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).

Li,-1.2670763858,0.0718659876,-0.0066783967
Si,0.984872737,-0.788050492,-0.0016007598
C,2.6874688772,-0.4511187283,-0.7641040981
H,2.845785709,0.5065375548,-1.2527984863
H,3.2178338753,-1.2623205049,-1.2566050507
C,2.6836752142,-0.4522597247,0.7698120684
H,3.2116251937,-1.2641691579,1.2637378344
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).

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/6-311+G(d,p).

Li,-1.3105661586,-0.0916139377,-0.0068435384
Si,1.0459922842,-0.7065734145,-0.0014861288
C,2.7716352788,-0.4830382789,-0.7606203625
H,3.0035459119,0.454296662,-1.2567218895
H,3.2227689753,-1.3400283759,-1.2554384664
C,2.7677825363,-0.4840910784,0.7666573517
H,3.216420012,-1.3417641325,1.2625607133
H,2.9971867429,0.4525583779,1.2652127142
Br,0.0994253072,1.7546557081,-0.0021388035

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

Table S4: Cartesian coordinates of the optimized structure and energy values for **5F** by B3LYP/6-311+G(d,p).

C,3.313897732,-1.1917164135,-0.2079515085
C,3.5503088347,0.0984189234,0.0430778793
H,3.201622531,-1.5660958315,-1.2209467744
H,3.2593807442,-1.9286078931,0.587644875
H,3.6415067582,0.8283417812,-0.7557206936
H,3.6991236363,0.4656175174,1.0541343994
Li,1.1122014336,-0.1777077343,0.0716241556
Si,-1.2902066689,-0.6171586198,0.0725559673
C,-2.8665645608,-0.1322610979,1.0152234871
H,-2.8167989795,0.7203824918,1.6873826506
H,-3.5268562654,-0.9136301034,1.3835664554
C,-2.9236174457,0.1756741546,-0.4859210226
H,-3.620790171,-0.4074385625,-1.0826667481
H,-2.9098601256,1.2245939274,-0.770294161
F,-0.2386614532,0.9026834603,0.3440570385

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).

C,1.3427615449,-0.8938833353,-0.4115559462
C,2.4456680368,-0.0718542004,0.3320240988
H,1.5222382699,-0.887975973,-1.494886228
H,1.2446042685,-1.956120328,-0.1324261839
H,3.4241325646,-0.3990542467,-0.0408675776
H,2.4282160001,-0.352201121,1.3955431005
Li,1.8767095023,1.8584022459,0.0701097097
Si,-0.2852138135,-0.0384324583,-0.1373790228
C,-1.6665728477,-0.286249801,1.0449567416
H,-2.0931025989,0.5556616103,1.5834958132
H,-1.7586403479,-1.2151673079,1.6016977385
C,-2.0573299397,-0.3694296078,-0.4961834616
H,-2.3816894849,-1.345806705,-0.8464057272
H,-2.7039151935,0.4273468199,-0.8538076399
F,0.0668200391,1.6233604083,-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= -554.103083
Sum of electronic and thermal Enthalpies= -554.102139
Sum of electronic and thermal Free Energies= -554.144595

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

C,1.3025139963,-1.4637326336,-0.0252040669
C,1.9188329599,0.0069221233,-0.0281181314
H,1.537857223,-2.0276545535,-0.9258150453
H,1.5607409016,-2.0328054775,0.8658847253
H,2.5048770888,0.2192184272,-0.9302166769
H,2.5312165458,0.2118716752,0.858026926
Li,1.3399403107,2.0238089761,-0.0111165914
Si,-0.0217172093,-0.165237915,-0.0026648767
C,-1.6561837672,-0.4569728134,0.8074409063
H,-2.1960086464,0.3628175985,1.2688079964
H,-1.8571252598,-1.4191327192,1.2699402102
C,-1.6731887129,-0.4471836814,-0.7809965799
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= 0.076338
Sum of electronic and zero-point Energies= -554.095281
Sum of electronic and thermal Energies= -554.086308
Sum of electronic and thermal Enthalpies= -554.085364
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).

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,1.3544433695,1.7315910533,0.779833679
H,1.908247356,0.957986799,1.3063475339
H,1.3118938968,2.6596169213,1.3454869685
C,1.6625918697,1.8748475663,-0.7335592797
H,1.8018408815,2.8842205462,-1.1110165649
H,2.3789772152,1.1730794183,-1.152793534
F,0.1348085852,-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).

C,1.1160954741,-1.4960141776,-0.3632895832
C,1.8898113691,-0.2154020449,0.1869338141
H,1.3636770288,-1.7250110702,-1.3984927122
H,1.2286545499,-2.3782838839,0.2638085361
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,-2.059504157,0.2807212894,1.605262847
H,-1.914046687,-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= -554.126961

Table S9: Cartesian coordinates of the optimized structure and energy values for **5Cl** by B3LYP/6-311+G(d,p).

