0.3320240988 |
| H    | 1.522382699  | -0.88975973   | 1.494886228  |
| H    | 1.2446042685 | -1.956120328  | -0.1324261839|
| H    | 3.4241325646 | -0.399052467  | -0.0408675776|
| Li   | 1.8767095023 | 1.8584022459  | 0.0701097097 |
| Si   | -0.2852138135| -0.0384324583 | -0.1373902228|
| C    | 1.6665728477 | -0.286249801  | 1.0449567416 |
| H    | -2.0931025989| 0.5556616103  | 1.5834958132 |
| H    | -1.7586403479| -1.2151673079 | 1.6016977385 |
| C    | -0.2057329937| -0.3694269678 | -0.4961834616|
| H    | -2.3816894849| -1.345806705  | -0.8464057272|
| H    | -2.7039151935| 0.4273468199  | -0.8538076399|
| F    | 0.0668203091 | 1.6233604083  | -0.306049415 |

Zero-point correction= 0.109726 (Hartree/Particle)
Thermal correction to Energy= 0.118502
Thermal correction to Enthalpy= 0.119446
Thermal correction to Gibbs Free Energy= 0.076989
Sum of electronic and zero-point Energies= -554.111858
Sum of electronic and thermal Energies= -554.102139
Sum of electronic and thermal Enthalpies= -554.144595

Table S6: Cartesian coordinates of the optimized structure and energy values for 7-LiF by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 1.3025139963 | -1.4637326336 | -0.0252040669 |
| C    | 1.9188329590 | 0.0069212233  | -0.0281181314|
| H    | 1.5378572223 | -2.0276545535 | -0.9258150453|
| H    | 1.607409016  | -0.232054775  | 0.8658847253 |
| H    | 2.5048770888 | 0.2192184272  | -0.9302166769|
| H    | -2.5311265458| 0.2118717675  | 0.858026926 |
| Li   | 1.3399403107 | 0.0238089761  | -0.0111165914|
| Si   | -0.0217172093| -0.165237915  | 0.0026648767 |
| C    | -1.6561837672| -0.4569728134 | 0.8074409063 |
| H    | -2.1960086464| 0.3628175895  | 1.2688079964 |
| H    | -1.857125298 | -1.4191327192 | 1.2699402102 |
| C    | -1.6731887129 | -0.4471836814 | -0.780965799 |
| H    | -1.8852903579 | -1.4031742805 | -1.2512082012|
| H    | -2.2221739157 | 0.3788406103  | -1.21994519 |
| F    | -0.326442157  | 1.8000236636  | 0.0133145955 |

Zero-point correction= 0.109835 (Hartree/Particle)
Thermal correction to Energy= 0.118807
Thermal correction to Enthalpy= 0.119751
Thermal correction to Gibbs Free Energy= 0.076989
Sum of electronic and zero-point Energies= -554.111858
Sum of electronic and thermal Energies= -554.103083
Sum of electronic and thermal Enthalpies= -554.144595
Sum of electronic and thermal Free Energies= -554.128778
**Table S7:** Cartesian coordinates of the optimized structure and energy values for **TS1F** by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -2.4776624721 | 1.1608776895 | -0.0795833075 |
| C    | -2.9923936911 | -0.1359919144 | 0.1768047654 |
| H    | -2.6957023268 | 1.6299747386 | -1.0312553045 |
| H    | -2.436605599 | 1.8766632423 | 0.7338164763 |
| H    | -3.6001224606 | -0.5932041826 | -0.6029538497 |
| H    | -3.2935728457 | -0.3647516824 | 1.1973272682 |
| Li   | -1.3341558941 | -1.3642345977 | -0.0255771583 |
| Si   | -0.0807668846 | 1.2503135708 | -0.3441126183 |
| C    | 1.3544433695 | 1.7315910533 | 0.7798333679 |
| H    | 1.908247356 | 0.957986799 | 1.3063475339 |
| H    | 1.3118938968 | 2.6596169213 | 1.3454869685 |
| C    | 1.6625918697 | 1.8748475663 | -0.7335927979 |
| H    | 1.8018408152 | 2.8842205462 | -1.1110165649 |
| H    | 2.3789772152 | 1.7307941831 | -1.152793534 |
| F    | 0.1348058582 | -0.5242941685 | -0.4400200744 |

