Supporting Information for

DFT Studies on a Carbenoid Mechanism for the Doering-Moore-Skattebøl Reaction

Alicia C. Voukides, Katharine J. Cahill and Richard P. Johnson*

Department of Chemistry
University of New Hampshire
Durham, NH 03824
rpj@cisunix.unh.edu

Contents

1-Bromo-1-Lithiocyclopropane Chemistry	**SI-2**
Solvated Models for 1-Bromo-1-Lithiocyclopropane Chemistry	**SI-3**
LiBr Dissociation Energetics with Explicit Solvation	**SI-3**
Complete Gaussian reference	**SI-4**
Summary Computational Results	**SI-5 to SI-34**

Table SI-1

Energies and Relative Energies of Stationary Points compared over several computational methods

	B3LYP/6-31+G(d)		B3LYP/6-311+G(d,p)		CCSD(T) // B3LYP/6-311+G(d,p)		MP2/6-31+G(d)	
Structure	E+ZPVE (au)	E_{rel} (kcal/mol)	E+ZPVE (au)	E_{rel} (kcal/mol)	E+ZPVE (au)	E_{rel} (kcal/mol)	E+ZPVE (au)	E_{rel} (kcal/mol)
18	-2695.88019	0.00	-2698.33347	0.00	-2696.30247	0.00	-2698.33347	0.00
TS19	-2695.86558	9.17	-2698.32169	7.39	-2696.28767	9.29	-2698.32169	13.29
20	-2695.86665	8.50	-2698.32182	7.31	-2696.28810	9.01	-2698.32182	12.12
TS22	-2695.86325	10.63	-2698.31890	9.14	-2696.28552	10.63	-2698.31890	13.31
23	-2695.86930	6.84	-2698.32469	5.51	-2696.28840	8.83	-2698.32469	9.41
24	-2695.95144	-44.71	-2698.41039	-48.27	-2696.37368	-44.69	-2698.41039	-44.23
TS21s	-2695.86147	11.75	-2698.31841	9.45	-2696.28516	10.86	-2698.31841	13.80
TS21a	-2695.85966	12.89	-2698.3172	10.24	-2696.28316	12.21	-2698.3172	14.6

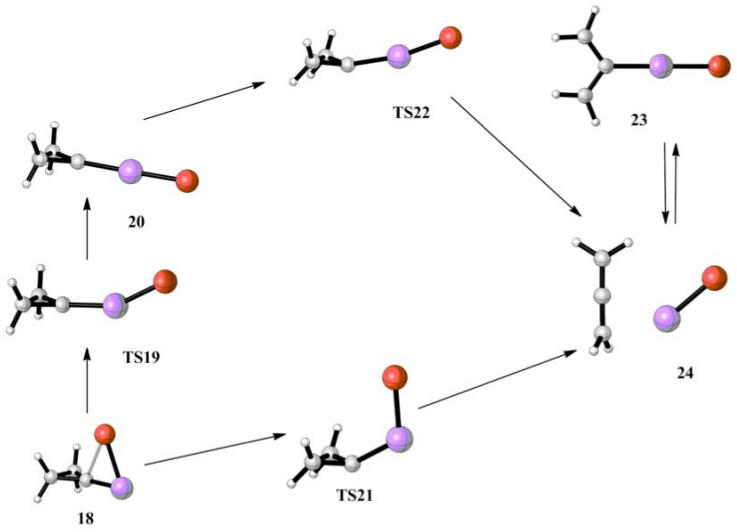


FIGURE S1. Structures for Stationary Points for Table S1

Table SI-2. Energies and Relative Energies of Stationary Points with PCM solvation[a]

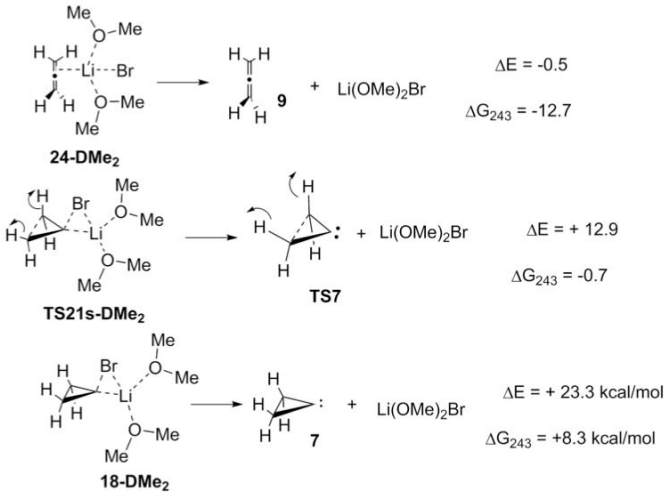
Structure	E_{tot} (au)[a]	Solvation Energy (kcal/mol)	G_{243} (au)
Carbenoid (**18-PCM**)	-2698.368464	-26.41	-2698.392477
TS21-PCM	-2698.353776	-28.09	-2698.379302
Allene-LiBr **24-PCM**	-2698.443992	-27.51	-2698.469486
Cyclopropylidene (**7-PCM**)	-116.536759	-3.92	-116.555140
Allene (**9-PCM**)	-116.642493	-1.17	-116.661382
LiBr-PCM	-2581.812237	-43.35	-2581.829754
Cyclopropylidene TS-PCM	-116.531157	-5.83	-116.555336

a) All calculations B3LYP/6-311+G(d,p) with PCM solvation in diethyl ether Free energies at 243 K (-30 °C).

Table S3. Explicit Solvation Models from B3LYP/6-311+g(d,p) Calculations

molecule	E+ZPVE (au)	Erel (kcal/mol)
18-DME2	-3008.373370	0.00
20-DME2	-3008.340531	20.61
TS21DME2	-3008.349264	15.13
24-DME2	-3008.444875	-44.87

SCHEME SI-1. B3LYP/6-311+G(d,p) Energetics of LiBr Dissociation with Explicit Solvation (two molecules of dimethyl ether)



Complete Gaussian Reference:

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

Summary Computational Results:

Note: All stationary points were characterized by vibrational frequency analysis, displaying zero imaginary modes for minima and one for transition states.

1-Bromo-1-Lithiocyclopropane Chemistry

18 B3LYP/6-31+G(d) 298K
Charge = 0 Multiplicity = 1
H,0,0.0018940986,-0.0122486908,-0.0090535377
C,0,-0.0001485907,0.0105405145,1.0773986951
C,0,1.3422910466,0.0105405134,1.7674891329
C,0,0.4708568142,1.2429538887,1.8119229613
H,0,-0.8487092774,-0.5094989199,1.5232359535
H,0,2.2246242415,-0.0122486926,1.1335563605
H,0,1.4735566732,-0.5094989218,2.7170129263
Br,0,1.2216596586,2.7572200425,0.3513788915
Li,0,0.1421175476,3.0461870051,2.4514226553

E(RB+HF-LYP) = -2695.94011863 A.U.

Zero-point correction= 0.059927 (Hartree/Particle)
Thermal correction to Energy= 0.065899
Thermal correction to Enthalpy= 0.066843
Thermal correction to Gibbs Free Energy= 0.029675
Sum of electronic and zero-point Energies= -2695.880192
Sum of electronic and thermal Energies= -2695.874220
Sum of electronic and thermal Enthalpies= -2695.873276
Sum of electronic and thermal Free Energies= -2695.910443

18 B3LYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1
H,0,0.0006916442,0.011421987,0.0070518043

C,0,-0.0006027324,-0.0028628076,1.0900492158
C,0,1.3361177255,-0.0028628058,1.7792959845
C,0,0.4500224381,1.2144312839,1.8569464765
H,0,-0.8436196452,-0.5374193014,1.5213024898
H,0,2.2176394161,0.0114219901,1.1501659679
H,0,1.4736946611,-0.5374192982,2.716168169
Br,0,1.2063145713,2.8179620862,0.3901986941
Li,0,0.1376987041,3.023141439,2.4626649801

E(RB+HF-LYP) = -2698.39273608 A.U.
E(CCSD(T)) = -2696.3617323 A.U.

Zero-point correction= 0.059267 (Hartree/Particle)
Thermal correction to Energy= 0.065306
Thermal correction to Enthalpy= 0.066250
Thermal correction to Gibbs Free Energy= 0.028935
Sum of electronic and zero-point Energies= -2698.333469
Sum of electronic and thermal Energies= -2698.327430
Sum of electronic and thermal Enthalpies= -2698.326486
Sum of electronic and thermal Free Energies= -2698.363801

18 MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0,0.0126015348,-0.0144363369,-0.0078105838
C,0,0.0046387658,0.017692422,1.0783582748
C,0,1.347855852,0.0176924206,1.7654686599
C,0,0.4828057801,1.2568299175,1.8000680899
H,0,-0.8339871159,-0.5074871831,1.5311076414
H,0,2.2239619644,-0.0144363393,1.123390569
H,0,1.4714850107,-0.5074871856,2.71045077
Br,0,1.187938828,2.6736873921,0.4216188969
Li,0,0.0747945225,3.0047885577,2.5976803905

E(MP2) = -2693.75772429 A.U.

Zero-point correction= 0.061614 (Hartree/Particle)
Thermal correction to Energy= 0.067369
Thermal correction to Enthalpy= 0.068313
Thermal correction to Gibbs Free Energy= 0.031643
Sum of electronic and zero-point Energies= -2693.696110
Sum of electronic and thermal Energies= -2693.690355
Sum of electronic and thermal Enthalpies= -2693.689411
Sum of electronic and thermal Free Energies= -2693.726081

TS19 B3LYP/6-31+G(d) 298K

Charge = 0 Multiplicity = 1
H,0,-0.0056544714,0.1372596137,0.0009565608
C,0,-0.0003967198,0.0358622787,1.0880201483
C,0,1.282735713,0.0366521726,1.8556521288
C,0,0.4141314286,1.2374680538,1.8500839034
H,0,-0.8689452882,-0.5062966385,1.467042129
H,0,2.2430578859,0.1386231293,1.3463391597
H,0,1.3598013158,-0.5049703496,2.8004678152

Br,0,0.8026174946,5.2496249996,1.2013022473
Li,0,0.2482386887,3.3012858764,2.1261909565

E(RB+HF-LYP) = -2695.92250822 A.U.
Imaginary Frequency = -39.87

Zero-point correction= 0.056930 (Hartree/Particle)
Thermal correction to Energy= 0.063096
Thermal correction to Enthalpy= 0.064040
Thermal correction to Gibbs Free Energy= 0.024998
Sum of electronic and zero-point Energies= -2695.865578
Sum of electronic and thermal Energies= -2695.859412
Sum of electronic and thermal Enthalpies= -2695.858468
Sum of electronic and thermal Free Energies= -2695.897511

TS19 B3LYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1
H,0,-0.005871324,-0.121873795,0.0106120239
C,0,-0.0029324865,-0.0346303942,1.0956805099
C,0,1.2800669203,-0.0281355692,1.8613892774
C,0,0.5353062697,1.2285034088,1.6408738933
H,0,-0.9189756469,-0.4041681241,1.5531275198
H,0,2.2371047082,-0.1105309349,1.3492536567
H,0,1.3150487769,-0.3928593505,2.8864280103
Br,0,0.9206077682,5.3848979898,0.956123119
Li,0,0.4851299424,3.3356543735,1.7061695481

Imaginary Frequency = -28.35
E(RB+HF-LYP) = -2698.37793370 A.U.
E(CCSD(T)) = -2696.3439127 A.U.