C,3.5812412078,-1.0716047521,-0.3751932713
C,3.804642307,0.1892026163,0.0039546099
H,3.3999068568,-1.3328663622,-1.4133267463
H,3.608797303,-1.8947676435,0.332292592
H,3.81172758,1.0078413287,-0.7092099343
H,4.0206273858,0.4459158456,1.0365547105
Li,1.3967531604,-0.1606684839,0.1771644657
Si,-0.9410011864,-0.9127151422,0.1863747015
C,-2.5768042096,-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).

C,-0.0812758077,1.653727016,-0.5439955789
C,-1.1150165391,2.1878717195,0.4860299568
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,1.9079116956,-0.633730538,0.9383637243
H,1.7820450952,-1.4262143561,1.6700185045
H,2.6788704353,0.0755737565,1.2288923971
C,1.938826672,-1.0984340943,-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=	-914.452294
Sum of electronic and thermal Energies=	-914.443000
Sum of electronic and thermal Enthalpies=	-914.442056
Sum of electronic and thermal Free Energies=	-914.486263

Table S11: Cartesian coordinates of the optimized structure and energy values for **8Cl** by B3LYP/6-311+G(d,p).

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,-0.3712723456
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,-1.1172545058,-2.1695346346,0.3166045516
C,-2.5124904182,-0.4442440159,0.2112724202
H,-3.3457536436,-1.1108137159,0.0024789625
H,-2.7819488152,0.3543760354,0.8949627906
Cl,-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

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

C,0.5161836944,2.4251988877,-0.586872233
C,-0.7462744593,1.6927456586,0.0372214553
H,0.4110585737,2.6941012654,-1.6333115282
H,0.9064185112,3.2423954646,0.0116663297
H,-1.571945767,1.5907305671,-0.6692435998
H,-1.074169208,2.1375663224,0.9783998701
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,-0.9545452623,-0.6221763561
H,2.2648732559,-1.0356116238,-1.3537838183
H,0.790612511,-1.8050350117,-0.6275236475
Cl,-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=	-914.461494
Sum of electronic and thermal Energies=	-914.451687
Sum of electronic and thermal Enthalpies=	-914.450743
Sum of electronic and thermal Free Energies=	-914.497795

Table S13: Cartesian coordinates of the optimized structure and energy values for **TS1Cl** by B3LYP/6-311+G(d,p).

C,-2.2612373281,1.1956461441,-0.4775749973
C,-2.581595902,0.1723779936,0.5037503571
H,-2.6747912961,1.0722526033,-1.4765842844
H,-2.3593498224,2.2363775317,-0.1648758608
H,-3.2095372682,-0.6406639586,0.145938654
H,-2.8498796239,0.5422684196,1.4921339084
Li,-0.6836007018,-0.6607152309,0.773325948
Si,-0.1773560753,1.160126752,-0.8844615008
C,0.8349001813,1.2482705944,0.7306683183
H,1.4363020058,0.4340758533,1.1395785504
H,0.4997065259,1.9277608022,1.5136670045
C,1.4918564332,1.9482776399,-0.4936581323
H,1.5549228786,3.0320029209,-0.4550311549
H,2.3914773423,1.4906123656,-0.8941126598
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).

C,1.7444757884,1.3384701949,-0.864857587
C,1.0862097471,1.9092215388,0.4508665956
H,1.2775229674,1.7296309909,-1.7683021882
H,2.828084268,1.4125243856,-0.9402866812
H,0.5395347573,2.8490763197,0.2599003324
H,1.8346244402,2.0895367884,1.2264846048
Li,-0.6834945775,1.4611875511,1.3607868269
Si,0.8961232979,-0.092540829,-0.1123461885
C,1.6398755319,-1.4060272724,0.9442100318
H,1.0897871113,-1.7973054443,1.797509253
H,2.7141850338,-1.4796147808,1.1018715474
C,1.086684014,-1.9091375013,-0.4653542352
H,1.8601389987,-2.2127533709,-1.1690337483
H,0.2731095932,-2.6271526106,-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= -914.441184
Sum of electronic and thermal Energies= -914.432493
Sum of electronic and thermal Enthalpies= -914.431549
Sum of electronic and thermal Free Energies= -914.474387

Table S15: Cartesian coordinates of the optimized structure and energy values for **TS3Cl** by B3LYP/6-311+G(d,p).