Zero-point correction=                           0.108439 (Hartree/Particle)
Thermal correction to Energy=                    0.117515
Thermal correction to Enthalpy=                  0.118459
Thermal correction to Gibbs Free Energy=         0.073773
Sum of electronic and zero-point Energies=           -554.091289
Sum of electronic and thermal Energies=              -554.082214
Sum of electronic and thermal Enthalpies=            -554.081270
Sum of electronic and thermal Free Energies=         -554.125955

**Table S8:** Cartesian coordinates of the optimized structure and energy values for **TS2F** by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 1.1160954741 | -1.4960141776 | -0.3632895832 |
| C    | 1.8898113691 | -0.2154020449 | 0.186938141 |
| H    | 1.3636770288 | -1.7250110702 | -1.3984927122 |
| H    | 1.2286545499 | -2.3782838839 | 0.263805361 |
| H    | 2.6146637254 | 0.1812676871 | -0.5366428144 |
| H    | 2.4015067262 | -0.4103087431 | 1.1355985785 |
| Li   | 1.5291748827 | 1.7853493244 | 0.6775356081 |
| Si   | 0.0677464304 | -0.1306891532 | 0.0412454837 |
| C    | 1.6460350392 | -0.4662878943 | 0.9347513037 |
| H    | 2.0595041570 | 0.2807212894 | 1.605262847 |
| H    | 1.9140466871 | 1.4807671981 | 1.2161842711 |
| C    | 1.8043594456 | -0.113254753 | -0.606069503 |
| H    | 2.1321805669 | -0.9352083543 | -1.2364640826 |
| H    | 2.3208756153 | 0.8181805062 | -0.8106288859 |
| F    | -0.1319488147 | 1.7901954654 | 0.3555671389 |

Zero-point correction=                           0.109706 (Hartree/Particle)
Thermal correction to Energy=                    0.117770
Thermal correction to Enthalpy=                  0.118714
Thermal correction to Gibbs Free Energy=         0.078112
Sum of electronic and zero-point Energies=           -554.095368
Sum of electronic and thermal Energies=              -554.087304
Sum of electronic and thermal Enthalpies=            -554.086360
Sum of electronic and thermal Free Energies=         -554.125955
Table S9: Cartesian coordinates of the optimized structure and energy values for 5Cl by B3LYP/6-311+G(d,p).

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 3.58124212078 | -1.0716047521 | -0.3751932713 |
| C    | 3.804642307  | 0.1892026163  | 0.0039546099  |
| H    | 3.399968568  | -1.3328663622 | -1.4133267463 |
| H    | 3.607977303  | -1.8947676435 | 0.332922592   |
| H    | 3.811727587  | 1.0078413287  | -0.7092099343 |
| H    | 4.0206723858 | 0.4459158456  | 1.0365547105  |
| Li   | 1.3967531604 | -0.1606684839 | 0.1771644657  |
| Si   | -0.9410011864| -0.9127151422 | -0.1863747015 |
| C    | -2.578042096 | -0.991518812 | 1.1507252754  |
| H    | -2.7505574621| -0.2624444468 | 1.936260669   |
| H    | -2.9803567488| -1.9718016506| 1.3936903271  |
| C    | -2.7363518588| -0.5124966595 | -0.2917846081 |
| H    | -3.2431972307| -1.1827818516| -0.9821933116 |
| H    | -3.0133678218| 0.5267530267  | -0.4402260433 |
| Cl   | -0.1170092824| 1.291631987  | 0.8273125638  |

Zero-point correction= 0.107871 (Hartree/Particle)
Thermal correction to Energy= 0.119328
Thermal correction to Enthalpy= 0.120273
Thermal correction to Gibbs Free Energy= 0.067317
Sum of electronic and zero-point Energies= -914.468164
Sum of electronic and thermal Energies= -914.456707
Sum of electronic and thermal Enthalpies= -914.455762
Sum of electronic and thermal Free Energies= -914.508718

Table S10: Cartesian coordinates of the optimized structure and energy values for 6Cl by B3LYP/6-311+G(d,p).

