

Supporting Information

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Table S1. Cartesian coordinates and energies of **1** (X = Cl) at the WB97XD/6-31+G(d,p) level of theory.

C,1.90032231,-0.8745856952,0.7604303106
C,1.9003418057,-0.8746052543,-0.7603777676
H,1.3227220383,-1.6529356823,1.2532499234
H,1.3227524125,-1.6529672453,-1.2531910853
H,2.8430280826,-0.6600715957,-1.2606791399
Li,-1.173611984,1.9601292247,-0.0001294396
H,2.842995471,-0.6600374923,1.2607501766
Ge,0.9203340632,0.635229446,-0.0000020299
Cl,-1.4328543492,-0.2601636355,-0.0000396783

Zero-point correction=	0.055666 (Hartree/Particle)
Thermal correction to Energy=	0.062679
Thermal correction to Enthalpy=	0.063623
Thermal correction to Gibbs Free Energy=	0.023472
Sum of electronic and zero-point Energies=	-2621.320313
Sum of electronic and thermal Energies=	-2621.313301
Sum of electronic and thermal Enthalpies=	-2621.312356
Sum of electronic and thermal Free Energies=	-2621.352507

Table S2. Cartesian coordinates and energies of **2** (X = Cl) at the WB97XD/6-31+G(d,p) level of theory.

C,-3.4880563492,0.7559539117,0.0002220829
C,-3.4882659451,-0.7559918305,0.0002085314
H,-3.816557048,1.2656660875,-0.9042082115
H,-3.8168992959,-1.2655980713,-0.9042349439
H,-3.8166505761,-1.2656384861,0.9047194689
Li,1.0118383381,0.0000774182,-0.0000728984
H,-3.8162931806,1.2656673982,0.9047478085
Ge,-1.6929465955,-0.0002649739,-0.0000200313
Cl,3.0849976123,0.0008637262,-0.0000467865

Zero-point correction=	0.054853 (Hartree/Particle)
Thermal correction to Energy=	0.062306
Thermal correction to Enthalpy=	0.063250
Thermal correction to Gibbs Free Energy=	0.020749
Sum of electronic and zero-point Energies=	-2621.304278
Sum of electronic and thermal Energies=	-2621.296825
Sum of electronic and thermal Enthalpies=	-2621.295881
Sum of electronic and thermal Free Energies=	-2621.338382

Table S3. Cartesian coordinates and energies of **3** (X = Cl) at the WB97XD/6-31+G(d,p) level of theory.

C,-0.9809473309,-1.7175371952,-0.2409465126
C,0.0834781004,1.6158830091,0.1518450258
H,-0.4984479866,-2.6862265618,-0.2675075004
H,-0.2503859717,2.1091829917,-0.7667503216
H,-0.5317990165,1.9451242958,0.9946309623
Li,2.1208986553,1.4875383491,0.3996955406
H,-2.0591595517,-1.6665858488,-0.3482266381
Ge,-0.0722514853,-0.2267102035,-0.0429560228
Cl,2.1886145869,-0.8606678364,0.1202144668

Zero-point correction= 0.052103 (Hartree/Particle)
Thermal correction to Energy= 0.059602
Thermal correction to Enthalpy= 0.060546
Thermal correction to Gibbs Free Energy= 0.019381
Sum of electronic and zero-point Energies= -2621.290338
Sum of electronic and thermal Energies= -2621.282839
Sum of electronic and thermal Enthalpies= -2621.281895
Sum of electronic and thermal Free Energies= -2621.323060

Table S4. Cartesian coordinates and energies of **4** (X = Cl) at the WB97XD/6-31+G(d,p) level of theory.

C,0.9931739103,1.5205899176,-0.2640097699
C,0.3385767631,0.4227624692,0.5877646138
H,0.5446512684,1.7647554867,-1.2267270734
H,1.3218731807,2.4020876923,0.2846013746
Li,-1.1526665144,0.4449506196,1.844326107
H,1.9300439576,-0.9282119239,-1.5423839118
H,3.2040374712,-0.3318888164,0.6131615239
Ge,1.9585712991,-0.1510775703,-0.2390659644
Cl,-1.1982676159,-0.2688696048,-0.3819903999

Zero-point correction= 0.049885 (Hartree/Particle)
Thermal correction to Energy= 0.056510
Thermal correction to Enthalpy= 0.057454
Thermal correction to Gibbs Free Energy= 0.018885
Sum of electronic and zero-point Energies= -2621.222983
Sum of electronic and thermal Energies= -2621.216358
Sum of electronic and thermal Enthalpies= -2621.215414
Sum of electronic and thermal Free Energies= -2621.253982

Table S5. Cartesian coordinates and energies of **5** (X = Cl) at the WB97XD/6–31+G(d,p) level of theory.