Zero-point correction= 0.056244 (Hartree/Particle)
Thermal correction to Energy= 0.062519
Thermal correction to Enthalpy= 0.063463
Thermal correction to Gibbs Free Energy= 0.024021
Sum of electronic and zero-point Energies= -2698.321690
Sum of electronic and thermal Energies= -2698.315415
Sum of electronic and thermal Enthalpies= -2698.314471
Sum of electronic and thermal Free Energies= -2698.353912

TS19 MP2/6-31+(d)

Charge = 0 Multiplicity = 1
H,0,0.0073636241,0.1436641756,0.0020880492
C,0,0.0050215047,0.0344768122,1.0863372771
C,0,1.2839201375,0.0344787796,1.8552419821
C,0,0.4191825181,1.2350906458,1.8454975295
H,0,-0.8600713626,-0.5053348995,1.4698476033
H,0,2.2404495951,0.1436804534,1.3447023789
H,0,1.3508979159,-0.505343199,2.7991533486
Br,0,1.1921266889,4.8695488737,0.5645733375
Li,0,0.3301647687,3.3589340072,1.9943548595

Imaginary Frequency = -33.10

E(MP2) = -2693.73308092 A.U.

Zero-point correction= 0.058157 (Hartree/Particle)
Thermal correction to Energy= 0.064277
Thermal correction to Enthalpy= 0.065221
Thermal correction to Gibbs Free Energy= 0.026035
Sum of electronic and zero-point Energies= -2693.674924
Sum of electronic and thermal Energies= -2693.668804
Sum of electronic and thermal Enthalpies= -2693.667860
Sum of electronic and thermal Free Energies= -2693.707046

20 RB3LYP/6-31+G(d) 298K

Charge = 0 Multiplicity = 1
H,0,-0.0005414727,-0.0006980361,-0.003063399
C,0,-0.0010784906,0.0033892656,1.0889316645
C,0,1.2836031917,0.0046148616,1.8534453935
C,0,0.4801520728,1.2436109128,1.7402671115
H,0,-0.902321736,-0.4457457492,1.5114476046
H,0,2.2430703287,0.0014081082,1.332012483
H,0,1.342829657,-0.443854137,2.8473447319
Br,0,-0.1514199895,5.4249386333,2.6525421748
Li,0,0.1933359162,3.2816757976,2.1802560129

E(RB+HF-LYP) = -2695.92369873 A.U.

Zero-point correction= 0.057050 (Hartree/Particle)
Thermal correction to Energy= 0.064041
Thermal correction to Enthalpy= 0.064985
Thermal correction to Gibbs Free Energy= 0.023938
Sum of electronic and zero-point Energies= -2695.866649
Sum of electronic and thermal Energies= -2695.859658
Sum of electronic and thermal Enthalpies= -2695.858714
Sum of electronic and thermal Free Energies= -2695.899760

20 RB3LYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1
H,0,0.0002182195,0.0030050132,0.003662154
C,0,0.0002454687,-0.0009128202,1.0922276791
C,0,1.284010088,-0.0000779902,1.8558683658
C,0,0.4791959117,1.2334452317,1.7468084478
H,0,-0.8987319362,-0.447878212,1.5130142969
H,0,2.2404103271,0.0046767049,1.3359770204
H,0,1.3438588318,-0.4466669519,2.8467905924
Br,0,-0.1698573631,5.4259749863,2.6767135592
Li,0,0.1852918498,3.2825369192,2.1975540205

E(RB+HF-LYP) = -2698.37801936 A.U.
E(CCSD(T)) = -2696.3442993 A.U.

Zero-point correction= 0.056196 (Hartree/Particle)
Thermal correction to Energy= 0.063429
Thermal correction to Enthalpy= 0.064373

Thermal correction to Gibbs Free Energy= 0.021769
Sum of electronic and zero-point Energies= -2698.321823
Sum of electronic and thermal Energies= -2698.314591
Sum of electronic and thermal Enthalpies= -2698.313646
Sum of electronic and thermal Free Energies= -2698.356250

20 MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0,0.0096149226,-0.0099941754,0.0001088186
C,0,0.0033444986,-0.0136332167,1.0898276985
C,0,1.2853323961,-0.0125099947,1.8521941994
C,0,0.480782611,1.2234482605,1.7445948952
H,0,-0.89253628,-0.4640648463,1.5165135701
H,0,2.2397622425,-0.0080985885,1.3262748025
H,0,1.3388624463,-0.4622658999,2.843355919
Br,0,-0.1618907184,5.4690039528,2.6882759569
Li,0,0.1852473573,3.3024184836,2.2012667451

E(MP2) = -2693.73504029 A.U.

Zero-point correction= 0.058247 (Hartree/Particle)
Thermal correction to Energy= 0.065218
Thermal correction to Enthalpy= 0.066162
Thermal correction to Gibbs Free Energy= 0.025125
Sum of electronic and zero-point Energies= -2693.676793
Sum of electronic and thermal Energies= -2693.669822
Sum of electronic and thermal Enthalpies= -2693.668878
Sum of electronic and thermal Free Energies= -2693.709915

TS21s B3LYP/6-31+G(d) 298K

Charge = 0 Multiplicity = 1
C,-0.0024129979,-0.052609595,-0.0274687338
C,0.0358524782,0.0341230012,1.6558176865
C,1.1675739878,-0.0340187881,0.7892821951
H,-0.0767417078,0.7293282356,-0.7848952205
H,-0.6486951057,-0.7720295972,1.9030996393
H,-0.005856744,0.8899463578,2.3314442156
Br,2.2077191914,3.367582212,0.5936838511
Li,2.8275089531,1.2063524737,0.6884587181
H,-0.6955632013,-0.8783128429,-0.1593560532

E(RB+HF-LYP) = -2695.91899887 A.U.
Imaginary Frequency = -273.39

Zero-point correction= 0.057526 (Hartree/Particle)
Thermal correction to Energy= 0.063917
Thermal correction to Enthalpy= 0.064861
Thermal correction to Gibbs Free Energy= 0.024816
Sum of electronic and zero-point Energies= -2695.861473
Sum of electronic and thermal Energies= -2695.855082
Sum of electronic and thermal Enthalpies= -2695.854138
Sum of electronic and thermal Free Energies= -2695.894183

TS21s B3LYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1
C,-0.0597103699,-0.0582243261,-0.0068987858
C,0.0217153096,0.0290595625,1.6451073771
C,1.1223708995,0.0485355399,0.7877582178
H,-0.207116545,0.7113293198,-0.7621149783
H,-0.6027077725,-0.8427835093,1.9181358177
H,-0.1282010845,0.879040054,2.3163726376
Br,2.3566343123,3.5271381122,1.0393718236
Li,2.7548766996,1.3389526236,0.8097649768
H,-0.6488084223,-0.9541846111,-0.1566473503

Imaginary Frequency = -299.65
E(RB+HF-LYP) = -2698.37496773 A.U.
E(CCSD(T)) = -2696.3419206 A.U.

Zero-point correction= 0.056762 (Hartree/Particle)
Thermal correction to Energy= 0.063289
Thermal correction to Enthalpy= 0.064234
Thermal correction to Gibbs Free Energy= 0.022935
Sum of electronic and zero-point Energies= -2698.318406
Sum of electronic and thermal Energies= -2698.311879
Sum of electronic and thermal Enthalpies= -2698.310935
Sum of electronic and thermal Free Energies= -2698.352233

TS21s MP2/6-31+G(d)
Charge = 0 Multiplicity = 1
C,0.0368918679,0.0934317825,0.054925281
C,0.000614100,3,0.0100544663,1.6576712584
C,1.2109178583,-0.0654934839,0.87718142
H,0.0334785289,0.9689877251,-0.5922631765
H,-0.649466658,-0.833566384,1.8648803487
H,-0.0340339289,0.8137849133,2.3913471902
Br,2.1865859974,3.1877587144,1.0696034801
Li,2.9945278598,1.059009087,0.976306955
H,-0.6012034878,-0.7226164345,-0.2677760147

Imaginary Frequency = -407.78
E(MP2) = -2693.73245840 A.U.

Zero-point correction= 0.058337 (Hartree/Particle)
Thermal correction to Energy= 0.064673
Thermal correction to Enthalpy= 0.065617
Thermal correction to Gibbs Free Energy= 0.026116
Sum of electronic and zero-point Energies= -2693.674121
Sum of electronic and thermal Energies= -2693.667785
Sum of electronic and thermal Enthalpies= -2693.666841
Sum of electronic and thermal Free Energies= -2693.706342

TS21a RB3LYP/6-31+G(d) 298K

Charge = 0 Multiplicity = 1
C,-3.060353,0.843146,-0.114007
C,-3.079807,-0.830587,-0.134608

C,-1.993493,-0.011332,0.2853
H,-3.41131,1.572061,0.618998
H,-3.417477,-0.999713,-1.152758
Br,1.793031,0.001154,-0.071755
Li,-0.094641,-0.032108, 1.12416
H,-3.447961,-1.569066,0.580201
H,-3.393512,1.045286,-1.127589

Imaginary Frequency = -246.54
E(RB+HF-LYP) = -2695.91712086 A.U.