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -0.0812758077| 1.653727016| -0.5439955789 |
| C    | -1.150165391| 2.187717195| 0.4860299568 |
| H    | -0.5276597777| 1.5755989952| -1.544036212 |
| H    | 0.8363036413| 2.255668238| -0.6756174791 |
| H    | -1.5478362138| 3.112141642| 0.0804162183 |
| H    | -0.5755749884| 2.4932834547| 1.3949068686 |
| Li   | -2.407046583| 0.687881253| 0.8789379964 |
| Si   | 0.4900333324| -0.0626386242| -0.089176921 |
| C    | 1.19079116956| -0.633730538| 0.9383637243 |
| H    | 1.7820450952| -1.4262143561| 1.6700185045 |
| H    | 2.6788704353| 0.0755737565| 1.2288923971 |
| C    | 1.938826672 | -1.0984304943| -0.5730159074 |
| H    | 2.7302684185| -0.6723960527| -1.184238551 |
| H    | 1.8213756171| -2.1652249068| -0.7390559051 |
| Cl   | 1.2719539977| -1.2851005029| 0.2668888885 |

Zero-point correction= 0.108562 (Hartree/Particle)
Thermal correction to Energy= 0.117856
Thermal correction to Enthalpy= 0.118800
Thermal correction to Gibbs Free Energy= 0.074594
Sum of electronic and zero-point Energies= -914.468164
Sum of electronic and thermal Energies= -914.456707
Sum of electronic and thermal Enthalpies= -914.455762
Sum of electronic and thermal Free Energies= -914.486263
Table S11: Cartesian coordinates of the optimized structure and energy values for \textbf{8Cl} by B3LYP/6-311+G(d,p).

\begin{verbatim}
C,2.8694904957,-1.2602117105,0.166367062  
C,3.1736303372,0.0138570061,0.4233512111  
H,2.8074637472,-1.6383782098,-0.8495825131  
H,2.7067249166,-1.9801637644,0.962451236  
H,3.3666391362,0.7278086474,-0.371273456  
H,3.2684044939,0.3845134682,1.4394056463  
Li,0.7436974669,-0.0296002546,0.120652247  
Si,-1.3776526662,-0.0033135554,-1.2649066551  
C,-1.1586949365,-1.0883335403,0.4331151228  
H,-0.6729230306,-0.7755594002,1.3654309633  
H,-1.1172540508,-2.1695436346,0.3166045516  
C,-2.5124904182,-0.4442440159,0.2112724202  
H,-3.3457536436,-1.1108371519,0.0024789625  
H,-2.7819488152,0.3543760354,0.8946927906  
C1,-0.2992825776,1.8947766445,-0.2379346997  

Zero-point correction=                           0.108304 (Hartree/Particle)
Thermal correction to Energy=                    0.119369     
Thermal correction to Enthalpy=                  0.120313     
Thermal correction to Gibbs Free Energy=         0.069252

Sum of electronic and zero-point Energies=           -914.474542
Sum of electronic and thermal Energies=              -914.463477
Sum of electronic and thermal Enthalpies=            -914.462533
Sum of electronic and thermal Free Energies=         -914.513595
\end{verbatim}

Table S12: Cartesian coordinates of the optimized structure and energy values for \textbf{7-LiCl} by B3LYP/6-311+G(d,p).

\begin{verbatim}
C,0.5161836944,2.4251988877,-0.586872233  
C,-0.7462744453,1.6927456586,0.0372214553  
H,0.4110585737,2.6941012654,-1.633115282  
H,0.9064185112,3.2423954646,0.0116663297  
H,-1.5719457671,1.5907305671,-0.6692435998  
H,-1.0741692082,2.1375663224,0.9783998701  
Li,-1.6351761976,-0.1355639228,0.9093012115  
Si,0.8519035213,0.6937643551,-0.1119712922  
C,1.9032657799,-0.4717916972,0.8314227063  
H,1.4738264793,-1.0504814532,1.6437265105  
H,2.9621345894,-0.2667805707,0.9628018607  
C,1.4656982777,-0.9545426233,-0.6221763561  
H,2.6248732559,-1.0356116238,-1.353783183  
H,0.790612511,-1.805305117,-0.6275236475  
C1,-1.6235385618,-2.0890859792,1.559660531  

