Rearrangements of Substituted Arenes via *Ipso* Arenium Ions: Supporting Information

Aida Ajaz, Erin C. McLaughlin, Sarah L. Skraba,

Rajesh Thamatam and Richard P. Johnson*

Department of Chemistry

University of New Hampshire

Durham, NH 03824

Corresponding Author: Richard.Johnson@unh.edu

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I. General Information

Complete Gaussian References:

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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.

(S-2) Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; 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.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

All structures reported were optimized at the B3LYP/6-31+G(d,p) level of theory. The polarizable continuum model (PCM) was employed to assess solvation by dichloroethane. Compound numbers refer to those shown in the text.

II. General 1,2- Aryl Shifts

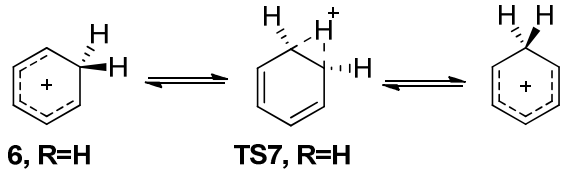

Figure S1. 1,2-Hydrogen shift

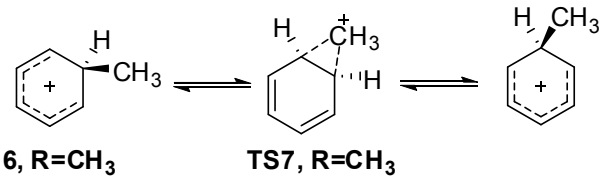

Figure S2. 1,2-Methyl shift

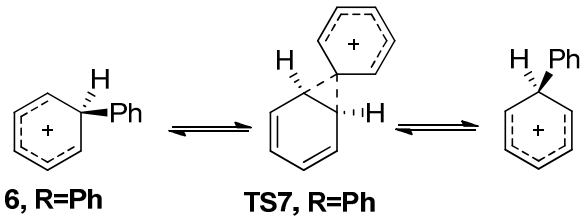

Figure S3. 1,2-Phenyl shift

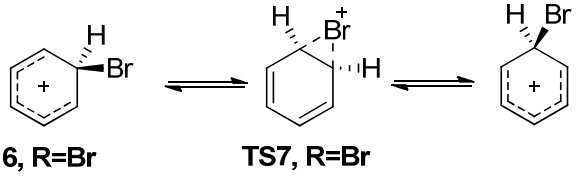

Figure S4. 1,2-Bromine shift

6, R=H: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.,0.,1.3993197929
C,0,0.,0.,-1.4171283638
C,0,1.2555269011,0.,0.6303878393
C,0,-1.2555269011,0.,0.6303878393
C,0,-1.2419302744,0.,-0.7423324191
C,0,1.2419302744,0.,-0.7423324191
H,0,2.1935774459,0.,1.1792926699
H,0,-2.1935774459,0.,1.1792926699
H,0,-2.1648832402,0.,-1.3120926531
H,0,2.1648832402,0.,-1.3120926531
H,0,0.,0.,-2.5048214599
H,0,0.,0.8519733546,2.1091110285
H,0,0.,-0.8519733546,2.1091110285

E(RB3LYP) = -232.570185197 A.U.

Zero-point correction= 0.110446 (Hartree/Particle)
Thermal correction to Energy= 0.115478
Thermal correction to Enthalpy= 0.116422
Thermal correction to Gibbs Free Energy= 0.083039
Sum of electronic and zero-point Energies= -232.459739
Sum of electronic and thermal Energies= -232.454708
Sum of electronic and thermal Enthalpies= -232.453763
Sum of electronic and thermal Free Energies= -232.487146

6, R=H: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.,0.,1.3974648038
C,0,0.,0.,-1.4162028188

C,0,1.2531366221,0.,0.6302340522
C,0,-1.2531366221,0.,0.6302340522
C,0,-1.2401289318,0.,-0.7419289587
C,0,1.2401289318,0.,-0.7419289587
H,0,2.1888790488,0.,1.1803923154
H,0,-2.1888790488,0.,1.1803923154
H,0,-2.1618904808,0.,-1.3116333261
H,0,2.1618904808,0.,-1.3116333261
H,0,0.,0.,-2.5025918998
H,0,0.,0.8508585174,2.1066523246
H,0,0.,-0.8508585174,2.1066523246

E(RB3LYP) = -232.644715343 A.U.

Zero-point correction= 0.110480 (Hartree/Particle)
Thermal correction to Energy= 0.115549
Thermal correction to Enthalpy= 0.116493
Thermal correction to Gibbs Free Energy= 0.083021
Sum of electronic and zero-point Energies= -232.534235
Sum of electronic and thermal Energies= -232.529166
Sum of electronic and thermal Enthalpies= -232.528222
Sum of electronic and thermal Free Energies= -232.561694

TS7, R=H: *in silico*

Charge = 1 Multiplicity = 1
C,0,-1.2335548604,0.7076151011,0.0041731064
C,0,1.1891447715,-0.7243761138,-0.048974282
C,0,-0.0473141664,1.4221540873,-0.0200922581
C,0,-1.233509442,-0.7076935027,0.0041744822
C,0,-0.0472226139,-1.4221560611,-0.0200893711
C,0,1.1890982853,0.724453846,-0.0489755239
H,0,-0.0437475555,2.5066787824,-0.0311085841
H,0,-2.1799569286,-1.2391829332,0.0208884501
H,0,-0.0435859945,-2.5066805751,-0.0311035478
H,0,2.1362871213,1.250556527,-0.1303289448
H,0,2.1363674199,-1.2504181418,-0.1303264165
H,0,1.295109407,0.000043811,1.0400367681
H,0,-2.1800365038,1.239043723,0.0208860314

E(RB3LYP) = -232.549449696 A.U.