Zero-point correction= 0.057129 (Hartree/Particle)
Thermal correction to Energy= 0.061981
Thermal correction to Enthalpy= 0.062926
Thermal correction to Gibbs Free Energy= 0.027206
Sum of electronic and zero-point Energies= -2695.859992
Sum of electronic and thermal Energies= -2695.855140
Sum of electronic and thermal Enthalpies= -2695.854195
Sum of electronic and thermal Free Energies= -2695.889914

TS21a RB3BLYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1

C	-1.97547800	-0.99940100	-0.20782700
H	-2.55713100	-1.70038300	0.35662900
H	-1.93739500	-1.11977500	-1.27287000
C	-1.19281300	-0.00197000	0.50408200
C	-1.97603100	1.00085200	-0.20155600
H	-1.93726000	1.12873600	-1.26536500
H	-2.55771200	1.69733900	0.36881400
Li	0.19249200	-0.00716200	2.04510400
Br	1.12222700	0.00053400	-0.13973500

Imaginary Frequency = -265.65
E(RB+HF-LYP) = -2698.37384285 A.U.
E(CCSD(T)) = -2696.3398422 A.U.

Zero-point correction= 0.056686 (Hartree/Particle)
Thermal correction to Energy= 0.062284
Thermal correction to Enthalpy= 0.063228
Thermal correction to Gibbs Free Energy= 0.025767
Sum of electronic and zero-point Energies= -2698.317157
Sum of electronic and thermal Energies= -2698.311559
Sum of electronic and thermal Enthalpies= -2698.310615
Sum of electronic and thermal Free Energies= -2698.348076

TS21a MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
C,0,2.7824818474,0.9178518392,-0.1384011067
H,0,3.2481503929,1.6922580254,0.4725587057
H,0,3.0064566766,0.9783328003,-1.2016299568
C,0,1.9242567978,0.0014891967,0.4976412851
C,0,2.7773991464,-0.9220104705,-0.1349100505
H,0,3.0010370528,-0.9877541625,-1.1978972913

H,0,3.2387865727,-1.6966536313,0.4789902487
Li,0,0.1124024774,0.0083229364,1.5404855096
Br,0,-1.195962964,0.0082634663,-0.3310043438

Imaginary Frequency = -51.63
E(MP2) = -2693.73169539 A.U.

Zero-point correction= 0.058831 (Hartree/Particle)
Thermal correction to Energy= 0.065081
Thermal correction to Enthalpy= 0.066025
Thermal correction to Gibbs Free Energy= 0.027257
Sum of electronic and zero-point Energies= -2693.672864
Sum of electronic and thermal Energies= -2693.666615
Sum of electronic and thermal Enthalpies= -2693.665670
Sum of electronic and thermal Free Energies= -2693.704438

TS22 RB3LYP/6-31+G(d) 298K

Charge = 0 Multiplicity = 1
H,0,-0.0142002529,-0.0344320123,-0.00409074
C,0,-0.0081114957,0.0028198489,1.0868354287
C,0,1.2189956935,0.0028198491,2.1550597734
C,0,0.5537557007,1.1839686195,1.6803215995
H,0,-0.7449596739,-0.6479671097,1.5491758024
H,0,2.3003564764,-0.0344320119,2.0107828316
H,0,0.8625875375,-0.6479671094,2.9485817234
Br,0,1.3499606504,5.3413273185,0.7656927356
Li,0,0.905030455,3.2232599666,1.2767998308

E(RB+HF-LYP) = -2695.92033985 A.U.
Imaginary Frequency = -307.15

Zero-point correction= 0.057092 (Hartree/Particle)
Thermal correction to Energy= 0.063657
Thermal correction to Enthalpy= 0.064601
Thermal correction to Gibbs Free Energy= 0.024346
Sum of electronic and zero-point Energies= -2695.863248
Sum of electronic and thermal Energies= -2695.856683
Sum of electronic and thermal Enthalpies= -2695.855739
Sum of electronic and thermal Free Energies= -2695.895994

TS22 RB3LYP/6-311+G(d,p) 298K

Charge = 0 Multiplicity = 1
H,0,0.1146118374,-0.0658315221,0.0244808607
C,0,0.0693867816,-0.0347281419,1.1116372257
C,0,1.2401264194,-0.0347281415,2.2204073224
C,0,0.5916584075,1.150604412,1.7326470463
H,0,-0.6960658747,-0.6716701963,1.537836721
H,0,2.3232199332,-0.0658315213,2.116183006
H,0,0.8561440679,-0.6716701957,3.0078851524
Br,0,1.6342286867,5.2083852898,0.6318071549
Li,0,0.9728363336,3.2014892211,1.3301649544

Imaginary Frequency = -317.32
E(RB+HF-LYP) = -2698.37516126 A.U.
E(CCSD(T)) = -2696.3417852 A.U.

Zero-point correction= 0.056263 (Hartree/Particle)
Thermal correction to Energy= 0.063001
Thermal correction to Enthalpy= 0.063945
Thermal correction to Gibbs Free Energy= 0.022386
Sum of electronic and zero-point Energies= -2698.318898
Sum of electronic and thermal Energies= -2698.312160
Sum of electronic and thermal Enthalpies= -2698.311216
Sum of electronic and thermal Free Energies= -2698.352775

TS22 MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0,0.0598677146,-0.0907610165,0.010001536
C,0,0.0314085858,-0.0450485429,1.0978993413
C,0,1.2113974854,-0.0450485433,2.1356645437
C,0,0.5581112714,1.1677417296,1.6887477201
H,0,-0.7779504207,-0.6159708118,1.5434310638
H,0,2.2867485542,-0.0907610173,1.9684771164
H,0,0.8728979236,-0.6159708124,2.9953031675
Br,0,1.152705788,5.477109555,1.0126651861
Li,0,0.8304130642,3.2815336671,1.3791274984

Imaginary Frequency = -393.00
E(MP2) = -2693.73284800 A.U.

Zero-point correction= 0.057947 (Hartree/Particle)
Thermal correction to Energy= 0.064494
Thermal correction to Enthalpy= 0.065438
Thermal correction to Gibbs Free Energy= 0.025272
Sum of electronic and zero-point Energies= -2693.674901
Sum of electronic and thermal Energies= -2693.668354
Sum of electronic and thermal Enthalpies= -2693.667410
Sum of electronic and thermal Free Energies= -2693.707576

TS23 UB3LYP/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0.0015654973,0.0000337364,-0.0048978677
C,0.0026702686,0.0000079105,1.0865008973
C,0.8569818878,0.0000018166,3.1860348117
C,1.1845008561,0.0001024476,1.8291866227
H,-0.9985697089,-0.0001420384,1.5425016893
H,1.6182135097,0.0000575515,3.968133919
H,-0.1781845665,-0.0001418845,3.5586589439
Br,5.204662104,0.0006768692,0.1933774398
Li,3.1240868905,0.0003767344,1.0399622016|

E(UB+HF-LYP) = -2695.92614144 A.U.
Imaginary Frequency = -969.21

Zero-point correction= 0.056847 (Hartree/Particle)

Thermal correction to Energy= 0.063784
Thermal correction to Enthalpy= 0.064728
Thermal correction to Gibbs Free Energy= 0.023802
Sum of electronic and zero-point Energies= -2695.869295
Sum of electronic and thermal Energies= -2695.862358
Sum of electronic and thermal Enthalpies= -2695.861413
Sum of electronic and thermal Free Energies= -2695.902339

TS23 UB3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
H,-0.175331406,0.0395704159,0.0644814627
C,0.0163622521,0.0300607622,1.1367759418
C,1.2202388696,-0.0777916265,3.0505266517
C,1.2995083109,-0.0999204226,1.6608411579
H,-0.8796304475,0.1307383227,1.7633355689
H,2.1018814067,-0.1643546009,3.6844554273
H,0.272745587,0.027367985,3.595241
Br,4.9653737186,-0.5092460361,-0.6687466141
Li,3.0733774968,-0.2979803339,0.5336969338

Imaginary Frequency = -1013.50
E(UB+HF-LYP) = -2698.38070573 A.U.
E(CCSD(T)) = -2696.3444099 A.U.

Zero-point correction= 0.056014 (Hartree/Particle)
Thermal correction to Energy= 0.063141
Thermal correction to Enthalpy= 0.064085
Thermal correction to Gibbs Free Energy= 0.022208
Sum of electronic and zero-point Energies= -2698.324692
Sum of electronic and thermal Energies= -2698.317564
Sum of electronic and thermal Enthalpies= -2698.316620
Sum of electronic and thermal Free Energies= -2698.358498

TS23 MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
H,-0.0218698889,0.,0.0117889541
C,-0.0070914162,0.,1.1018431367
C,0.8398185183,0.,3.1892486752
C,1.184422128,0.,1.8339263203
H,-0.9995023103,0.,1.5749144866
H,1.5887169548,0.,3.9814529771
H,-0.2016624424,0.,3.541375489
Br,5.2484508813,0.,0.1850534241
Li,3.1538986979,0.,1.0348629609

Imaginary Frequency = -83.87
E(MP2) = -2693.73838550 A.U.

Zero-point correction= 0.057279 (Hartree/Particle)
Thermal correction to Energy= 0.063720
Thermal correction to Enthalpy= 0.064664
Thermal correction to Gibbs Free Energy= 0.024425
Sum of electronic and zero-point Energies= -2693.681107

Sum of electronic and thermal Energies= -2693.674665
Sum of electronic and thermal Enthalpies= -2693.673721
Sum of electronic and thermal Free Energies= -2693.713961

24 RB3LYP/6-31+G(d)

Charge = 0 Multiplicity = 1
C,0,0.,0.,0.
C,0,0.,0.,2.62453395
C,0,0.01951219,0.,1.3054220734
H,0,-0.9460982309,0.,-0.5413830505
H,0,0.0554864295,0.9304149987,3.1913945068
H,0,0.0554864295,-0.9304149987,3.1913945068
Br,0,-3.9154343401,0.,0.5253478997
Li,0,-2.312065132,0.,2.0574587048
H,0,0.9260683883,0.,-0.5717911289

E(RB+HF-LYP) = -2696.00962932 A.U.