C,0.2320037463,1.6182261608,-0.7127178078
C,-0.3490583627,0.5979830717,-0.0643484813
H,1.2298609826,1.6066848375,-1.1649209547
H,-0.2880156769,2.572372238,-0.8325225249
Li,-2.0776842389,0.1652408263,0.8879553928
H,0.5656448894,-2.1082292821,-0.9278171154
H,1.5545539524,-1.2973996156,1.2352886032
Ge,0.4394073164,-1.0826390395,0.2050252684
Cl,-1.3067126086,-2.0722391971,1.3740576197

Zero-point correction= 0.050169 (Hartree/Particle)
Thermal correction to Energy= 0.057255
Thermal correction to Enthalpy= 0.058199
Thermal correction to Gibbs Free Energy= 0.018345
Sum of electronic and zero-point Energies= -2621.295844
Sum of electronic and thermal Energies= -2621.288758
Sum of electronic and thermal Enthalpies= -2621.287814
Sum of electronic and thermal Free Energies= -2621.327668

Table S6. Cartesian coordinates and energies of **6** at the WB97XD/6-31+G(d,p) level of theory.

C,-0.7771686876,1.0036466,-0.0857946719
C,0.7274238256,1.0426618059,-0.111867913
H,-1.2915338842,1.6520911128,0.6224349058
H,1.2321924824,1.7170940044,0.5790491512
H,1.2228383963,0.999249956,-1.0811767122
H,-1.3027610067,0.9331486943,-1.0372942177
Ge,0.0313628741,-0.6482601733,0.6249394577

Zero-point correction=	0.051633 (Hartree/Particle)
Thermal correction to Energy=	0.055503
Thermal correction to Enthalpy=	0.056447
Thermal correction to Gibbs Free Energy=	0.024984
Sum of electronic and zero-point Energies=	-2153.500115
Sum of electronic and thermal Energies=	-2153.496245
Sum of electronic and thermal Enthalpies=	-2153.495301
Sum of electronic and thermal Free Energies=	-2153.526764

Table S7. Cartesian coordinates and energies of **7** at the WB97XD/6-31+G(d,p) level of theory.

C,-1.7568489908,0.7620278578,0.2053925713
C,1.7060556987,0.8690695087,-0.2481065292
H,-2.2212764793,1.3238447546,1.0056379629
H,2.1505815637,1.618798914,-0.8899858278
H,2.3462959667,0.153322451,0.251341873
H,-2.3771561506,0.1671052379,-0.4526049472
Ge,-0.0252976086,0.815463276,-0.0213851029

Zero-point correction=	0.048281 (Hartree/Particle)
Thermal correction to Energy=	0.053293
Thermal correction to Enthalpy=	0.054237
Thermal correction to Gibbs Free Energy=	0.020954
Sum of electronic and zero-point Energies=	-2153.453950
Sum of electronic and thermal Energies=	-2153.448938
Sum of electronic and thermal Enthalpies=	-2153.447994
Sum of electronic and thermal Free Energies=	-2153.481277

Table S8. Cartesian coordinates and energies of **8** at the WB97XD/6-31+G(d,p) level of theory.

C,1.5235744665,-0.3200001576,-0.0000134488
H,1.784754247,-0.8518175817,-0.921781301
H,1.784816744,-0.8516577585,0.9218289111
C,1.1897604149,1.0230201933,-0.0001181941
Ge,-0.6008895981,0.3992850192,-0.000003815
H,-1.1523924084,-0.239020641,1.2760687464
H,-1.1524782358,-0.2392406838,-1.2759292485

Zero-point correction=	0.043217 (Hartree/Particle)
Thermal correction to Energy=	0.047262
Thermal correction to Enthalpy=	0.048206
Thermal correction to Gibbs Free Energy=	0.015455
Sum of electronic and zero-point Energies=	-2153.381572
Sum of electronic and thermal Energies=	-2153.377527
Sum of electronic and thermal Enthalpies=	-2153.376583
Sum of electronic and thermal Free Energies=	-2153.409334

Table S9. Cartesian coordinates and energies of **9** at the WB97XD/6-31+G(d,p) level of theory.

C,	2.1891962489,-0.4861564676,-0.0000003931
H,	2.7673276726,-0.572889993,-0.9247229484
H,	2.7673644346,-0.5727333824,0.9247136612
C,	0.8919614575,-0.2973639882,0.0000082232
Ge,	-0.9265707574,0.0298468509,0.0000078698
H,	-1.6108964628,-0.501482305,1.2648422686
H,	-1.6109435933,-0.5017457146,-1.2646906813
Zero-point correction=	0.044201 (Hartree/Particle)
Thermal correction to Energy=	0.048837
Thermal correction to Enthalpy=	0.049781
Thermal correction to Gibbs Free Energy=	0.016091
Sum of electronic and zero-point Energies=	-2153.432335
Sum of electronic and thermal Energies=	-2153.427699
Sum of electronic and thermal Enthalpies=	-2153.426755
Sum of electronic and thermal Free Energies=	-2153.460446

Table S10. Cartesian coordinates and energies of **TS1** at the WB97XD/6–31+G(d,p) level of theory.