Imaginary Frequency = -794.7372

Zero-point correction= 0.108183 (Hartree/Particle)
Thermal correction to Energy= 0.112704
Thermal correction to Enthalpy= 0.113648
Thermal correction to Gibbs Free Energy= 0.080561
Sum of electronic and zero-point Energies= -232.441266
Sum of electronic and thermal Energies= -232.436746

Sum of electronic and thermal Enthalpies= -232.435802
Sum of electronic and thermal Free Energies= -232.468889

TS7, R=H: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.2328147343,0.7073515864,0.0043803309
C,0,1.1880718027,-0.7221129754,-0.0511137894
C,0,-0.0478200473,1.4202142431,-0.0217254967
C,0,-1.2327691415,-0.7074298671,0.0043814311
C,0,-0.0477285924,-1.4202162812,-0.021722473
C,0,1.1880251778,0.722190407,-0.051115527
H,0,-0.0422353347,2.5036200486,-0.0323743216
H,0,-2.1785413949,-1.2381668264,0.022972291
H,0,-0.0420746201,-2.5036217179,-0.0323694192
H,0,2.1343840997,1.2474747621,-0.1258420321
H,0,2.1344648764,-1.2473361475,-0.1258386097
H,0,1.2947380709,0.000043572,1.0365568917
H,0,-2.1786212224,1.2380277464,0.022970634

E(RB3LYP) = -232.625355130 A.U.

Imaginary Frequency = -748.3635

Zero-point correction= 0.108415 (Hartree/Particle)
Thermal correction to Energy= 0.112930
Thermal correction to Enthalpy= 0.113874
Thermal correction to Gibbs Free Energy= 0.080799
Sum of electronic and zero-point Energies= -232.516941
Sum of electronic and thermal Energies= -232.512425
Sum of electronic and thermal Enthalpies= -232.511481
Sum of electronic and thermal Free Energies= -232.544557

6, R=CH_3: *in silico*

Charge = 1 Multiplicity = 1
C,0,-0.9526111254,-0.4402548934,0.0484810627
C,0,1.8534912863,-0.0236119638,0.1571625721
C,0,-0.2230080236,-0.3218773906,1.3250725379
C,0,-0.1278747238,-0.3123227395,-1.1678506955
C,0,1.2306278484,-0.1201093609,-1.1065461866
C,0,1.1361595261,-0.1295972254,1.3689516242
H,0,-0.7979994332,-0.404909731,2.2442675043
H,0,-0.6311172495,-0.3881490274,-2.1288013764
H,0,1.8254066711,-0.0347049716,-2.0097038581
H,0,1.660353436,-0.0512819859,2.3154382884
H,0,2.9285196838,0.1360860137,0.198799176
H,0,-1.313746005,-1.4960696881,0.0306530389

C,0,-2.2714681003,0.4090136246,0.0014067083
H,0,-2.8272575951,0.1762749932,-0.9087372717
H,0,-2.8949358154,0.1694777752,0.864738558
H,0,-2.0341982052,1.4744181317,0.0145446325

E(RB3LYP) = -271.890245047 A.U.

Zero-point correction= 0.139067 (Hartree/Particle)
Thermal correction to Energy= 0.145499
Thermal correction to Enthalpy= 0.146443
Thermal correction to Gibbs Free Energy= 0.108874
Sum of electronic and zero-point Energies= -271.751178
Sum of electronic and thermal Energies= -271.744746
Sum of electronic and thermal Enthalpies= -271.743802
Sum of electronic and thermal Free Energies= -271.781371

6, R=CH_3: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.9513102799,-0.4191905101,0.0486114384
C,0,1.8560714524,-0.0377320218,0.1572069166
C,0,-0.2235757619,-0.3024532781,1.3246888894
C,0,-0.1284757227,-0.2929019675,-1.1673627664
C,0,1.2323127055,-0.1230946494,-1.1052369619
C,0,1.1379401319,-0.1325728974,1.3677517996
H,0,-0.8006895427,-0.3761058539,2.2421183961
H,0,-0.6339717336,-0.3593616591,-2.1266431269
H,0,1.8280188497,-0.04479506,-2.0072881236
H,0,1.6631450694,-0.0613540509,2.3131514949
H,0,2.9321997313,0.1056195274,0.1988228424
H,0,-1.2848534318,-1.4848542144,0.0317986039
C,0,-2.2800841749,0.3991978792,0.0010402865
H,0,-2.8289514882,0.1552091774,-0.9099633042
H,0,-2.8967120656,0.1484036879,0.8656706551
H,0,-2.0607215681,1.4683674556,0.0135092749

E(RB3LYP) = -271.961709629 A.U.

Zero-point correction= 0.139406 (Hartree/Particle)
Thermal correction to Energy= 0.145738
Thermal correction to Enthalpy= 0.146683
Thermal correction to Gibbs Free Energy= 0.109421
Sum of electronic and zero-point Energies= -271.822304
Sum of electronic and thermal Energies= -271.815971
Sum of electronic and thermal Enthalpies= -271.815027
Sum of electronic and thermal Free Energies= -271.852288

TS7, R=CH_3: *in silico*

Charge = 1 Multiplicity = 1
C,0,-1.0019395409,-1.1115630184,-0.1126246964
C,0,0.3132358134,-1.2912309108,-0.4712586038
C,0,-0.6670398007,1.2761629786,0.2547968427
C,0,-1.4942690921,0.1778616731,0.2520126068
H,0,-1.6866486033,-1.9538710911,-0.1269135295
H,0,0.6854486347,-2.2620005203,-0.780137922
H,0,-1.0425507255,2.2637644721,0.4996970726
H,0,-2.5433790305,0.289927699,0.507593633
C,0,0.7078906765,1.1196893784,-0.1085668762
H,0,1.3127389063,1.9974285784,-0.311371461
C,0,1.1996077507,-0.1681750775,-0.4728055969
H,0,2.1717023334,-0.2521337253,-0.9475499932
C,0,1.6847736669,0.2864920651,1.365275032
H,0,2.5780598506,-0.322602277,1.2453030557
H,0,0.9112931932,-0.1788598162,1.9664409444
H,0,1.9649877273,1.283071322,1.6994432319

E(RB3LYP) = -271.861434499 A.U.