Zero-point correction= 0.058189 (Hartree/Particle)
Thermal correction to Energy= 0.065467
Thermal correction to Enthalpy= 0.066411
Thermal correction to Gibbs Free Energy= 0.024980
Sum of electronic and zero-point Energies= -2695.951440
Sum of electronic and thermal Energies= -2695.944162
Sum of electronic and thermal Enthalpies= -2695.943218
Sum of electronic and thermal Free Energies= -2695.984650

24 RB3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
C,0,0.0623919328,0.,-0.0164407393
C,0,-0.01955035,0.,2.5949140906
C,0,0.0346232263,0.,1.2827391648
H,0,-0.8574129086,0.,-0.5952355085
H,0,0.0199406795,0.9292354831,3.1589727534
H,0,0.0199406795,-0.9292354831,3.1589727534
Br,0,-3.981706169,0.,0.534408337
Li,0,-2.3243604616,0.,1.9958619807
H,0,1.008594197,0.,-0.5486413715

E(RB+HF-LYP) = -2698.46811413 A.U.
E(CCSD(T)) = -2696.4314068 A.U.

Zero-point correction= 0.057728
Thermal correction to Energy= 0.065065
Thermal correction to Enthalpy= 0.066009
Thermal correction to Gibbs Free Energy= 0.024319
Sum of electronic and zero-point Energies= -2698.410386
Sum of electronic and thermal Energies= -2698.403050
Sum of electronic and thermal Enthalpies= -2698.402105
Sum of electronic and thermal Free Energies= -2698.443795

24 MP2/6-31+G(d)

Charge = 0 Multiplicity = 1
C,0,-0.0374647625,0.,0.0102758829
C,0,0.0277086111,0.,2.6474447608
C,0,0.0145373728,0.,1.3227389563
H,0,-0.9945673935,0.,-0.508273071
H,0,0.0905948485,0.9305588731,3.2097336169
H,0,0.0905948485,-0.9305588731,3.2097336169
Br,0,-3.8805571884,0.,0.4364426446
Li,0,-2.3053643987,0.,2.0306030288
H,0,0.8774735849,0.,-0.5763249657

E(MP2) = -2693.82537782 A.U.

Zero-point correction= 0.058776 (Hartree/Particle)
Thermal correction to Energy= 0.066124
Thermal correction to Enthalpy= 0.067068
Thermal correction to Gibbs Free Energy= 0.025671
Sum of electronic and zero-point Energies= -2693.766602
Sum of electronic and thermal Energies= -2693.759254
Sum of electronic and thermal Enthalpies= -2693.758310
Sum of electronic and thermal Free Energies= -2693.799706

*****Implicit (PCM) Solvated Models for 1-Bromo-1-Lithiocyclopropane Chemistry****

LiBr: RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
Li,0,0.,0.,-0.0070055511
Br,0,0.,0.,2.3770055511

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2581.744030
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2581.813107
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2581.809287

(Polarized solute)-Solvent (kcal/mol) = -43.35

Cavitation energy (kcal/mol) = 6.23
Dispersion energy (kcal/mol) = -4.36
Repulsion energy (kcal/mol) = 0.53
Total non electrostatic (kcal/mol) = 2.40

Zero-point correction= 0.000870 (Hartree/Particle)
Thermal correction to Energy= 0.002996
Thermal correction to Enthalpy= 0.003766
Thermal correction to Gibbs Free Energy= -0.016647
Sum of electronic and zero-point Energies= -2581.812237
Sum of electronic and thermal Energies= -2581.810111
Sum of electronic and thermal Enthalpies= -2581.809341
Sum of electronic and thermal Free Energies= -2581.829754

7-PCM-243 Cycloproplyidene– RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
C,0,0.0275525584,0.,0.0477148135
C,0,0.0276840371,0.,1.5382899129
C,0,1.3184657624,0.,0.7929377626
H,0,-0.3393236007,-0.9092353674,2.0120862025
H,0,-0.3393236007,0.9092353674,2.0120862025
H,0,1.9122780086,0.9092353674,0.711915873
H,0,1.9122780086,-0.9092353674,0.711915873

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -116.583245
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -116.589485
Total free energy in solution:
with all non electrostatic terms (a.u.) = -116.584389

(Polarized solute)-Solvent (kcal/mol) = -3.92

Cavitation energy (kcal/mol) = 8.13
Dispersion energy (kcal/mol) = -5.26
Repulsion energy (kcal/mol) = 0.32
Total non electrostatic (kcal/mol) = 3.20

Zero-point correction= 0.052726 (Hartree/Particle)
Thermal correction to Energy= 0.056342
Thermal correction to Enthalpy= 0.057286
Thermal correction to Gibbs Free Energy= 0.029277
Sum of electronic and zero-point Energies= -116.536759
Sum of electronic and thermal Energies= -116.533143
Sum of electronic and thermal Enthalpies= -116.532199
Sum of electronic and thermal Free Energies= -116.560209

9-PCM-243 Allene RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
C,0,-0.0019223175,0.,0.0030990811
C,0,-0.0229230099,0.,2.6113250211
C,0,-0.0116067846,0.,1.3072047077
H,0,0.9303132744,0.0000000001,-0.55515403
H,0,-0.0275004882,-0.9283453583,3.1760524
H,0,-0.0275004883,0.9283453583,3.1760524
H,0,-0.9262074476,-0.0000000001,-0.5682462712

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -116.695248
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -116.697106
Total free energy in solution:
with all non electrostatic terms (a.u.) = -116.690631

(Polarized solute)-Solvent (kcal/mol) = -1.17

Cavitation energy (kcal/mol) = 8.92
Dispersion energy (kcal/mol) = -5.12
Repulsion energy (kcal/mol) = 0.27
Total non electrostatic (kcal/mol) = 4.06

Zero-point correction= 0.054613 (Hartree/Particle)
Thermal correction to Energy= 0.057440
Thermal correction to Enthalpy= 0.058210
Thermal correction to Gibbs Free Energy= 0.035724
Sum of electronic and zero-point Energies= -116.642493
Sum of electronic and thermal Energies= -116.639666
Sum of electronic and thermal Enthalpies= -116.638896
Sum of electronic and thermal Free Energies= -116.661382

TS7-PCM-243 CyclopropylideneTS RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
H,0,0.0044969902,-0.0181218401,0.0029406477
C,0,-0.013879211,-0.0031785717,1.0991791779
C,0,2.0002599071,-0.0007956757,1.181269499
C,0,0.9544753942,0.5595502483,1.9251241382
H,0,1.993453654,-0.2063257513,0.1029457731
H,0,2.8770880653,-0.3910841392,1.7028023228
H,0,-0.8595097014,-0.5337086482,1.5448086559

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -116.574484
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -116.583769
Total free energy in solution:
with all non electrostatic terms (a.u.) = -116.577980

(Polarized solute)-Solvent (kcal/mol) = -5.83

Cavitation energy (kcal/mol) = 8.48
Dispersion energy (kcal/mol) = -5.15
Repulsion energy (kcal/mol) = 0.29
Total non electrostatic (kcal/mol) = 3.63

Zero-point correction= 0.052612 (Hartree/Particle)
Thermal correction to Energy= 0.056038
Thermal correction to Enthalpy= 0.056982
Thermal correction to Gibbs Free Energy= 0.028433
Sum of electronic and zero-point Energies= -116.531157
Sum of electronic and thermal Energies= -116.527731
Sum of electronic and thermal Enthalpies= -116.526786
Sum of electronic and thermal Free Energies= -116.555336

18-PCM 1-Bromo-1-Lithiocyclopropane RB3LYP/6-311+G(d,p) + PCM solvation/ 298 K

Charge = 0 Multiplicity = 1
H,0,0.0146634058,-0.0464004668,-0.0143553555
C,0,0.0068909,0.0219438161,1.0676310163

C,0,1.3461375927,0.021943815,1.7560800986
C,0,0.4982449067,1.2783356662,1.7586446388
H,0,-0.8477957596,-0.4667019316,1.5306052401
H,0,2.2215045478,-0.0464004685,1.1200866912
H,0,1.4670322098,-0.4667019334,2.7205586669
Br,0,1.2764171816,2.6719241866,0.2448585495
Li,0,0.0450472424,3.0560038348,2.6402544636

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2698.383337
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2698.427022
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2698.420105

(Polarized solute)-Solvent (kcal/mol) = -27.41

Cavitation energy (kcal/mol) = 11.59
Dispersion energy (kcal/mol) = -7.82
Repulsion energy (kcal/mol) = 0.57
Total non electrostatic (kcal/mol) = 4.34

Zero-point correction= 0.058451 (Hartree/Particle)
Thermal correction to Energy= 0.064822
Thermal correction to Enthalpy= 0.065766
Thermal correction to Gibbs Free Energy= 0.027474
Sum of electronic and zero-point Energies= -2698.368570
Sum of electronic and thermal Energies= -2698.362200
Sum of electronic and thermal Enthalpies= -2698.361256
Sum of electronic and thermal Free Energies= -2698.399547

18-PCM-243 1-Bromo-1-Lithiocyclopropane RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
C,0,0.0059517224,-0.0124551257,0.0023238064
C,0,0.003914566,-0.0142784694,1.5068721864
C,0,1.3204448538,-0.0349632198,0.7562920237
H,0,-0.2052794593,0.9061129488,-0.5412379214
H,0,-0.3570655563,-0.9087047329,2.0013088852
H,0,-0.2111890085,0.9031654485,2.0507556413
Br,0,2.0881976108,-2.1340054251,0.7543889298
Li,0,3.3474851662,0.1817489849,0.7497676334
H,0,-0.3532516237,-0.9055717696,-0.4957480683

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2698.384760
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2698.426842
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2698.419969

(Polarized solute)-Solvent (kcal/mol) = -26.41

Cavitation energy (kcal/mol) = 11.58
Dispersion energy (kcal/mol) = -7.83
Repulsion energy (kcal/mol) = 0.57
Total non electrostatic (kcal/mol) = 4.31

Zero-point correction= 0.058378 (Hartree/Particle)
Thermal correction to Energy= 0.063054
Thermal correction to Enthalpy= 0.063824
Thermal correction to Gibbs Free Energy= 0.034365
Sum of electronic and zero-point Energies= -2698.368464
Sum of electronic and thermal Energies= -2698.363788
Sum of electronic and thermal Enthalpies= -2698.363018
Sum of electronic and thermal Free Energies= -2698.392477

TS21s-PCM RB3LYP/6-311+G(d,p) + PCM solvation 298 K

Charge = 0 Multiplicity = 1
C,0,0.000919752,-0.0006533606,-0.0000260578
C,0,-0.0004713918,0.0003572996,1.7357401358
C,0,1.1181565908,0.0003556534,0.8689340228
H,0,-0.0515018881,0.791908465,-0.7473299199
H,0,-0.7321650668,-0.7900791007,1.8677982178
H,0,-0.054999507,0.7934418979,2.4823313645
Br,0,3.7284168432,-2.2341436643,0.9732659527
Li,0,3.2453127146,0.1350550258,0.8873397374
H,0,-0.7317789869,-0.7900741728,-0.1323941655