C,-3.0505597497,0.5611910176,0.7581319252
C,-3.036828316,0.5631040982,-0.7552372281
H,-2.9111277022,1.5130722514,1.268147306
H,-2.8862918531,1.5164585024,-1.2591300806
H,-3.7503231783,-0.0749601419,-1.2743364398
Li,1.0223521551,-1.1385896099,0.0124179561
H,-3.7739948914,-0.0775957209,1.2625245201
Ge,-1.467573106,-0.2926557166,0.0150321023
Cl,2.6867204817,0.1170243197,-0.0270488712

Zero-point correction= 0.054556 (Hartree/Particle)
Thermal correction to Energy= 0.061348
Thermal correction to Enthalpy= 0.062292
Thermal correction to Gibbs Free Energy= 0.021279
Sum of electronic and zero-point Energies= -2621.300721
Sum of electronic and thermal Energies= -2621.293929
Sum of electronic and thermal Enthalpies= -2621.292985
Sum of electronic and thermal Free Energies= -2621.333998

Table S11. Cartesian coordinates and energies of **TS2** at the WB97XD/6-31+G(d,p) level of theory.

C,-3.0522655971,-1.4903327427,0.0191220928
C,-2.8110570848,1.3773277671,-0.0260221002
H,-2.8002152323,-2.5377084491,0.1831914765
H,-2.3860611933,2.364761757,-0.2073451106
H,-3.7933608168,1.4146408446,0.4465540124
Li,0.9350195786,0.0484487387,0.0028919906
H,-4.0447892888,-1.3461500573,-0.4081150446
Ge,-1.7719969339,-0.1577937595,-0.0267896616
Cl,2.9991545684,0.3268268736,0.0165240069

Zero-point correction= 0.051326 (Hartree/Particle)
Thermal correction to Energy= 0.058987
Thermal correction to Enthalpy= 0.059931
Thermal correction to Gibbs Free Energy= 0.016629
Sum of electronic and zero-point Energies= -2621.222273
Sum of electronic and thermal Energies= -2621.214612
Sum of electronic and thermal Enthalpies= -2621.213668
Sum of electronic and thermal Free Energies= -2621.256970

Table S12. Cartesian coordinates and energies of **TS3** at the WB97XD/6-31+G(d,p) level of theory.

C,0.9155800708,1.4806713063,-0.1342767103
C,0.3847584205,0.4658139199,0.7338631388
H,0.8108315443,1.4370032671,-1.2230920383
H,1.0392222514,2.500644449,0.2314770076
Li,-1.3049583627,0.5548287238,1.8168740708
H,2.0010904272,-0.6794829646,-1.5371172744
H,3.0620741637,-0.6798526488,0.7966735429
Ge,1.8586535055,-0.3338053839,-0.066513448
Cl,-1.7489903808,-0.3036095489,-0.1535676091

Zero-point correction= 0.048440 (Hartree/Particle)
Thermal correction to Energy= 0.054990
Thermal correction to Enthalpy= 0.055934
Thermal correction to Gibbs Free Energy= 0.017088
Sum of electronic and zero-point Energies= -2621.216050
Sum of electronic and thermal Energies= -2621.209500
Sum of electronic and thermal Enthalpies= -2621.208556
Sum of electronic and thermal Free Energies= -2621.247402

Table S13. Cartesian coordinates and energies of **TS4** at the WB97XD/6–31+G(d,p) level of theory.

C,-1.3349795197,0.5772578845,-0.0369519124
C,1.3356059304,0.6181444966,0.0183442276
H,-1.2698295594,1.5171955845,0.516824607
H,1.1103376418,1.6791595762,-0.1034730775
H,2.3677029339,0.3753577604,-0.2440780695
H,-2.3161508816,0.429109594,-0.4944938843
Ge,0.0126043744,-0.7203997263,-0.006246531

Zero-point correction= 0.047628 (Hartree/Particle)
Thermal correction to Energy= 0.051728
Thermal correction to Enthalpy= 0.052673
Thermal correction to Gibbs Free Energy= 0.020616
Sum of electronic and zero-point Energies= -2153.413396
Sum of electronic and thermal Energies= -2153.409297
Sum of electronic and thermal Enthalpies= -2153.408352
Sum of electronic and thermal Free Energies= -2153.440409

Table S14. Cartesian coordinates and energies of **TS5** at the WB97XD/6–31+G(d,p) level of theory.

C,1.5235744665,-0.3200001576,-0.0000134488
H,1.784754247,-0.8518175817,-0.921781301
H,1.784816744,-0.8516577585,0.9218289111
C,1.1897604149,1.0230201933,-0.0001181941
Ge,-0.6008895981,0.3992850192,-0.000003815
H,-1.1523924084,-0.239020641,1.2760687464
H,-1.1524782358,-0.2392406838,-1.2759292485

Zero-point correction=	0.043217 (Hartree/Particle)
Thermal correction to Energy=	0.047262
Thermal correction to Enthalpy=	0.048206
Thermal correction to Gibbs Free Energy=	0.015455
Sum of electronic and zero-point Energies=	-2153.381572
Sum of electronic and thermal Energies=	-2153.377527
Sum of electronic and thermal Enthalpies=	-2153.376583
Sum of electronic and thermal Free Energies=	-2153.409334