Zero-point correction=                           0.109511 (Hartree/Particle)
Thermal correction to Energy=                    0.119318     
Thermal correction to Enthalpy=                  0.120262     
Thermal correction to Gibbs Free Energy=         0.073210

Sum of electronic and zero-point Energies=           -914.474542
Sum of electronic and thermal Energies=              -914.463477
Sum of electronic and thermal Enthalpies=            -914.462533
Sum of electronic and thermal Free Energies=         -914.513595
\end{verbatim}
Table S13: Cartesian coordinates of the optimized structure and energy values for TS1Cl by B3LYP/6-311+G(d,p).

| Atom  | Coordinates          | Energy Values       |
|-------|----------------------|---------------------|
| C     | -2.2612373281,1.1956461441,-0.477549973 |                     |
| C     | -2.581595902,0.1723779936,0.5037503571 |                     |
| H     | -2.6747912961,1.0722526033,-1.4765842844 |                     |
| H     | -2.359349224,2.2363775317,-0.1648758608 |                     |
| H     | -3.2095372682,-0.640639586,0.14593654 |                     |
| Li    | -0.6836007018,-0.6607152309,0.773328549 |                     |
| Si    | -0.173560753,1.160126752,-0.8844615008 |                     |
| C     | 0.8349001813,1.2482705944,0.7306683183 |                     |
| H     | 1.4363020058,0.434075833,1.1395785504 |                     |
| H     | 0.4997065259,1.9277608022,1.5136670045 |                     |
| C     | 1.4918564332,1.9482776399,-0.4936581323 |                     |
| H     | 0.5549228786,0.3020009290,-0.4550311549 |                     |
| H     | 2.3914773423,1.4906123656,-0.894126598 |                     |
| Cl    | 0.2300036508,-0.9419754311,-1.4340191505 |                     |

Zero-point correction= 0.107767 (Hartree/Particle)
Thermal correction to Energy= 0.116818
Thermal correction to Enthalpy= 0.117762
Thermal correction to Gibbs Free Energy= 0.074287
Sum of electronic and zero-point Energies= -914.435802
Sum of electronic and thermal Energies= -914.426751
Sum of electronic and thermal Enthalpies= -914.425807
Sum of electronic and thermal Free Energies= -914.469282

Table S14: Cartesian coordinates of the optimized structure and energy values for TS2Cl by B3LYP/6-311+G(d,p).

| Atom  | Coordinates          | Energy Values       |
|-------|----------------------|---------------------|
| C     | 1.7444757884,1.3384701949,-0.864857587 |                     |
| C     | 1.0862097471,1.9092215388,0.450865956 |                     |
| H     | 1.2775229674,1.7296309909,-1.7683021882 |                     |
| H     | 2.828084268,1.4125243856,-0.9402866812 |                     |
| H     | 0.5395347573,2.8490763197,0.2599003324 |                     |
| Li    | 0.6834945775,1.461187551,1.3607868269 |                     |
| Si    | 0.8961232979,-0.092540829,-0.1123461885 |                     |
| C     | 1.6398755319,-1.4060272274,0.9442100318 |                     |
| H     | 1.0897871113,-1.7973054443,1.797509253 |                     |
| H     | 2.714850338,-1.4796147808,1.1018715474 |                     |
| C     | 1.086684014,-1.9091375013,-0.465342352 |                     |
| H     | 1.8601389987,-2.2127533709,-1.1690337483 |                     |
| H     | 0.2731095932,-2.6271256106,-0.4178439711 |                     |
| Cl    | 1.4627259819,-0.06080347,0.0317867775 |                     |

Zero-point correction= 0.108094 (Hartree/Particle)
Thermal correction to Energy= 0.116785
Thermal correction to Enthalpy= 0.117729
Thermal correction to Gibbs Free Energy= 0.074892
Sum of electronic and zero-point Energies= -914.435802
Sum of electronic and thermal Energies= -914.426751
Sum of electronic and thermal Enthalpies= -914.425807
Sum of electronic and thermal Free Energies= -914.469282
Table S15: Cartesian coordinates of the optimized structure and energy values for TS3Cl by B3LYP/6-31+G(d,p).