Imaginary Frequency = -159.58

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2698.365099
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2698.409849
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2698.400970

(Polarized solute)-Solvent (kcal/mol) = -28.08

Cavitation energy (kcal/mol) = 13.10
Dispersion energy (kcal/mol) = -8.19
Repulsion energy (kcal/mol) = 0.66
Total non electrostatic (kcal/mol) = 5.57

Zero-point correction= 0.056074 (Hartree/Particle)
Thermal correction to Energy= 0.062801
Thermal correction to Enthalpy= 0.063746
Thermal correction to Gibbs Free Energy= 0.023242
Sum of electronic and zero-point Energies= -2698.353776
Sum of electronic and thermal Energies= -2698.347048
Sum of electronic and thermal Enthalpies= -2698.346104
Sum of electronic and thermal Free Energies= -2698.386607

TS21s-PCM-243 RB3LYP/6-311+G(d,p) + PCM solvation 243 K

Charge = 0 Multiplicity = 1
C,0,0.000919752,-0.0006533606,-0.0000260578
C,0,-0.0004713918,0.0003572996,1.7357401358
C,0,1.1181565908,0.0003556534,0.8689340228
H,0,-0.0515018881,0.791908465,-0.7473299199
H,0,-0.7321650668,-0.7900791007,1.8677982178
H,0,-0.054999507,0.7934418979,2.4823313645
Br,0,3.7284168432,-2.2341436643,0.9732659527
Li,0,3.2453127146,0.1350550258,0.8873397374
H,0,-0.7317789869,-0.7900741728,-0.1323941655

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2698.365099
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2698.409849
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2698.400970

(Polarized solute)-Solvent (kcal/mol) = -28.08

Cavitation energy (kcal/mol) = 13.10
Dispersion energy (kcal/mol) = -8.19
Repulsion energy (kcal/mol) = 0.66
Total non electrostatic (kcal/mol) = 5.57

Imaginary Frequency = -159.5831

Zero-point correction= 0.056074 (Hartree/Particle)
Thermal correction to Energy= 0.061113
Thermal correction to Enthalpy= 0.061883
Thermal correction to Gibbs Free Energy= 0.030547
Sum of electronic and zero-point Energies= -2698.353776
Sum of electronic and thermal Energies= -2698.348736
Sum of electronic and thermal Enthalpies= -2698.347967
Sum of electronic and thermal Free Energies= -2698.379302

TS21a-PCM RB3LYP/6-311+G(d,p) + PCM solvation 298 K

Charge = 0 Multiplicity = 1
C,0,0.000919752,-0.0006533606,-0.0000260578
C,0,-0.0004713918,0.0003572996,1.7357401358
C,0,1.1181565908,0.0003556534,0.8689340228
H,0,-0.0515018881,0.791908465,-0.7473299199
H,0,-0.7321650668,-0.7900791007,1.8677982178
H,0,-0.054999507,0.7934418979,2.4823313645
Br,0,3.7284168432,-2.2341436643,0.9732659527
Li,0,3.2453127146,0.1350550258,0.8873397374
H,0,-0.7317789869,-0.7900741728,-0.1323941655

E(RB+HF-LYP) = -2698.40984936 A.U.
Imaginary Freq = -159.58

Variational PCM results
 ======================
 <psi(f)| H |psi(f)>   (a.u.) =   -2698.365099
 <psi(f)|H+V(f)/2|psi(f)>   (a.u.) =   -2698.409849
 Total free energy in solution:
  with all non electrostatic terms   (a.u.) =   -2698.400970

 (Polarized solute)-Solvent   (kcal/mol) =   -28.08

 Cavitation energy   (kcal/mol) =   13.10
 Dispersion energy   (kcal/mol) =   -8.19
 Repulsion energy   (kcal/mol) =   0.66
 Total non electrostatic   (kcal/mol) =   5.57

Zero-point correction=   0.056074 (Hartree/Particle)
 Thermal correction to Energy=   0.062801
 Thermal correction to Enthalpy=   0.063746
 Thermal correction to Gibbs Free Energy=   0.023242
 Sum of electronic and zero-point Energies=   -2698.353776
 Sum of electronic and thermal Energies=   -2698.347048
 Sum of electronic and thermal Enthalpies=   -2698.346104
 Sum of electronic and thermal Free Energies=   -2698.386607

24-PCM Allene-LiBr complex RB3LYP/6-311+G(d,p) + PCM solvation/ 298 K

Charge = 0 Multiplicity = 1
 C,0,-0.0187868277,0.,-0.0163544812
 C,0,0.0800173102,0.,2.5922986724
 C,0,0.0232391907,0.,1.2837619612
 H,0,-0.9704466823,0.,-0.5396208295
 H,0,0.1438986079,0.9299072986,3.1535162892
 H,0,0.1438986079,-0.9299072986,3.1535162892
 Br,0,-3.8547833097,0.,0.4201468564
 Li,0,-2.6720601666,0.,2.46940738
 H,0,0.8966018287,0.,-0.6019459223

Variational PCM results
 ======================
 <psi(f)| H |psi(f)>   (a.u.) =   -2698.455815
 <psi(f)|H+V(f)/2|psi(f)>   (a.u.) =   -2698.500592
 Total free energy in solution:
  with all non electrostatic terms   (a.u.) =   -2698.490647

 (Polarized solute)-Solvent   (kcal/mol) =   -28.10

 Cavitation energy   (kcal/mol) =   13.64
 Dispersion energy   (kcal/mol) =   -8.02
 Repulsion energy   (kcal/mol) =   0.62
 Total non electrostatic   (kcal/mol) =   6.24

Zero-point correction=   0.056717 (Hartree/Particle)
 Thermal correction to Energy=   0.064452

Thermal correction to Enthalpy= 0.065396
Thermal correction to Gibbs Free Energy= 0.022700
Sum of electronic and zero-point Energies= -2698.443875
Sum of electronic and thermal Energies= -2698.436140
Sum of electronic and thermal Enthalpies= -2698.435196
Sum of electronic and thermal Free Energies= -2698.477892

24-PCM-243 Allene-LiBr complex RB3LYP/6-311+G(d,p) + PCM solvation/ 243 K

Charge = 0 Multiplicity = 1
C,0,-0.0319095271,0.,-0.0290710544
C,0,0.0544496111,0.,2.5803131433
C,0,0.0180896308,0.,1.2705851125
H,0,0.8807909804,0.,-0.6177932925
H,0,0.0285599785,-0.9301004864,3.1444748848
H,0,0.0285599785,0.9301004864,3.1444748848
Br,0,3.8063636121,0.,0.1649667006
Li,0,2.7134504794,0.,2.265475628
H,0,-0.9865359851,0.,-0.5482631702

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -2698.456727
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -2698.500567
Total free energy in solution:
with all non electrostatic terms (a.u.) = -2698.490783

(Polarized solute)-Solvent (kcal/mol) = -27.51

Cavitation energy (kcal/mol) = 13.55
Dispersion energy (kcal/mol) = -8.03
Repulsion energy (kcal/mol) = 0.62
Total non electrostatic (kcal/mol) = 6.14

Zero-point correction= 0.056575 (Hartree/Particle)
Thermal correction to Energy= 0.061746
Thermal correction to Enthalpy= 0.062515
Thermal correction to Gibbs Free Energy= 0.031081
Sum of electronic and zero-point Energies= -2698.443992
Sum of electronic and thermal Energies= -2698.438822
Sum of electronic and thermal Enthalpies= -2698.438052
Sum of electronic and thermal Free Energies= -2698.469486

*******Explicit Solvated Models for 1-Bromo-1-Lithiocyclopropane Chemistry******

Li(OMe$_2$)Br: RB3LYP/6-311+G(d,p) / 243 K

Charge = 0 Multiplicity = 1
Li,0,-0.238762,0.136576,-0.001277
Br,0,1.47387,-1.384002,-0.000061
O,0,-2.099155,-0.31462,-0.000599

O,0,0.184796,2.048605,-0.000398
C,0,-3.231571,0.549766,-0.0021
H,0,-2.859343,1.574046,-0.003835
H,0,-3.843808,0.381128,-0.895282
H,0,-3.843863,0.384182,0.891616
C,0,-2.442137,-1.707823,0.00154
H,0,-3.023286,-1.953819,-0.893636
H,0,-1.504379,-2.26225,0.002619
H,0,-3.023713,-1.950953,0.897223
C,0,0.870142,2.463164,-1.188536
H,0,1.860098,1.999915,-1.241682
H,0,0.27176,2.136184,-2.038921
H,0,0.961673,3.554415,-1.208524
C,0,0.865807,2.462702,1.190401
H,0,0.264182,2.1356,2.038449
H,0,1.855475,1.99925,1.247073
H,0,0.957471,3.553925,1.211031

E(RB+HF-LYP) = -2891.96917836 A.U.

Zero-point correction= 0.163988 (Hartree/Particle)
Thermal correction to Energy= 0.174345
Thermal correction to Enthalpy= 0.175115
Thermal correction to Gibbs Free Energy= 0.129529
Sum of electronic and zero-point Energies= -2891.805191
Sum of electronic and thermal Energies= -2891.794833
Sum of electronic and thermal Enthalpies= -2891.794063
Sum of electronic and thermal Free Energies= -2891.839649

18-DME2 RB3LYP/6-311+G(d,p) 298 K

Charge = 0 Multiplicity = 1
H,0,0.1126995498,-0.0321344061,-0.0115089527
C,0,0.124790916,-0.078839819,1.0755233161
C,0,1.4283996369,0.0270305291,1.8213225033
C,0,0.4833721345,1.2099511183,1.7866874589
H,0,-0.6239408724,-0.7427232031,1.4912957711
H,0,2.3606341204,0.1548351052,1.2755533632
H,0,1.5273603338,-0.5690932846,2.7207668726
Br,0,-0.6219307872,1.3005575216,3.7067398916
Li,0,0.1940748235,3.1635996424,2.145649033
H,0,-1.3576629878,5.6097288749,2.7678030847
C,0,-2.0545018823,5.092014926,2.1091178983
C,0,-2.1096803648,3.3889068982,0.4480757374
O,0,-1.3003227324,4.1522842761,1.3478093092
H,0,-2.8120970613,4.5810161628,2.7136969999
H,0,-1.4534950667,2.6683643166,-0.0363984103
H,0,-2.8887658793,2.8503965559,0.997617821
H,0,1.4121562455,5.7260840646,1.3093814888
C,0,2.0902423175,5.4713562482,2.1238509745
C,0,2.2454901989,4.0390840929,4.0212844875
O,0,1.4578666278,4.4622606964,2.9041628616
H,0,3.0372394608,5.1069986014,1.7084292888
H,0,2.4217921834,4.8813855892,4.6998061734

H,0,1.6819208247,3.259864034,4.5322228433
H,0,3.204924388,3.6337035971,3.6815821647
H,0,2.2823659119,6.3641308076,2.7304774506
H,0,-2.5427960536,5.8178397139,1.448313014
H,0,-2.5688549253,4.0470719097,-0.2984551353

E(RB+HF-LYP) = -3008.59517254 A.U.