Imaginary Frequency = -416.5234

Zero-point correction= 0.138823 (Hartree/Particle)
Thermal correction to Energy= 0.144796
Thermal correction to Enthalpy= 0.145741
Thermal correction to Gibbs Free Energy= 0.109453
Sum of electronic and zero-point Energies= -271.722611
Sum of electronic and thermal Energies= -271.716638
Sum of electronic and thermal Enthalpies= -271.715694
Sum of electronic and thermal Free Energies= -271.751982

TS7, R=CH_3: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.9971042593,-1.1114131058,-0.1094343324
C,0,0.3162966627,-1.2899333229,-0.4693927853
C,0,-0.6642026195,1.2757052569,0.2520612023
C,0,-1.4899040816,0.1781198853,0.2532189006
H,0,-1.6799646542,-1.9544753822,-0.1166603082
H,0,0.6923250704,-2.2604057266,-0.7714947727
H,0,-1.036323622,2.262780826,0.5004318101
H,0,-2.5371783399,0.2886274049,0.51419851
C,0,0.7116514449,1.1195093724,-0.1105212113
H,0,1.3179216629,1.9957032275,-0.3084456801
C,0,1.2030605451,-0.1663182502,-0.4720469694
H,0,2.176705701,-0.2514266463,-0.9402818312
C,0,1.6709924839,0.2857647511,1.3574623212
H,0,2.5640742735,-0.3218885863,1.2369501675
H,0,0.8953026212,-0.1790627594,1.9548476311
H,0,1.9502588708,1.2826747855,1.6884410878

E(RB3LYP) = -271.933341501 A.U.

Imaginary Frequency = -392.5545

Zero-point correction= 0.138961 (Hartree/Particle)
Thermal correction to Energy= 0.144965
Thermal correction to Enthalpy= 0.145910
Thermal correction to Gibbs Free Energy= 0.109542
Sum of electronic and zero-point Energies= -271.794380
Sum of electronic and thermal Energies= -271.788376
Sum of electronic and thermal Enthalpies= -271.787432
Sum of electronic and thermal Free Energies= -271.823800

6, R=Ph: *in silico*

Charge = 1 Multiplicity = 1
C,0,-0.1399325206,-0.5148386412,0.2714020542
C,0,1.2657968963,-0.6239611546,0.1905865156
C,0,2.0082923069,0.5013513116,-0.0732103345
C,0,1.3779641893,1.8268720204,-0.2510201699
C,0,-0.0976797696,1.8467466672,-0.1614942276
C,0,-0.8223955393,0.7100757239,0.1030479763
H,0,-0.7213242708,-1.4116448835,0.4734302575
H,0,1.7412930051,-1.589605208,0.3255167006
H,0,3.0915053188,0.4518091945,-0.1464261496
H,0,1.7048889782,2.3977383085,0.6500094589
H,0,-0.5916091013,2.8047582242,-0.3008250527
H,0,-1.9045483903,0.7395320823,0.1726803835
C,0,1.9426579677,2.63254229,-1.4435843761
C,0,2.6801432602,3.8010827493,-1.2280767054
C,0,1.7059124418,2.1763671727,-2.7479749215
C,0,3.1819009974,4.5148487616,-2.3198980901
H,0,2.8671261194,4.1599685884,-0.219253578
C,0,2.2103005557,2.8946767802,-3.8333009748
H,0,1.1332788228,1.2686471937,-2.9211901916
C,0,2.9477986647,4.0630623676,-3.6204600269
H,0,3.7539332548,5.4213900961,-2.1502996051
H,0,2.0266378787,2.5409392025,-4.8428694241
H,0,3.3384749192,4.6190721816,-4.46659622

E(RB3LYP) = -463.637668641 A.U.

Zero-point correction= 0.191628 (Hartree/Particle)
Thermal correction to Energy= 0.201168
Thermal correction to Enthalpy= 0.202113
Thermal correction to Gibbs Free Energy= 0.155474
Sum of electronic and zero-point Energies= -463.446040
Sum of electronic and thermal Energies= -463.436500
Sum of electronic and thermal Enthalpies= -463.435556

Sum of electronic and thermal Free Energies= -463.482195

6, R=Ph: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.1404886476,-0.5119502397,0.3284979798
C,0,1.2620584566,-0.6256776815,0.2205899015
C,0,2.0002657593,0.4849815499,-0.1018941591
C,0,1.3679333943,1.8083210442,-0.2942721913
C,0,-0.1074377464,1.8314999535,-0.1902394931
C,0,-0.8241688144,0.7071220812,0.1331497923
H,0,-0.7177352543,-1.3995400174,0.5719619344
H,0,1.7389082001,-1.5862370575,0.3779664381
H,0,3.0804213805,0.429325993,-0.1970922987
H,0,1.6793070038,2.3562607102,0.6285204261
H,0,-0.6043104851,2.7833387308,-0.3515376461
H,0,-1.9036138461,0.7408105294,0.2252961033
C,0,1.9382157396,2.6241403222,-1.4654845732
C,0,2.6739129706,3.7910185261,-1.2330602226
C,0,1.7152384482,2.1888443684,-2.7797670399
C,0,3.1856340587,4.5213799912,-2.3098464762
H,0,2.8494589425,4.1324967833,-0.216947654
C,0,2.2282968381,2.9215868414,-3.8521417435
H,0,1.1449936684,1.2837504315,-2.9695682023
C,0,2.9637993563,4.0881872811,-3.6194333128
H,0,3.7555879685,5.425902078,-2.1218349784
H,0,2.0527333329,2.5801249224,-4.8675964921
H,0,3.3614052605,4.6557438874,-4.4550727934

E(RB3LYP) = -463.705211854 A.U.