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -2.940327775 | -1.0149297469 | 0.3041109003 |
| C       | -3.3196214285 | 0.1479234722 | 1.3759539473 |
| H       | -2.9662686681 | -1.185923722 | 0.3812796205 |
| H       | -3.6703072506 | 0.9724603774 | -0.3109729986 |
| Li      | -0.9181201988 | 0.3211931888 | 0.1841474497 |
| Si      | 1.4083629641 | -0.1975400753 | 0.8181295075 |
| C       | 2.1814340657 | -0.3767340182 | -1.7785861706 |
| H       | 2.600183837 | -1.9551773522 | -0.9417242907 |
| C       | 3.1681738213 | -0.1978156839 | 0.0682005247 |
| H       | 3.9051505511 | -0.8165215999 | 0.5733272465 |
| Cl      | 0.558479705 | 1.901964568 | -0.1404305209 |

Zero-point correction= 0.107732 (Hartree/Particle)
Thermal correction to Energy= 0.118427
Thermal correction to Enthalpy= 0.119371
Thermal correction to Gibbs Free Energy= 0.068646
Sum of electronic and zero-point Energies= -914.465863
Sum of electronic and thermal Energies= -914.455168
Sum of electronic and thermal Enthalpies= -914.454224
Sum of electronic and thermal Free Energies= -914.504949

Table S16: Cartesian coordinates of the optimized structure and energy values for 5Br by B3LYP/6-31+G(d,p).

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | -3.625221579 | 1.5155054386 | -0.000060736 |
| C       | -3.8271966401 | 0.1953375784 | 0.0002327884 |
| H       | -3.5582093012 | 0.2832823303 | -0.9231455585 |
| H       | -3.5583596213 | 0.083714927 | 0.922766187 |
| Li      | -1.4146322378 | 0.4964638872 | -0.0001570002 |
| Si      | 0.9478891641 | 1.1832345371 | -0.0000910102 |
| C       | 2.6822170481 | 1.028631784 | 0.7636850259 |
| C       | 2.6823164699 | 1.0276008442 | -0.7635316977 |
| H       | 2.3052011652 | 0.101185167 | 1.2600373724 |
| H       | 2.3094052464 | 0.9029209161 | 1.258909493 |
| H       | 2.3052185226 | 0.1002476369 | -1.259167518 |
| H       | 2.3094568815 | 1.9019904516 | -1.258723311 |
| Br      | 1.1231711116 | -1.296103652 | -0.0001766659 |

Zero-point correction= 0.107564 (Hartree/Particle)
Thermal correction to Energy= 0.119202
Thermal correction to Enthalpy= 0.120146
Thermal correction to Gibbs Free Energy= 0.065917
Sum of electronic and zero-point Energies= -3028.390603
Sum of electronic and thermal Energies= -3028.378965
Sum of electronic and thermal Enthalpies= -3028.378021
Sum of electronic and thermal Free Energies= -3028.432250
Table S17: Cartesian coordinates of the optimized structure and energy values for 6\textit{Br} by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 0.930505   | 1.839513   | -0.580651  |
| C    | 0.022700   | 2.684322   | 0.350615   |
| H    | 0.610644   | 1.923912   | -1.627253  |
| H    | 2.006376   | 2.773727   | 1.330587   |
| Li   | -1.759338  | 1.753414   | 0.531138   |
| Si   | 1.918631   | -0.970277  | 0.990662   |
| C    | -0.011319  | 3.706172   | -0.051236  |
| H    | 0.514933   | 2.773727   | 1.330587   |
| Li   | -1.759338  | 1.753414   | 0.531138   |