Zero-point correction= 0.221803 (Hartree/Particle)
Thermal correction to Energy= 0.239699
Thermal correction to Enthalpy= 0.240643
Thermal correction to Gibbs Free Energy= 0.172241
Sum of electronic and zero-point Energies= -3008.373370
Sum of electronic and thermal Energies= -3008.355474
Sum of electronic and thermal Enthalpies= -3008.354530
Sum of electronic and thermal Free Energies= -3008.422932

18-DME2 RB3LYP/6-311+G(d,p) 243 K

Charge = 0 Multiplicity = 1
H,0,2.3964858227,0.8630016729,2.6263791018
C,0,2.5317058947,0.3685621272,1.6665843818
C,0,2.3621230434,-1.1233191484,1.5549062981
C,0,1.2776383766,-0.2021072078,1.0365641185
H,0,3.2974131409,0.8210522296,1.0475587339
H,0,2.0998821338,-1.7103260776,2.4323594513
H,0,3.0186322117,-1.6397191013,0.8645963821
Br,0,1.4518700304,-0.0574182625,-1.1680424007
Li,0,-0.6038365244,-0.0008893184,0.367643594
H,0,-2.8274883443,1.2367991717,-1.1510658903
C,0,-2.2972327306,2.1252981626,-0.8091725675
C,0,-0.7384273395,2.8250346699,0.8468575143
O,0,-1.5033790424,1.7411568,0.3105514221
H,0,-1.6650119877,2.5037305245,-1.6201428643
H,0,-0.1323794102,2.4178206576,1.6539283678
H,0,-0.0784592352,3.243682755,0.0799637549
H,0,-3.3346579145,-0.5865419857,1.3442210657
C,0,-3.0804171079,-1.5682933832,0.9447394108
C,0,-1.5168554174,-2.6244733127,-0.5098621016
O,0,-1.9528670137,-1.4015447198,0.0915937763
H,0,-2.8462424667,-2.2483721077,1.7722690673
H,0,-2.312376641,-3.0410937461,-1.1379733457
H,0,-0.6457808849,-2.3877350858,-1.1190102317
H,0,-1.2378565497,-3.3517608304,0.2604977854
H,0,-3.9340364879,-1.9649145594,0.3826131932
H,0,-3.0212514809,2.8960805404,-0.5200602583
H,0,-1.4058920753,3.6057415355,1.229360241

E(RB+HF-LYP) = -3008.59517293 A.U.

Zero-point correction= 0.221810 (Hartree/Particle)
Thermal correction to Energy= 0.234965
Thermal correction to Enthalpy= 0.235734
Thermal correction to Gibbs Free Energy= 0.184428
Sum of electronic and zero-point Energies= -3008.373363
Sum of electronic and thermal Energies= -3008.360208

Sum of electronic and thermal Enthalpies= -3008.359439
Sum of electronic and thermal Free Energies= -3008.410745

TS21s-DME2 RB3LYP/6-311+G(d,p) 298 K

Charge = 0 Multiplicity = 1

C	2.11115800	2.42115600	1.09362600
C	2.75610000	0.85406800	1.30580200
C	1.38331100	1.22855300	1.35097400
H	1.83467700	2.98144100	0.20169900
H	3.53203800	1.09532400	2.02274700
H	3.00180700	0.08421600	0.57502500
Br	0.99023400	-0.73981000	-1.54265700
Li	-0.22505500	0.15191600	0.34229600
H	2.77414700	2.95028200	1.76774900
H	-2.64718100	-1.46887000	0.20572200
C	-1.91709000	-2.15870100	0.62693300
C	-0.00967400	-2.18789500	2.03192500
O	-1.00128500	-1.37930600	1.39929300
H	-2.42719600	-2.88792200	1.26758500
H	0.60008100	-2.70363600	1.28247700
H	0.62247200	-1.52160500	2.61816200
H	-1.39347400	-2.67110000	-0.18649400
H	-0.48377800	-2.91980400	2.69680200
H	-3.70715500	1.74306900	0.51497000
C	-2.64955300	1.94479600	0.72563800
C	-2.02341800	1.59809800	-1.54717500
O	-1.81173600	1.23972700	-0.17939400
H	-2.47303500	3.02570400	0.66101300
H	-1.83590000	2.66850100	-1.69482200
H	-1.31853800	1.01311900	-2.13678000
H	-2.41002500	1.59829100	1.73082500
H	-3.05279900	1.36676000	-1.84611900

Imaginary Frequency = -218.83
E(RB+HF-LYP) = -3008.56831577 A.U.

Zero-point correction= 0.219052 (Hartree/Particle)
Thermal correction to Energy= 0.237302
Thermal correction to Enthalpy= 0.238247
Thermal correction to Gibbs Free Energy= 0.168905
Sum of electronic and zero-point Energies= -3008.349264
Sum of electronic and thermal Energies= -3008.331013
Sum of electronic and thermal Enthalpies= -3008.330069
Sum of electronic and thermal Free Energies= -3008.399411

TS21s-DME2 RB3LYP/6-311+G(d,p) 243 K

Charge = 0 Multiplicity = 1
C,0,2.111158,2.421156,1.093626
C,0,2.7561,0.854068,1.305802
C,0,1.383311,1.228553,1.350974
H,0,1.834677,2.981441,0.201699
H,0,3.532038,1.095324,2.022747
H,0,3.001807,0.084216,0.575025

Br,0,0.990234,-0.73981,-1.542657
Li,0,-0.225055,0.151916,0.342296
H,0,2.774147,2.950282,1.767749
H,0,-2.647181,-1.46887,0.205722
C,0,-1.91709,-2.158701,0.626933
C,0,-0.009674,-2.187895,2.031925
O,0,-1.001285,-1.379306,1.399293
H,0,-2.427196,-2.887922,1.267585
H,0,0.600081,-2.703636,1.282477
H,0,0.622472,-1.521605,2.618162
H,0,-1.393474,-2.6711,-0.186494
H,0,-0.483778,-2.919804,2.696802
H,0,-3.707155,1.743069,0.51497
C,0,-2.649553,1.944796,0.725638
C,0,-2.023418,1.598098,-1.547175
O,0,-1.811736,1.239727,-0.179394
H,0,-2.473035,3.025704,0.661013
H,0,-1.8359,2.668501,-1.694822
H,0,-1.318538,1.013119,-2.13678
H,0,-2.410025,1.598291,1.730825
H,0,-3.052799,1.36676,-1.846119

E(RB+HF-LYP) = -3008.56831577 A.U.

Zero-point correction= 0.219052 (Hartree/Particle)
Thermal correction to Energy= 0.232551
Thermal correction to Enthalpy= 0.233320
Thermal correction to Gibbs Free Energy= 0.181237
Sum of electronic and zero-point Energies= -3008.349264
Sum of electronic and thermal Energies= -3008.335765
Sum of electronic and thermal Enthalpies= -3008.334996
Sum of electronic and thermal Free Energies= -3008.387079

20-DME2 RB3LYP/6-311+G(d,p) 298 K

Charge = 0 Multiplicity = 1
H,0,0.0019552966,0.0059582406,0.0041609096
C,0,0.0013698361,0.0018150726,1.0913734029
C,0,1.2865434143,0.0016491573,1.8471120836
C,0,0.4817548338,1.2508352968,1.7455425749
H,0,-0.8908515716,-0.4457564222,1.5222668589
H,0,2.2364269302,0.0055916439,1.3181741772
H,0,1.3437115935,-0.4460959756,2.8362158072
Br,0,-0.1044683553,5.6462404302,2.7071825326
Li,0,0.199852146,3.3397439702,2.2006505856
H,0,-0.4011571953,3.6089888476,-0.8049534253
C,0,0.5195031351,4.1844135159,-0.6997945143
C,0,2.5644447402,4.1929661998,0.4960798565
O,0,1.3064553397,3.5437351026,0.3054495854
H,0,1.053998235,4.1875728807,-1.6578053305
H,0,3.1109060074,3.6237787393,1.2491868447
H,0,3.137341078,4.1960342489,-0.4394724355
H,0,-2.6423859603,2.4786937607,3.0118930107
C,0,-2.2168254083,2.8018266025,3.9628187087
C,0,-0.1762666701,2.803911422,5.166136177

O,0,-0.8292665863,2.4634027626,3.9422311842
H,0,-2.3454511579,3.8834950059,4.066388722
H,0,-0.6458082255,2.279262375,6.0074211108
H,0,0.8624893388,2.4828989518,5.0782932634
H,0,-2.724872319,2.2776868074,4.7817510893
H,0,-0.2068334092,3.8856050109,5.3282877649
H,0,0.2730774785,5.207173219,-0.3989170149
H,0,2.416716475,5.2161943389,0.8544898658

E(RB+HF-LYP) = -3008.55852497 A.U.