C,-2.9403277753,-1.0149297469,0.3041109003
C,-3.3196214285,0.1479201795,-0.2320299575
H,-2.9662686681,-1.1859234722,1.3759593473
H,-2.6234500472,-1.8516615887,-0.3109729986
H,-3.6703072506,0.9724603774,0.3812792305
H,-3.3272069793,0.3062678594,-1.3062254017
Li,-0.9181201838,0.3211931888,0.1841474497
Si,1.4083629641,-0.1975400753,0.8181295075
C,2.1814340657,-0.8748108412,-0.8442266283
H,1.9442679968,-0.3767340182,-1.7785861706
H,2.2600183837,-1.9551773522,-0.9417242907
C,3.1681738213,-0.1978156839,0.0682005247
H,3.9051505511,-0.8165215999,0.5733327465
H,3.563221735,0.7653169854,-0.2378719483
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/6-311+G(d,p).

C,-3.625221579,1.5155054386,-0.0000607363
C,-3.8271966401,0.1953375784,0.0002327884
H,-3.5582093012,2.0832823303,-0.9231455585
H,-3.5583596313,2.083714927,0.922766187
H,-3.9290904275,-0.3678757271,-0.9223211385
H,-3.9292408737,-0.3674458501,0.9230293454
Li,-1.4146322378,0.4964638872,-0.0001570002
Si,0.9478891641,1.1832345371,-0.0000901202
C,2.6822171048,1.0281631784,0.7636850259
C,2.6823164699,1.0276008442,-0.7635316977
H,2.9520211852,0.1011785167,1.2600373724
H,3.0984052464,1.902920916,1.2582909493
H,2.9521815226,0.1002476369,-1.2591617518
H,3.0985768815,1.9019904516,-1.2587273311
Br,0.123171116,-1.2961036652,0.0007166659

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 **6Br** by B3LYP/6-311+G(d,p).

C,0.9305050437,1.8395137762,-0.5806507562
C,0.0227000012,2.6843221772,0.3506155966
H,0.6106443158,1.9239122331,-1.6272537532
H,2.0063764857,2.0963914111,-0.5783390412
H,-0.0113199074,3.7061721766,-0.0512356723
H,0.5149326721,2.773727992,1.3305873626
Li,-1.7593386122,1.7534141862,0.5311380458
Si,0.8694839533,0.0198497709,-0.1591387622
C,1.9186312484,-0.9702772611,0.9906662183
C,2.0085572836,-1.3887586577,-0.5284512644
H,2.8145092692,-0.5198537484,1.4109246177
H,1.4774343683,-1.7061497066,1.6559829296
H,2.9589145783,-1.196489172,-1.0200357717
H,1.6125546518,-2.37013724,-0.7715081012
Br,-1.3696223518,-0.6588899374,-0.0774726484

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 **8Br** by B3LYP/6-311+G(d,p).

C,-3.0754651703,-1.0320788915,0.2583162841
C,-3.2743078272,0.2281387682,-0.1347185902
H,-2.9149775906,-1.2859073347,1.3017966171
H,-3.1024114848,-1.8600125413,-0.4434343426
H,-3.2788880107,1.0537691454,0.5699944577
H,-3.468251856,0.4789202133,-1.1730657859
Li,-0.8458880196,-0.0750431132,-0.1425431254
Si,1.4554886825,-0.1659503989,0.9482999625
C,0.8563777648,-1.4131664144,-0.5352676
H,0.3046605115,-1.1469467058,-1.4444355745
H,0.6676110286,-2.446553952,-0.2500275075
C,2.3081336369,-0.9844908052,-0.5586663322
H,3.0499728629,-1.74832454,-0.3381809499
H,2.6069327411,-0.3423276814,-1.3806461809
Br,0.4931686109,1.8925156015,-0.2895550623

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=	-3028.396764
Sum of electronic and thermal Energies=	-3028.385440
Sum of electronic and thermal Enthalpies=	-3028.384495
Sum of electronic and thermal Free Energies=	-3028.437419

Table S19: Cartesian coordinates of the optimized structure and energy values for **7-LiBr** by B3LYP/6-311+G(d,p).

C,-3.1221622371,-1.2498678829,-0.0055800151
C,-1.5996400969,-1.6961130463,0.0012670261
H,-3.6650026324,-1.5085324684,-0.9092400267
H,-3.6725090169,-1.5059103427,0.8942768249
H,-1.3116167932,-2.2408310501,-0.8996763446
H,-1.3182498166,-2.2367218002,0.9067621541
Li,0.5381865747,-1.1636265655,0.0088067374
Si,-1.9614987058,0.1599115936,-0.0029319925
C,-1.430361634,1.7215625177,0.7929230963
H,-0.4471195151,1.7922138196,1.2483320434
H,-2.1649717819,2.3706819751,1.2613188744
C,-1.4243189986,1.7192334908,-0.7995883236
H,-2.1561068509,2.3663145578,-1.275214691
H,-0.4379560194,1.7902638482,-1.2481176328
Br,2.3556555241,0.1041113534,0.0371862696

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/6-311+G(d,p).