Zero-point correction= 0.108087 (Hartree/Particle)
Thermal correction to Energy= 0.117638
Thermal correction to Enthalpy= 0.118582
Thermal correction to Gibbs Free Energy= 0.072897
Sum of electronic and zero-point Energies= -3028.371897
Sum of electronic and thermal Energies= -3028.362346
Sum of electronic and thermal Enthalpies= -3028.361402
Sum of electronic and thermal Free Energies= -3028.407086

Table S18: Cartesian coordinates of the optimized structure and energy values for 8\textit{Br} by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -3.075465  | -1.032078  | 0.258316   |
| C    | -3.274307  | 0.228138   | -0.134718  |
| H    | -2.914978  | -1.285907  | 1.301796   |
| H    | -3.102448  | -1.860012  | -0.443434  |
| Li   | 1.455489   | -0.165950  | 0.948299   |
| Si   | 0.856378   | -1.413166  | -0.535267  |
| C    | -0.304660  | -1.469467  | -1.344435  |
| H    | 0.667611   | -2.446553  | 0.250027   |
| C    | 2.308133   | -0.984490  | -0.558666  |
| Si   | 3.049972   | -1.748324  | 0.338180   |
| C    | 0.493169   | 1.892515   | 0.289555   |

Zero-point correction= 0.107846 (Hartree/Particle)
Thermal correction to Energy= 0.119170
Thermal correction to Enthalpy= 0.120114
Thermal correction to Gibbs Free Energy= 0.067190
Sum of electronic and zero-point Energies= -3028.371897
Sum of electronic and thermal Energies= -3028.362346
Sum of electronic and thermal Enthalpies= -3028.361402
Sum of electronic and thermal Free Energies= -3028.407086
Table S19: Cartesian coordinates of the optimized structure and energy values for 7-LiBr by B3LYP/6-31+G(d,p).

| Atom | Coordinates | Energy Values |
|------|-------------|---------------|
| C    | -3.1221622371, -1.2498678829, -0.0055800151 |               |
| C    | -1.5996400969, -1.6961304630, 0.0012670261 |               |
| H    | -3.6650026324, -1.5083246840, -0.99024000267 |               |
| H    | -3.6725090169, -1.5059103427, 0.8942768249 |               |
| H    | -1.3116179322, -2.2408310501, -0.8996763446 |               |
| Li   | 0.5381865747, -1.1636265655, 0.0088067374 |               |
| Si   | 0.9614987058, 0.1599115936, 0.0029319925 |               |
| C    | -1.4303616341, 1.7215625177, 0.7929230963 |               |
| H    | -0.4471195151, 1.7922138196, 1.2483320434 |               |
| H    | -2.1649717819, 2.3706819751, 1.2613187442 |               |
| C    | -1.4243189986, 1.7192334908, -0.7995883236 |               |
| H    | -2.1561068590, 2.363145578, -1.275214691 |               |
| H    | -0.4379560194, 1.7902638482, -1.2481176328 |               |
| Br   | 2.3565555241, 1.0411135340, 0.0371862969 |               |

Zero-point correction= 0.109257 (Hartree/Particle)
Thermal correction to Energy= 0.119209
Thermal correction to Enthalpy= 0.120153
Thermal correction to Gibbs Free Energy= 0.071434
Sum of electronic and zero-point Energies= -3028.383954
Sum of electronic and thermal Energies= -3028.374002
Sum of electronic and thermal Enthalpies= -3028.373058
Sum of electronic and thermal Free Energies= -3028.421777

Table S20: Cartesian coordinates of the optimized structure and energy values for TS1Br by B3LYP/6-31+G(d,p).