Zero-point correction= 0.217994 (Hartree/Particle)
Thermal correction to Energy= 0.235357
Thermal correction to Enthalpy= 0.236301
Thermal correction to Gibbs Free Energy= 0.169593
Sum of electronic and zero-point Energies= -3008.340531
Sum of electronic and thermal Energies= -3008.323168
Sum of electronic and thermal Enthalpies= -3008.322224
Sum of electronic and thermal Free Energies= -3008.388932

24-DME2 RB3LYP/6-311+G(d,p) 298 K

Charge = 0 Multiplicity = 1
C,0,0.0727934584,0.0001976695,-0.0328614138
C,0,0.0050026844,-0.00062445,2.5763344801
C,0,0.0495191921,-0.0002029221,1.2690211114
H,0,-0.856542692,0.0011216741,-0.5987350324
H,0,0.0052796357,0.9244053214,3.1452837265
H,0,0.0035962694,-0.926059948,3.1446188982
Br,0,-3.7822425,0.0022326868,-0.070250354
Li,0,-2.747230712,0.0010797663,2.0386523667
H,0,1.014214471,-0.000356374,-0.5738241886
H,0,-1.5476756633,2.5877997919,1.7050505712
C,0,-2.5353441024,2.8482851785,2.0826990776
C,0,-4.2543380509,2.0322346236,3.4945198331
O,0,-2.968428455,1.7739428949,2.9291424644
H,0,-2.4751091921,3.7761890574,2.6622174377
H,0,-5.0167762638,2.0849925577,2.7101429084
H,0,-4.4842497728,1.2120193144,4.1746255291
H,0,-3.2193509186,2.966101871,1.2376333701
H,0,-4.238430267,2.96982513,4.0612491678
H,0,-4.483420191,-1.2097574864,4.1757908731
C,0,-4.2551560345,-2.0296344395,3.4947190026
C,0,-2.5383732343,-2.8464929867,2.0806413176
O,0,-2.9695775166,-1.7722751045,2.9282063939
H,0,-4.2397059427,-2.9677312207,4.060622929
H,0,-3.2232534959,-2.9630115755,1.2361076891
H,0,-1.5507837116,-2.5867586431,1.7022705015
H,0,-5.0184840072,-2.080894025,2.7111045065
H,0,-2.4785791488,-3.7748451781,2.6594863504

E(RB+HF-LYP) = -3008.66497037 A.U.

Zero-point correction= 0.220095 (Hartree/Particle)

Thermal correction to Energy= 0.238427
Thermal correction to Enthalpy= 0.239371
Thermal correction to Gibbs Free Energy= 0.170328
Sum of electronic and zero-point Energies= -3008.444875
Sum of electronic and thermal Energies= -3008.426543
Sum of electronic and thermal Enthalpies= -3008.425599
Sum of electronic and thermal Free Energies= -3008.494642

24-DME2 RB3LYP/6-311+G(d,p) 243 K

Charge = 0 Multiplicity = 1
C,0,-0.001566,3.278493,0.08075
C,0,-0.001649,1.982294,-2.184665
C,0,-0.001606,2.640997,-1.054607
H,0,-0.000886,2.728264,1.019437
H,0,0.923507,1.712971,-2.685578
H,0,-0.926873,1.711868,-2.684856
Br,0,0.000444,-0.098313,1.944509
Li,0,0.000058,-0.189567,-0.4025
H,0,-0.002209,4.363836,0.110943
H,0,2.584384,1.027128,-0.679323
C,0,2.846241,-0.02124,-0.544123
C,0,2.031456,-2.205072,-0.970148
O,0,1.771902,-0.805062,-1.082503
H,0,3.773491,-0.241936,-1.084419
H,0,2.082596,-2.504404,0.082038
H,0,1.212769,-2.730774,-1.461612
H,0,2.965957,-0.222734,0.524019
H,0,2.970248,-2.458766,-1.4749
H,0,-1.210537,-2.731964,-1.461161
C,0,-2.02955,-2.207075,-0.969371
C,0,-2.846412,-0.024054,-0.543186
O,0,-1.771475,-0.806808,-1.081911
H,0,-2.968299,-2.461761,-1.473705
H,0,-2.96562,-0.225705,0.524983
H,0,-2.585608,1.024572,-0.678412
H,0,-2.079929,-2.506392,0.082856
H,0,-3.773609,-0.245629,-1.083215

E(RB3LYP) = -3008.66497042 A.U.

Zero-point correction= 0.220091 (Hartree/Particle)
Thermal correction to Energy= 0.233622
Thermal correction to Enthalpy= 0.234391
Thermal correction to Gibbs Free Energy= 0.182561
Sum of electronic and zero-point Energies= -3008.444879
Sum of electronic and thermal Energies= -3008.431349
Sum of electronic and thermal Enthalpies= -3008.430579
Sum of electronic and thermal Free Energies= -3008.482409

Dimers

Bent Dimer (25) B3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
H,0,0.2388250948,-0.2912843986,-0.1620714025

C,0,0.0970091342,-0.2340631851,0.9105060894
C,0,1.3249867707,-0.0297901138,1.7456298633
C,0,0.3078761484,1.0932002995,1.6330613253
H,0,-0.7133084755,-0.8532406683,1.285712327
H,0,2.2681976781,0.0531421497,1.2192045978
H,0,1.4087477625,-0.5186432703,2.7133235638
Br,0,0.9745775807,2.5613640199,0.2426270404
Li,0,-1.1936315175,2.5246441045,1.4153050697
H,0,-3.6956572408,4.4835805247,3.644076128
C,0,-2.7528008914,4.5664163649,3.1169983288
C,0,-1.5240929067,4.7691649858,3.9514085376
C,0,-1.7364415939,3.4426522673,3.2276370348
H,0,-2.8370159343,5.0562524251,2.1498461291
H,0,-1.6650972952,4.8254446568,5.0241464308
H,0,-0.7136988431,5.3882337834,3.5761894939
Br,0,-2.4027588007,1.9736855062,4.6170048834
Li,0,-0.23406767,2.0125418413,3.4448483858

E(RB+HF-LYP) = -5396.84021793 A.U.

Zero-point correction= 0.121500 (Hartree/Particle)
Thermal correction to Energy= 0.134676
Thermal correction to Enthalpy= 0.135620
Thermal correction to Gibbs Free Energy= 0.077931
Sum of electronic and zero-point Energies= -5396.718718
Sum of electronic and thermal Energies= -5396.705542
Sum of electronic and thermal Enthalpies= -5396.704598
Sum of electronic and thermal Free Energies= -5396.762287

Bent Dimer PCM solvation (25-PCM) B3LYP/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0,-0.0082684375,0.0025887805,0.0032445872
C,0,-0.005095301,0.0043918811,1.0916970438
C,0,1.3412257297,-0.0052740156,1.7603232309
C,0,0.4960448662,1.2416138839,1.8755335637
H,0,-0.8290929553,-0.5528986321,1.5410486774
H,0,2.2112378321,-0.0158024769,1.1075049694
H,0,1.4783287388,-0.5759839092,2.6796141934
Br,0,1.1469786396,2.676775182,0.4716952267
Li,0,-1.3825740541,2.2126184838,1.3894556487
H,0,-3.567113539,4.6622330891,3.7864094381
C,0,-2.6711867606,4.6569954943,3.169571907
C,0,-1.3532006299,4.6295160209,3.8917789881
C,0,-1.8288924185,3.4059458726,3.0701264061
H,0,-2.7670616195,5.2434838741,2.2550349462
H,0,-1.392206559,4.6128876076,4.9793378578
H,0,-0.5106189564,5.191993775,3.4847507226
Br,0,-2.5467416191,1.9601688296,4.4223429555
Li,0,0.0565771401,2.46642669,3.5267938188

E(RB+HF-LYP) = -5391.97630940 A.U.

Variational PCM results
==========

<psi(f)| H |psi(f)> (a.u.) = -5391.944098
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -5391.976309
Total free energy in solution:
with all non electrostatic terms (a.u.) = -5391.963064

(Polarized solute)-Solvent (kcal/mol) = -20.21

Cavitation energy (kcal/mol) = 20.68
Dispersion energy (kcal/mol) = -13.31
Repulsion energy (kcal/mol) = 0.94
Total non electrostatic (kcal/mol) = 8.31

Zero-point correction= 0.121220 (Hartree/Particle)
Thermal correction to Energy= 0.134725
Thermal correction to Enthalpy= 0.135670
Thermal correction to Gibbs Free Energy= 0.077460
Sum of electronic and zero-point Energies= -5391.855090
Sum of electronic and thermal Energies= -5391.841584
Sum of electronic and thermal Enthalpies= -5391.840640
Sum of electronic and thermal Free Energies= -5391.898850

Bent Dimer explicit solvation 2 dimethylethers (25-DME2)

Charge = 0 Multiplicity = 1
H,0,3.3048535334,-1.5186425746,-1.0025842318
C,0,2.3135948289,-1.8141425228,-0.6667856154
C,0,2.14584678,-2.0716897187,0.8028352042
C,0,1.4816263678,-0.8533228502,0.1797529385
H,0,1.7702160307,-2.4267009951,-1.3875799283
H,0,3.0309719561,-1.9459602982,1.422810287
H,0,1.4853278103,-2.8729943006,1.1371502156
Br,0,2.5576799982,0.8718584005,0.5987109508
Li,0,0.2606641043,0.2010943698,-1.1373242251
H,0,-3.0332999294,1.945172015,-1.4190339123
C,0,-2.1481215905,2.0706560468,-0.7990841949
C,0,-2.3158570699,1.8129288638,0.6705042715
C,0,-1.4841090858,0.8520618498,-0.1762175673
H,0,-1.4874812747,2.8718955932,-1.1333166063
H,0,-3.3071625805,1.517576076,1.0062971301
H,0,-1.7723341722,2.4252805641,1.3913663559
Br,0,-2.5604223213,-0.8728232735,-0.5953806248
Li,0,-0.263041528,-0.202097338,1.1409807412
O,0,-0.3703935568,-0.3468312029,3.0637707289
O,0,0.3685214294,0.3456135824,-3.0601164005
C,0,-0.2504277721,-0.6446136245,-3.8837576134
H,0,-1.3114805853,-0.410125872,-4.0368821007
H,0,0.2648702335,-0.7020526557,-4.8518810837
H,0,-0.163213974,-1.600159007,-3.3637971556
C,0,0.3245206323,1.6474026313,-3.6429810772
H,0,0.8632937986,1.6532491216,-4.599979327
H,0,-0.7151480362,1.963194936,-3.8021490475
H,0,0.8161605767,2.3316351128,-2.9480234754
C,0,0.2494722399,0.642646136,3.8876227814
H,0,-0.2657077798,0.7002814064,4.8557972264
H,0,1.3103314731,0.4071958229,4.0406125614
H,0,0.1630719291,1.5983959222,3.3679044876

C,0,-0.3275266348,-1.6488053865,3.6463063385
H,0,0.7118689915,-1.9655333839,3.8054008935
H,0,-0.8663128462,-1.6544333531,4.6032986538
H,0,-0.8197506462,-2.332440793,2.951172171

E(RB+HF-LYP) = -5702.07160207 A.U.