Zero-point correction= 0.192023 (Hartree/Particle)
Thermal correction to Energy= 0.201494
Thermal correction to Enthalpy= 0.202438
Thermal correction to Gibbs Free Energy= 0.155695
Sum of electronic and zero-point Energies= -463.513189
Sum of electronic and thermal Energies= -463.503718
Sum of electronic and thermal Enthalpies= -463.502774
Sum of electronic and thermal Free Energies= -463.549516

TS7, R=Ph: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.2462394818,-0.4068182237,-0.3125180879
C,0,1.5750927119,-0.1163617612,-0.2006558783
C,0,1.9991976329,1.238661969,0.0870800544
C,0,0.9938875998,2.2660115992,0.2544389112
C,0,-0.4037007481,1.9055778314,0.1289191403
C,0,-0.7542767203,0.615507088,-0.1458907578

H,0,-0.0721353528,-1.4291973493,-0.4912037553
H,0,2.3309648168,-0.8902567705,-0.2800520593
H,0,2.9853618313,1.3742260964,0.5163984966
H,0,1.2309327431,3.1670246839,0.808697814
H,0,-1.1536173631,2.6703020625,0.3003436888
H,0,-1.8024951033,0.3389033892,-0.2031318654
C,0,1.9372914312,2.4090289662,-1.2090475387
C,0,2.9520954036,3.3894946385,-1.1336223451
C,0,1.376095095,2.0628602127,-2.4557580055
C,0,3.3969858643,4.0133102052,-2.2932527393
H,0,3.3851325147,3.6571072968,-0.1738901124
C,0,1.8292701292,2.6930655505,-3.6049811264
H,0,0.5972318086,1.3118757159,-2.5216561069
C,0,2.8374493728,3.6667247166,-3.5280352714
H,0,4.1760421482,4.7659136921,-2.2346394208
H,0,1.3995662718,2.429049924,-4.5655282055
H,0,3.1850341607,4.1539383167,-4.4336095193

E(RB3LYP) = -463.624691656 A.U.

Imaginary Frequency = -202.8178

Zero-point correction= 0.191888 (Hartree/Particle)
Thermal correction to Energy= 0.200692
Thermal correction to Enthalpy= 0.201636
Thermal correction to Gibbs Free Energy= 0.158006
Sum of electronic and zero-point Energies= -463.432804
Sum of electronic and thermal Energies= -463.424000
Sum of electronic and thermal Enthalpies= -463.423056
Sum of electronic and thermal Free Energies= -463.466686

TS7, R=Ph: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.2508385287,-0.4033412134,-0.319657163
C,0,1.5787109023,-0.1123868232,-0.1974147751
C,0,1.9980700985,1.2406570304,0.0991364528
C,0,0.9929107109,2.2648163981,0.2634278168
C,0,-0.4025501426,1.9062234899,0.1265430383
C,0,-0.7507365924,0.6171247179,-0.1559375511
H,0,-0.065906235,-1.4233484587,-0.5108608427
H,0,2.3371283496,-0.8824722225,-0.2806718479
H,0,2.984464329,1.3819289879,0.5237201997
H,0,1.2305735113,3.1687559769,0.8107905531
H,0,-1.1519001307,2.6723445783,0.2899301266
H,0,-1.7975812211,0.3409840497,-0.2277804848
C,0,1.9376285819,2.409861735,-1.2059968554
C,0,2.948911928,3.3904179812,-1.1299397335
C,0,1.3763277926,2.0579934694,-2.4487866468
C,0,3.3922532006,4.0122040136,-2.2924089403

H,0,3.3791710822,3.6589540959,-0.1702702948
C,0,1.8281106389,2.6863096496,-3.6001483557
H,0,0.5994119443,1.3054003735,-2.5126012393
C,0,2.8339505334,3.6619755525,-3.5259675176
H,0,4.1696069351,4.7662398326,-2.234970767
H,0,1.3981170393,2.4179622132,-4.5590319269
H,0,3.1801339452,4.1473444221,-4.4326979353

E(RB3LYP) = -463.687471064 A.U.

Imaginary Frequency = -220.4862

Zero-point correction= 0.191900 (Hartree/Particle)
Thermal correction to Energy= 0.200729
Thermal correction to Enthalpy= 0.201673
Thermal correction to Gibbs Free Energy= 0.157979
Sum of electronic and zero-point Energies= -463.495571
Sum of electronic and thermal Energies= -463.486742
Sum of electronic and thermal Enthalpies= -463.485798
Sum of electronic and thermal Free Energies= -463.529492

6, R=Br: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.0635667468,0.8922900531,0.
C,0,2.5114072072,-0.5152019389,0.
C,0,0.7434245401,0.5168625128,-1.2546747969
C,0,0.7434245401,0.5168625128,1.2546747969
C,0,1.9312614644,-0.168127985,1.24196357
C,0,1.9312614644,-0.168127985,-1.24196357
H,0,0.2620673936,0.7916902008,-2.1888178315
H,0,0.2620673936,0.7916902008,2.1888178315
H,0,2.4178185292,-0.4560254319,2.1673471685
H,0,2.4178185292,-0.4560254319,-2.1673471685
H,0,3.4430433024,-1.0765695255,0.
Br,0,-1.6052176126,-0.2351350604,0.
H,0,-0.3107005584,1.9209560886,0.

E(RB3LYP) = -2803.67676400 A.U.