| Atom | Coordinates | Energy Values |
|------|-------------|---------------|
| C    | -2.2205292894, 1.1678636021, -0.5412143197 |               |
| C    | -2.5952433599, 0.2232758538, 0.5023321754 |               |
| H    | -2.6222621140, 0.9892415406, -1.5369127058 |               |
| H    | -2.3007123492, 0.2303019489, -0.2999909527 |               |
| H    | -2.2480524912, -0.5871579712, 0.1860748197 |               |
| Li   | 0.7176594748, -0.6060983956, 0.8812832563 |               |
| Si   | -0.3984509191, -0.797548955, -0.9021800145 |               |
| C    | -0.8138193585, 1.2503491651, -0.7483084046 |               |
| H    | 1.4451777759, 0.4773770341, 1.1889682114 |               |
| H    | 0.4124934604, 1.9228456245, 1.5064399609 |               |
| C    | 0.4668413262, 1.9673462583, -0.4645217325 |               |
| H    | 1.4625674813, 0.5356750709, 0.4465937365 |               |
| H    | 0.24051601464, 1.5588392491, -0.8268213756 |               |
| Br   | 0.3573378866, -1.18398654966, -1.4297208056 |               |

Zero-point correction= 0.107265 (Hartree/Particle)
Thermal correction to Energy= 0.116578
Thermal correction to Enthalpy= 0.117522
Thermal correction to Gibbs Free Energy= 0.072487
Sum of electronic and zero-point Energies= -3028.383954
Sum of electronic and thermal Energies= -3028.374002
Sum of electronic and thermal Enthalpies= -3028.373058
Sum of electronic and thermal Free Energies= -3028.421777
Table S21: Cartesian coordinates of the optimized structure and energy values for TS2Br by B3LYP/6-311+G(d,p).

| Atom | X-Coordinate   | Y-Coordinate   | Z-Coordinate   |
|------|----------------|----------------|----------------|
| C    | 1.6903990792   | 1.3403306697   | -0.8620371065  |
| C    | 1.1036955004   | 1.9349010022   | 0.4714024475   |
| H    | 1.1838323006   | 1.7289403857   | -1.7460069376  |
| H    | 2.7698551997   | 1.4004815711   | -1.0023834954  |
| H    | 0.6455698249   | 2.9628786066   | 0.3078493679   |
| H    | 1.8850953333   | 0.0382558487   | 1.2290057573   |
| Li   | -0.6746240386  | 1.5039705069   | 1.3635872755   |
| Si   | 0.8804103895   | -0.1298219207  | -0.1464149095  |
| C    | 1.6172453765   | -1.4119883777  | 0.9512361293   |
| H    | 1.0509410139   | -1.8135274537  | 1.788557518    |
| C    | 3.3208358743   | -1.16269025    | -0.1512245409  |
| C    | 3.6129939318   | 0.0654028369   | 0.284704874    |
| H    | 3.3612913934   | -1.4197492847  | -1.2053726544  |
| H    | 3.0673577003   | -1.9665966436  | 0.5332432504   |
| H    | 3.9008872273   | 0.8605440406   | -0.3962605905  |
| H    | 3.6067051904   | 0.3133407936   | 1.3417453417   |
| Li   | 1.2151678678   | 0.0544211438   | -0.135796817   |
| Si   | -1.116982645   | -0.4867035506  | -0.7355166629  |
| C    | -1.8858310049  | -0.1083935884  | 0.9625775418   |
| H    | -1.6815365447  | -0.5184318566  | 1.8654486682   |
| H    | -1.918026505   | -2.1586186099  | 1.1268163755   |
| C    | -2.885359256   | -0.510518976   | -0.0024336229  |
| H    | -3.5871915348  | -1.1913031642  | -0.4770252075  |
| H    | -3.3256581778  | 0.4523622352   | 0.2343701444   |
| Br   | 0.2768510321   | 1.8550790199   | 0.1241150149   |

Zero-point correction= 0.107600 (Hartree/Particle)
Thermal correction to Energy= 0.116536
Thermal correction to Enthalpy= 0.117480
Thermal correction to Gibbs Free Energy= 0.073265

Sum of electronic and zero-point Energies= -3028.361266
Sum of electronic and thermal Energies= -3028.352330
Sum of electronic and thermal Enthalpies= -3028.351386
Sum of electronic and thermal Free Energies= -3028.395601

Table S22: Cartesian coordinates of the optimized structure and energy values for TS3Br by B3LYP/6-311+G(d,p).