C,-2.2205292894,1.1678636021,-0.5412143197
C,-2.5952433599,0.2232758538,0.5023321754
H,-2.622262114,0.9892415406,-1.5369127058
H,-2.3007122349,2.2303019489,-0.2999909527
H,-3.2480524912,-0.5871579712,0.1860748197
H,-2.8772721054,0.6731752186,1.4532938146
Li,-0.7176597478,-0.6060983956,0.8812832563
Si,-0.1398450919,1.0797548955,-0.9021800145
C,0.8138193585,1.2503491651,0.7483084046
H,1.4451777759,0.477377034,1.1889682114
H,0.4124934604,1.9228456425,1.5064399609
C,1.4668413262,1.9673462583,-0.4645217325
H,1.462567481,3.0535675079,-0.4465937365
H,2.4051601464,1.5588392491,-0.8268213756
Br,0.357337886,-1.1839865496,-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=	-3028.357167
Sum of electronic and thermal Energies=	-3028.347854
Sum of electronic and thermal Enthalpies=	-3028.346909
Sum of electronic and thermal Free Energies=	-3028.391945

Table S21: Cartesian coordinates of the optimized structure and energy values for **TS2Br** by B3LYP/6-311+G(d,p).

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,0.6455698249,2.9262878606,0.3078493679
H,1.8850953333,2.0382558487,1.2290057573
Li,-0.6746240386,1.5039705069,1.3635872755
Si,0.8804103895,-0.1298219207,-0.1464149095
C,1.6172453765,-1.4119883977,0.9512361293
H,1.0509410139,-1.8135274537,1.788557518
H,2.6870717508,-1.4413043258,1.1496958826
C,1.1401300984,-1.9451234259,-0.4739860536
H,1.9507927754,-2.2346621158,-1.1410116089
H,0.3483632759,-2.6884624997,-0.4520176741
Br,-1.6046378799,-0.0823477056,-0.0805875924

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).

C,3.3208358743,-1.16269025,-0.1512245409
C,3.6129933918,0.0654028369,0.284704874
H,3.3612913934,-1.4197492847,-1.2053726544
H,3.0673577003,-1.9665966436,0.5332432504
H,3.9008872273,0.8605440406,-0.3962605905
H,3.6067051904,0.3133407936,1.3417454317
Li,1.2151678678,0.0544211438,-0.1357966817
Si,-1.116982645,-0.4867035506,-0.7355166629
C,-1.8858310049,-1.0839358846,0.9625775418
H,-1.6815365447,-0.5184318566,1.8654486682
H,-1.9180206505,-2.1586186099,1.1268163755
C,-2.8853539256,-0.510518976,-0.0024336229
H,-3.5871915348,-1.1913031642,-0.4770252075
H,-3.3256581778,0.4523622352,0.2343701444
Br,-0.276851032,1.8550790199,0.1241150149

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=	-3028.377307
Sum of electronic and thermal Enthalpies=	-3028.376362
Sum of electronic and thermal Free Energies=	-3028.428668

Table S23: Cartesian coordinates of the optimized structure and energy values for **Ethylene** by B3LYP/6-311+G(d,p).

C,-0.5086633202,1.7954103949,0.
H,0.0053896326,0.8397939025,0.
H,-1.593252131,1.7622644652,0.
C,0.1554912202,2.9463064551,0.
H,-0.3585617326,3.9019229475,0.
H,1.240080031,2.9794523848,0

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).

C,2.5494196783,-0.9647723648,-0.0005612624
C,1.1114187556,-1.6461157698,-0.0001906584
H,3.1376999069,-1.1170566403,0.9003211923
H,3.1370797603,-1.1166101446,-0.9019303909
H,0.8581773396,-2.1975278646,0.9011739589
H,0.8576304852,-2.1978752053,-0.9011836283
Si,1.1202556023,0.1930433994,-0.0000520411
C,0.4100647466,1.6919035926,-0.7946580202
H,-0.570243147,1.6615814351,-1.2623689774
H,1.0595317514,2.4293342783,-1.2588644069
C,0.4102050677,1.6916273102,0.7951975275
H,1.0596207217,2.428915025,1.2596803181
H,-0.5700886685,1.661060949,1.2629263889

Zero-point correction=	0.106320 (Hartree/Particle)
Thermal correction to Energy=	0.112469
Thermal correction to Enthalpy=	0.113413
Thermal correction to Gibbs 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