Zero-point correction= 0.286704 (Hartree/Particle)
Thermal correction to Energy= 0.310775
Thermal correction to Enthalpy= 0.311719
Thermal correction to Gibbs Free Energy= 0.227579
Sum of electronic and zero-point Energies= -5701.784898
Sum of electronic and thermal Energies= -5701.760827
Sum of electronic and thermal Enthalpies= -5701.759883
Sum of electronic and thermal Free Energies= -5701.844023

TS26 B3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
H,0,-0.0203838151,-0.2377622775,0.0023092182
C,0,0.0305282912,-0.0070427241,1.0588311002
C,0,1.6771126887,0.0001429718,1.2939818657
C,0,0.7795038489,1.0467905009,1.6644693996
H,0,-0.7782096745,-0.4266306428,1.6544368076
H,0,2.0247023183,-0.2289177334,0.2945970284
H,0,2.2893324544,-0.4117403134,2.094218584
Br,0,0.3663590656,0.5054282776,5.2109402039
Li,0,0.5769793118,2.7637087357,5.8745805181
H,0,-0.3918453857,5.9886338642,5.3264925638
C,0,-0.5811334117,5.2031896029,4.6044143469
C,0,0.2153994624,5.2460464388,3.3343372171
C,0,0.4882462682,4.1406659598,4.3342527988
H,0,-1.6114849602,4.8578160969,4.5836138125
H,0,0.9262016193,6.0571001852,3.2300085009
H,0,-0.2461371601,4.9504455291,2.3951854573
Br,0,2.2204106336,4.5868354438,5.4774010286
Li,0,0.5866311018,2.1931694009,3.4357986516

Imaginary Frequency = -268.48
E(RB+HF-LYP) = -5396.82260076 A.U.

Zero-point correction= 0.117915 (Hartree/Particle)
Thermal correction to Energy= 0.131951
Thermal correction to Enthalpy= 0.132895
Thermal correction to Gibbs Free Energy= 0.071304
Sum of electronic and zero-point Energies= -5396.704686
Sum of electronic and thermal Energies= -5396.690649
Sum of electronic and thermal Enthalpies= -5396.689705
Sum of electronic and thermal Free Energies= -5396.751297

TS26-PCM B3LYP/6-31+G(d)

Charge = 0 Multiplicity = 1
H,0.0318283936, 0.0168334701,-0.0203887828
C,0.0008212438, 0.0191138691,1.0665592122

C,1.5971552823,-0.0215645618,1.4575883152
C,0.6589940867,0.9532250705,1.9315165705
H,-0.8578409821,-0.5081426825,1.4887570092
H,2.0728153667,-0.0346957107,0.4797884907
H,2.1369641838,-0.5836831363,2.2231470825
Br,-0.1247664803,0.0251274229,5.3767831067
Li,-0.4370460332,2.285827155,6.3628916756
H,0.1223225157,5.9363910794,4.8253118943
C,-0.5770992149,5.1087801069,4.7321002619
C,-0.5106828974,4.3030103412,3.4670928225
C,-0.0722911738,3.6838553314,4.8130267559
H,-1.5451335432,5.3016926057,5.1962787032
H,0.2354450539,4.6008532139,2.7334720842
H,-1.4309639 413,3.9128171639,3.0296192794
Br,2.0340295167,3.6746547866,4.8700725845
Li,0.3416582313,1.876697124,3.8006879202

Imaginary Frequency = -284.98
E(RB+HF-LYP) = -5391.95462432 A.U.

Variational PCM results
 ======================
 <psi(f)| H |psi(f)> (a.u.) = -5391.920133
 <psi(f)|H+V(f)/2|psi(f)> (a.u.) = -5391.954624
 Total free energy in solution:
 with all non electrostatic terms (a.u.) = -5391.938669

 (Polarized solute)-Solvent (kcal/mol) = -21.64

 Cavitation energy (kcal/mol) = 22.31
 Dispersion energy (kcal/mol) = -13.25
 Repulsion energy (kcal/mol) = 0.95
 Total non electrostatic (kcal/mol) = 10.01

Zero-point correction= 0.117995 (Hartree/Particle)
 Thermal correction to Energy= 0.132220
 Thermal correction to Enthalpy= 0.133164
 Thermal correction to Gibbs Free Energy= 0.072147
 Sum of electronic and zero-point Energies= -5391.836630
 Sum of electronic and thermal Energies= -5391.822404
 Sum of electronic and thermal Enthalpies= -5391.821460
 Sum of electronic and thermal Free Energies= -5391.882477

TS27 B3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
 H,0,-0.0116408842,0.0331268697,-0.0323798891
 C,0,-0.01653743,0.0304810165,1.0520267981
 C,0,1.7312564635,-0.0459316605,1.2507972639
 C,0,0.8049733585,0.7843024066,1.9183420961
 H,0,-0.8490648548,-0.5126422901,1.4983183832
 H,0,1.968298062,-0.0538965343,0.1926012441
 H,0,2.3936161701,-0.6551253065,1.8652051401
 Br,0,0.8101518865,4.2245715159,2.1610602058
 Li,0,0.1296441555,4.435675466,4.4131521583

H,0,0.6540262055,3.4853909276,7.6342267298
C,0,1.0853085236,2.9441856821,6.8003789708
C,0,0.5258549209,1.581449063,6.5180626377
C,0,0.2557069935,2.7025436966,5.5355576641
H,0,2.1441014526,3.1354632595,6.6462542226
H,0,-0.2713422557,1.2367425527,7.1658492915
H,0,1.1844654971,0.7851444646,6.1794534483
Br,0,-1.6960604633,3.4856298031,5.8210327438
Li,0,0.6057911733,2.162608789,3.4881562962

Imaginary Frequency = -127.90
E(RB+HF-LYP) = -5396.82172789 A.U.

Zero-point correction= 0.118045 (Hartree/Particle)
Thermal correction to Energy= 0.132087
Thermal correction to Enthalpy= 0.133031
Thermal correction to Gibbs Free Energy= 0.071620
Sum of electronic and zero-point Energies= -5396.703683
Sum of electronic and thermal Energies= -5396.689641
Sum of electronic and thermal Enthalpies= -5396.688697
Sum of electronic and thermal Free Energies= -5396.750108

28 B3LYP/6-311+G(d,p)

Charge = 0 Multiplicity = 1
C,0,0.9950333515,1.0033770807,-0.0211765183
C,0,0.4986887438,0.0708566655,2.3670404973
C,0,0.746445325,0.5389863416,1.1679441475
H,0,0.1919600346,1.2723595075,-0.7000218306
H,0,0.4377309365,0.7298355473,3.2294751337
H,0,0.4318185709,-0.9977163623,2.5548828007
Br,0,-2.9376855233,1.1304819505,-0.2288166968
Li,0,-1.8041866558,0.3151911089,1.6860676939
H,0,2.018296682,1.1321036716,-0.3598127163
H,0,-5.3594117395,-2.4972508474,3.9305227647
C,0,-5.9382449549,-1.7615868101,3.3854388931
C,0,-6.1463063922,-0.4302624085,4.0558057867
C,0,-5.2713166762,-0.5256955902,2.8283586166
H,0,-6.7125433186,-2.1949120932,2.7573654666
H,0,-5.702858242,-0.3028596511,5.0358795037
H,0,-7.0744803818,0.1199345857,3.9233698318
Br,0,-3.1316822125,-0.5436888116,3.5372480264
Li,0,-4.7346504595,0.3893107316,1.1291481951

E(RB+HF-LYP) = -5396.91494974 A.U.

Zero-point correction= 0.118062 (Hartree/Particle)
Thermal correction to Energy= 0.133323
Thermal correction to Enthalpy= 0.134267
Thermal correction to Gibbs Free Energy= 0.070405
Sum of electronic and zero-point Energies= -5396.796888
Sum of electronic and thermal Energies= -5396.781627
Sum of electronic and thermal Enthalpies= -5396.780683
Sum of electronic and thermal Free Energies= -5396.844545

28-PCM B3LYP/6-31+G(d)

Charge = 0 Multiplicity = 1
C,0,-0.0104544623,-0.0048446058,-0.0034532799
C,0,0.0120671779,-0.0053766674,2.6185656283
C,0,0.0102314124,-0.0084648206,1.3036838135
H,0,-0.3834333812,-0.8687847697,-0.5496941764
H,0,-0.8327090219,0.395826455,3.1807986657
H,0,0.8850792811,-0.323684034,3.1862312203
Br,0,-1.1670689411,-3.5382884722,0.4685936111
Li,0,-0.9036177307,-2.5016744563,2.6734446488
H,0,0.3429425667,0.8547724523,-0.5712960398
H,0,3.3707508382,-1.523125,2.6092378073
C,0,3.5067979556,-2.3171413645,1.8786238041
C,0,4.0305085156,-3.6330854632,2.3978220816
C,0,2.6060316353,-3.5392544937,1.880336833
H,0,3.8036068385,-1.9523412478,0.8942656636
H,0,4.2318675814,-3.6950479858,3.4650215087
H,0,4.7141526247,-4.2320270394,1.7939956511
Br,0,1.3013523936,-3.4006185873,3.6382538703
Li,0,1.1377261153,-4.4456289851,0.7538106267

E(RB+HF-LYP) = -5392.04680856 A.U.

Variational PCM results
==========
<psi(f)| H |psi(f)> (a.u.) = -5392.004529
<psi(f)|H+V(f)/2|psi(f)> (a.u.) = -5392.046809
Total free energy in solution:
with all non electrostatic terms (a.u.) = -5392.030183

(Polarized solute)-Solvent (kcal/mol) = -26.53

Cavitation energy (kcal/mol) = 22.38
Dispersion energy (kcal/mol) = -12.81
Repulsion energy (kcal/mol) = 0.87
Total non electrostatic (kcal/mol) = 10.43

Zero-point correction= 0.117668 (Hartree/Particle)
Thermal correction to Energy= 0.132364
Thermal correction to Enthalpy= 0.133309
Thermal correction to Gibbs Free Energy= 0.072727
Sum of electronic and zero-point Energies= -5391.929140
Sum of electronic and thermal Energies= -5391.914444
Sum of electronic and thermal Enthalpies= -5391.913500
Sum of electronic and thermal Free Energies= -5391.974082