Zero-point correction= 0.101585 (Hartree/Particle)
Thermal correction to Energy= 0.107877
Thermal correction to Enthalpy= 0.108821
Thermal correction to Gibbs Free Energy= 0.069816
Sum of electronic and zero-point Energies= -2803.575179
Sum of electronic and thermal Energies= -2803.568887
Sum of electronic and thermal Enthalpies= -2803.567943
Sum of electronic and thermal Free Energies= -2803.606948

6, R=Br: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.0586748391,0.8759043221,0.
C,0,2.5176376513,-0.5061296454,0.
C,0,0.7367822507,0.4964516026,-1.2552232098
C,0,0.7367822507,0.4964516026,1.2552232098
C,0,1.9354196454,-0.1647053665,1.2421195111
C,0,1.9354196454,-0.1647053665,-1.2421195111
H,0,0.2520941368,0.7648894068,-2.1881680859
H,0,0.2520941368,0.7648894068,2.1881680859
H,0,2.4278478818,-0.4444252842,2.1656063934
H,0,2.4278478818,-0.4444252842,-2.1656063934
H,0,3.4541920963,-1.0567498863,0.
Br,0,-1.6500131348,-0.1815195128,0.
H,0,-0.2735363413,1.9192122151,0.

E(RB3LYP) = -2803.75023313 A.U.

Zero-point correction= 0.101650 (Hartree/Particle)
Thermal correction to Energy= 0.107985
Thermal correction to Enthalpy= 0.108929
Thermal correction to Gibbs Free Energy= 0.069651
Sum of electronic and zero-point Energies= -2803.648583
Sum of electronic and thermal Energies= -2803.642248
Sum of electronic and thermal Enthalpies= -2803.641304
Sum of electronic and thermal Free Energies= -2803.680582

TS7, R=Br: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.2051245625,-0.7355180866,0.9491609463
C,0,2.1431904698,0.7213870787,-0.4968826984
C,0,0.2057308893,0.7366563156,0.9486732952
C,0,1.1951737095,-1.4378322353,0.1816388346
C,0,2.14258962,-0.7228056818,-0.4964098478
C,0,1.1963611974,1.4376444333,0.1806862751
H,0,1.2013261759,-2.5219408865,0.1948367239
H,0,2.9272364696,-1.2427278884,-1.0373420345
H,0,1.2034126193,2.5217560256,0.1931728984
H,0,2.928279176,1.2403027711,-1.0381401311
H,0,-0.3270192389,-1.2541798994,1.7408334168
H,0,-0.3259730232,1.2562822158,1.7400117821
Br,0,-1.4960804773,0.0008855279,-0.2229034004

E(RB3LYP) = -2803.66617509 A.U.

Imaginary Frequency = -235.7027

Zero-point correction= 0.100725 (Hartree/Particle)

Thermal correction to Energy= 0.106509
Thermal correction to Enthalpy= 0.107453
Thermal correction to Gibbs Free Energy= 0.069849
Sum of electronic and zero-point Energies= -2803.565450
Sum of electronic and thermal Energies= -2803.559666
Sum of electronic and thermal Enthalpies= -2803.558722
Sum of electronic and thermal Free Energies= -2803.596326

TS7, R=Br: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.2083256029,-0.7348835741,0.951823635
C,0,2.1421414028,0.7210347044,-0.4959085613
C,0,0.2089323701,0.7360196303,0.9513371132
C,0,1.1950129292,-1.437272549,0.1820542317
C,0,2.1415409074,-0.7224515683,-0.4954354614
C,0,1.196199293,1.4370846869,0.1811005747
H,0,1.1978385072,-2.520378163,0.1946738248
H,0,2.9246648269,-1.2410937967,-1.0379922444
H,0,1.1999210672,2.5201956424,0.1930078065
H,0,2.9257046395,1.2386700108,-1.0387924313
H,0,-0.3263914615,-1.2525103961,1.7408138686
H,0,-0.3253429664,1.2546108665,1.7399950782
Br,0,-1.489194968,0.0008841961,-0.2293413744

E(RB3LYP) = -2803.73778659 A.U.

Imaginary Frequency = -245.4588

Zero-point correction= 0.100856 (Hartree/Particle)
Thermal correction to Energy= 0.106652
Thermal correction to Enthalpy= 0.107596
Thermal correction to Gibbs Free Energy= 0.069969
Sum of electronic and zero-point Energies= -2803.636930
Sum of electronic and thermal Energies= -2803.631134
Sum of electronic and thermal Enthalpies= -2803.630190
Sum of electronic and thermal Free Energies= -2803.667818

III. Trifluoromethane Sulfonic Acid (4)

4: *in silico*

Charge = 0 Multiplicity = 1
S,0,0.8657711959,0.1468617277,0.0750841907
O,0,1.232105121,1.3524596492,-0.6357441624
O,0,1.2609286613,-0.1471797874,1.4446133895
C,0,-1.0119325999,-0.0052602085,-0.0028224888
O,0,1.2621182211,-1.1151703835,-0.8769283288
H,0,1.4189029578,-1.8981454802,-0.3180385023

F,0,-1.5498820172,0.9368669743,0.7726471111
F,0,-1.3746737585,-1.2141622292,0.4460236718
F,0,-1.4355242815,0.1479820676,-1.2562054109

E(RB3LYP) = -962.040045961 A.U.