| Atom | X-Coordinate   | Y-Coordinate   | Z-Coordinate   |
|------|----------------|----------------|----------------|
| C    | 3.3208358743   | -1.16269025    | -0.1512245409  |
| C    | 3.6129939318   | 0.0654028369   | 0.284704874    |
| H    | 3.3612913934   | -1.4197492847  | -1.2053726544  |
| H    | 3.0673577003   | -1.9665966436  | 0.5332432504   |
| H    | 3.9008872273   | 0.8605440406   | -0.3962605905  |
| H    | 3.6067051904   | 0.3133407936   | 1.3417453417   |
| Li   | 1.2151678678   | 0.0544211438   | -0.135796817   |
| Si   | -1.116982645   | -0.4867035506  | -0.7355166629  |
| C    | -1.8858310049  | -0.1083935884  | 0.9625775418   |
| H    | -1.6815365447  | -0.5184318566  | 1.8654486682   |
| H    | -1.918026505   | -2.1586186099  | 1.1268163755   |
| C    | -2.885359256   | -0.510518976   | -0.0024336229  |
| H    | -3.5871915348  | -1.1913031642  | -0.4770252075  |
| H    | -3.3256581778  | 0.4523622352   | 0.2343701444   |
| Br   | 0.2768510321   | 1.8550790199   | 0.1241150149   |

Zero-point correction= 0.107405 (Hartree/Particle)
Thermal correction to Energy= 0.118298
Thermal correction to Enthalpy= 0.119242
Thermal correction to Gibbs Free Energy= 0.066937

Sum of electronic and zero-point Energies= -3028.388200
Sum of electronic and thermal Energies= -3028.352330
Sum of electronic and thermal Enthalpies= -3028.351386
Sum of electronic and thermal Free Energies= -3028.395601
**Table S23:** Cartesian coordinates of the optimized structure and energy values for Ethylene by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -0.508663  | 1.795410   | 0.0000     |
| H    | 0.005389   | 0.839793   | 0.0000     |
| H    | -1.593252  | 1.762264   | 0.0000     |
| C    | 0.155491   | 2.946306   | 0.0000     |
| H    | -0.358581  | 3.901922   | 0.0000     |
| H    | 1.240080   | 2.979452   | 0.0000     |

Zero-point correction= 0.050782 (Hartree/Particle)

Thermal correction to Energy= 0.053824

Thermal correction to Enthalpy= 0.054768

Thermal correction to Gibbs Free Energy= 0.029257

Sum of electronic and zero-point Energies= -78.564731

Sum of electronic and thermal Energies= -78.561689

Sum of electronic and thermal Enthalpies= -78.560745

Sum of electronic and thermal Free Energies= -78.586255

**Table S24:** Cartesian coordinates of the optimized structure and energy values for 11 by B3LYP/6-311+G(d,p).

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 2.549419   | -0.964772  | -0.0005    |
| C    | 1.111418   | -1.646115  | -0.0001    |
| H    | 3.137659   | -1.117056  | 0.9003     |
| H    | 3.137079   | -1.116610  | -0.9020    |
| H    | 0.858177   | -2.197528  | 0.9011     |
| H    | 0.857630   | -2.197875  | -0.9012    |
| Si   | 1.120256   | 0.193043   | -0.0000    |
| C    | 0.410064   | 1.691903   | -0.7946    |
| H    | -0.570243  | 1.661581   | -1.2623    |
| H    | 1.059531   | 2.429334   | -1.2588    |
| C    | 0.410205   | 1.691627   | 0.7951     |
| H    | 1.059620   | 2.428915   | 1.2596     |
| H    | -0.570088  | 1.661060   | 1.2629     |

Zero-point correction= 0.106320 (Hartree/Particle)

Thermal correction to Energy= 0.112469

Thermal correction to Enthalpy= 0.113413

Thermal correction to Gibb's Free Energy= 0.077115

Sum of electronic and zero-point Energies= -446.611916

Sum of electronic and thermal Energies= -446.605767

Sum of electronic and thermal Enthalpies= -446.604823

Sum of electronic and thermal Free Energies= -446.641121