Zero-point correction= 0.038219 (Hartree/Particle)
Thermal correction to Energy= 0.046064
Thermal correction to Enthalpy= 0.047008
Thermal correction to Gibbs Free Energy= 0.005171
Sum of electronic and zero-point Energies= -962.001827
Sum of electronic and thermal Energies= -961.993982
Sum of electronic and thermal Enthalpies= -961.993038
Sum of electronic and thermal Free Energies= -962.034875

4: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
S,0,0.8631815369,0.1313525255,0.0834372007
O,0,1.2254140002,1.3523252474,-0.6129905795
O,0,1.2581368142,-0.1462606661,1.4576000346
C,0,-1.0175545173,-0.0100829172,0.0022705985
O,0,1.2756404508,-1.0955945586,-0.8829883792
H,0,1.4342761374,-1.9101380931,-0.3671089839
F,0,-1.5457917752,0.9643397312,0.7449462483
F,0,-1.3984985631,-1.1960900088,0.4833446197
F,0,-1.4269905839,0.1144010698,-1.2598812892

E(RB3LYP) = -962.048017287 A.U.

Zero-point correction= 0.037898 (Hartree/Particle)
Thermal correction to Energy= 0.045754
Thermal correction to Enthalpy= 0.046698
Thermal correction to Gibbs Free Energy= 0.004762
Sum of electronic and zero-point Energies= -962.010119
Sum of electronic and thermal Energies= -962.002263
Sum of electronic and thermal Enthalpies= -962.001319
Sum of electronic and thermal Free Energies= -962.043255

4 (Anion): *in silico*

Charge = -1 Multiplicity = 1
S,0,-0.9398513714,0.000168533,0.000280313
O,0,-1.256017134,-0.4282330448,-1.3827300847
O,0,-1.2549738784,-0.9834962384,1.0629689545
C,0,0.9526776744,-0.0000912438,-0.0001974741
O,0,-1.2547185036,1.4123816098,0.3209931183
F,0,1.460899366,-1.2257752575,-0.2803155592
F,0,1.4610058092,0.3702288654,1.2013373894

F,0,1.4609385378,0.8547560062,-0.9223435171

E(RB3LYP) = -961.553375697 A.U.

Zero-point correction= 0.026464 (Hartree/Particle)
Thermal correction to Energy= 0.033739
Thermal correction to Enthalpy= 0.034683
Thermal correction to Gibbs Free Energy= -0.006110
Sum of electronic and zero-point Energies= -961.526911
Sum of electronic and thermal Energies= -961.519637
Sum of electronic and thermal Enthalpies= -961.518693
Sum of electronic and thermal Free Energies= -961.559485

4 (Anion): *1,2-dichloroethane*

Charge = -1 Multiplicity = 1
S,0,-0.9203673556,0.0001476924,0.0004024147
O,0,-1.2533858799,-0.428649162,-1.3803596016
O,0,-1.2533267647,-0.9811302468,1.062228449
C,0,0.9614883608,-0.0002580596,-0.0001061635
O,0,-1.2526948238,1.410555931,0.3191186054
F,0,1.4493614034,-1.2266597448,-0.2818658829
F,0,1.4501890681,0.3692055456,1.2024635461
F,0,1.4486964917,0.8567272743,-0.9218882273

E(RB3LYP) = -961.630439918 A.U.

Zero-point correction= 0.026332 (Hartree/Particle)
Thermal correction to Energy= 0.033600
Thermal correction to Enthalpy= 0.034545
Thermal correction to Gibbs Free Energy= -0.006206
Sum of electronic and zero-point Energies= -961.604108
Sum of electronic and thermal Energies= -961.596840
Sum of electronic and thermal Enthalpies= -961.595895
Sum of electronic and thermal Free Energies= -961.636646

IV. Terphenyl Rearrangement

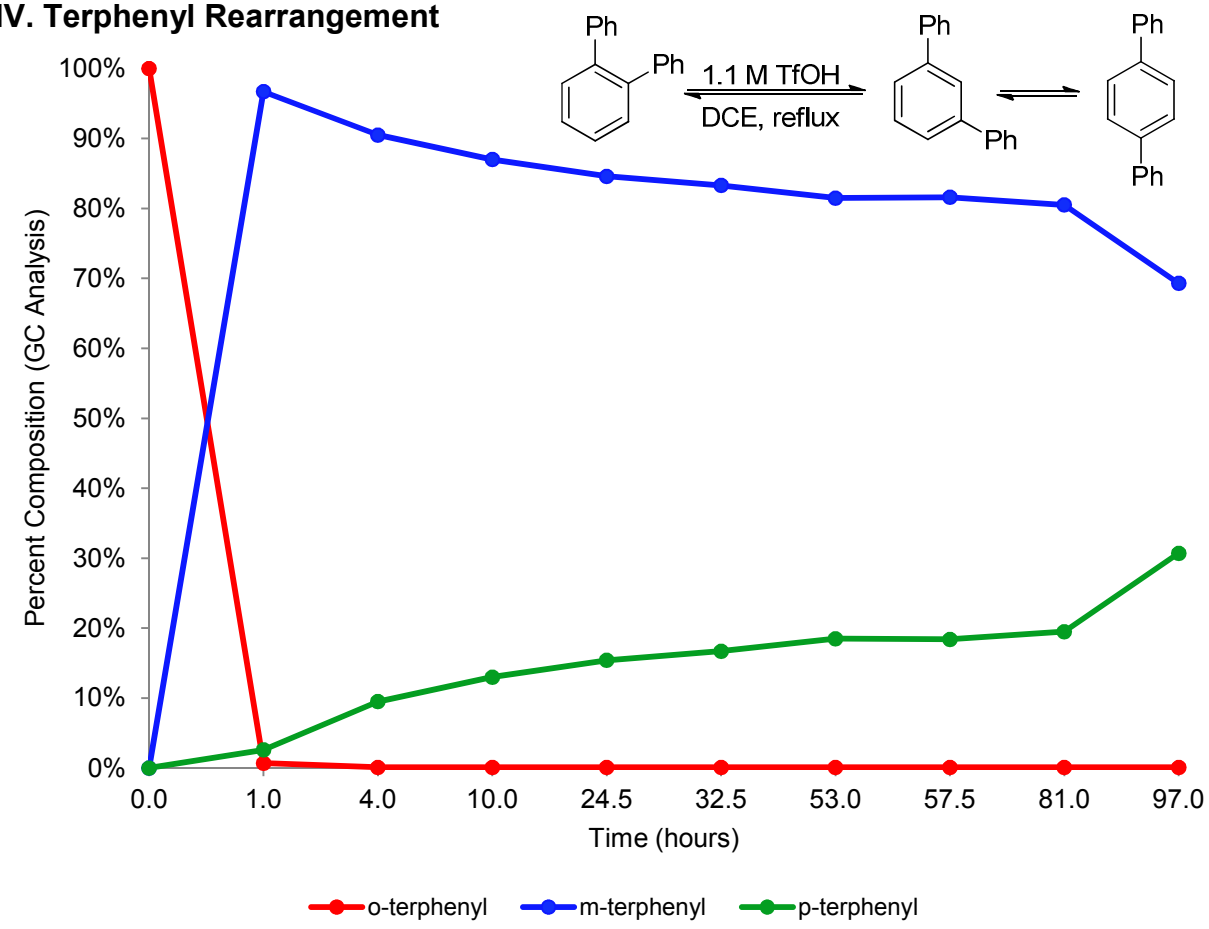

Figure S5. Evolution of terphenyl isomers in a 1.1 M TfOH reflux of *o*-terphenyl

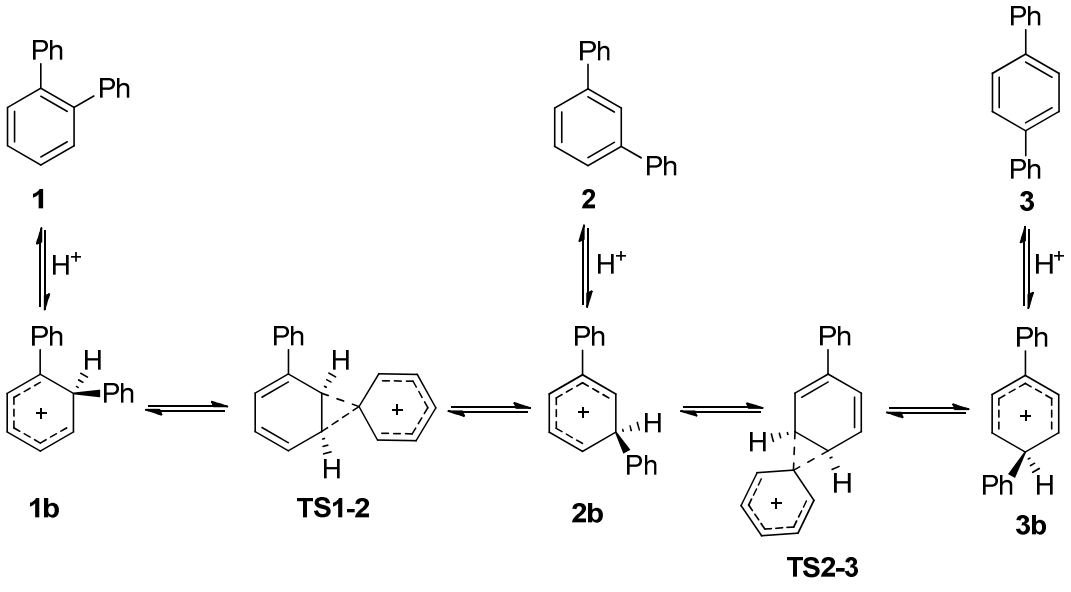

Figure S6. Rearrangement of terphenyl isomers

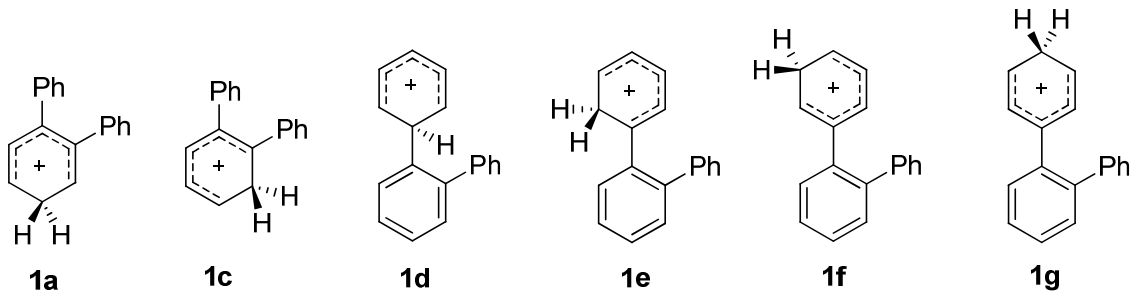

Figure S7. *o*-Terphenyl cations

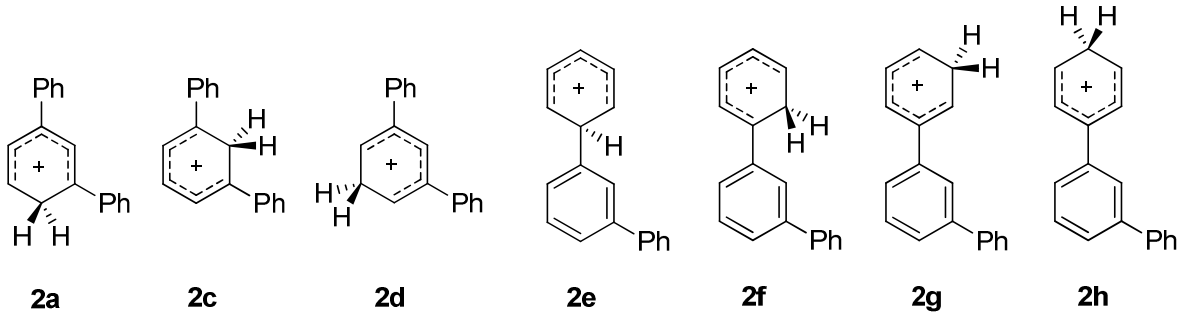

Figure S8. *m*-Terphenyl cations

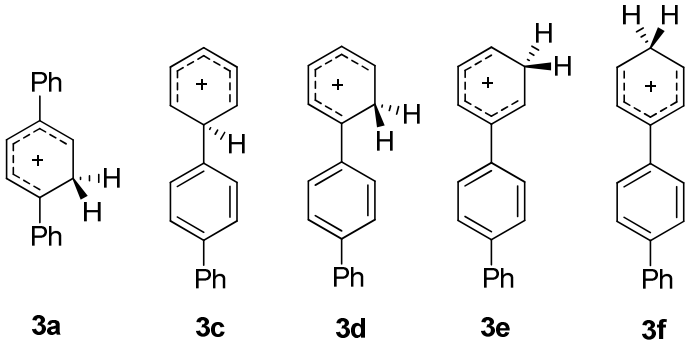

Figure S9. *p*-Terphenyl cations

1: *in silico*

Charge = 0 Multiplicity = 1
C,0,0.7083196993,-0.0257747927,1.2566666497
C,0,-0.6977193135,0.0155125992,3.7039348152
C,0,-0.7083196993,0.0257747927,1.2566666497
C,0,1.3836703013,-0.0374767958,2.4902909745
C,0,0.6977193135,-0.0155125992,3.7039348152
C,0,-1.3836703013,0.0374767958,2.4902909745
H,0,2.4682775606,-0.0960748115,2.4880629788
H,0,1.249394638,-0.0332350734,4.6394134616
H,0,-2.4682775606,0.0960748115,2.4880629788
H,0,-1.249394638,0.0332350734,4.6394134616
C,0,1.5271538887,-0.1076267723,0.0105153135

C,0,3.157494092,-0.3048184736,-2.2837130795
C,0,2.5909470329,0.7866120986,-0.19771624
C,0,1.2984199533,-1.1060107631,-0.9515474715
C,0,2.1058510062,-1.2046064248,-2.0854212269
C,0,3.3971177062,0.6920554106,-1.3348512834
H,0,2.7777206139,1.5707297404,0.5310465522
H,0,0.4875640727,-1.8126387015,-0.8053887648
H,0,1.9144566464,-1.9874962059,-2.8139150141
H,0,4.2090202619,1.3994310801,-1.4793183543
H,0,3.7835222702,-0.3810719372,-3.168059291
C,0,-1.5271538887,0.1076267723,0.0105153135
C,0,-3.157494092,0.3048184736,-2.2837130795
C,0,-1.2984199533,1.1060107631,-0.9515474715
C,0,-2.5909470329,-0.7866120986,-0.19771624
C,0,-3.3971177062,-0.6920554106,-1.3348512834
C,0,-2.1058510062,1.2046064248,-2.0854212269
H,0,-0.4875640727,1.8126387015,-0.8053887648
H,0,-2.7777206139,-1.5707297404,0.5310465522
H,0,-4.2090202619,-1.3994310801,-1.4793183543
H,0,-1.9144566464,1.9874962059,-2.8139150141
H,0,-3.7835222702,0.3810719372,-3.168059291

E(RB3LYP) = -694.403597538 A.U.

Zero-point correction= 0.261900 (Hartree/Particle)
Thermal correction to Energy= 0.275545
Thermal correction to Enthalpy= 0.276489
Thermal correction to Gibbs Free Energy= 0.221241
Sum of electronic and zero-point Energies= -694.141698
Sum of electronic and thermal Energies= -694.128053
Sum of electronic and thermal Enthalpies= -694.127109
Sum of electronic and thermal Free Energies= -694.182357

1: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,0.7086219415,-0.0224557732,1.2562804607
C,0,-0.6982298446,0.0098241449,3.7044379657
C,0,-0.7086219415,0.0224557732,1.2562804607
C,0,1.3847549298,-0.0278113606,2.4901272523
C,0,0.6982298446,-0.0098241449,3.7044379657
C,0,-1.3847549298,0.0278113606,2.4901272523
H,0,2.4698690149,-0.0756717908,2.489695891
H,0,1.2500734493,-0.0219234735,4.6397772308
H,0,-2.4698690149,0.0756717908,2.489695891
H,0,-1.2500734493,0.0219234735,4.6397772308
C,0,1.5272282916,-0.1078608119,0.0096650502
C,0,3.1585743209,-0.3177184062,-2.284293262
C,0,2.586072586,0.7908625196,-0.2070199284
C,0,1.304305899,-1.1178507213,-0.9426291969

C,0,2.1122552986,-1.2230226766,-2.0767276315
C,0,3.3925088161,0.6901629109,-1.3443346761
H,0,2.770885188,1.5823320653,0.514042447
H,0,0.49959183,-1.8301685722,-0.7887672652
H,0,1.9264977238,-2.0150915103,-2.7966928798
H,0,4.2001225663,1.4008566844,-1.4956054839
H,0,3.7848765575,-0.3986476353,-3.167955954
C,0,-1.5272282916,0.1078608119,0.0096650502
C,0,-3.1585743209,0.3177184062,-2.284293262
C,0,-1.304305899,1.1178507213,-0.9426291969
C,0,-2.586072586,-0.7908625196,-0.2070199284
C,0,-3.3925088161,-0.6901629109,-1.3443346761
C,0,-2.1122552986,1.2230226766,-2.0767276315
H,0,-0.49959183,1.8301685722,-0.7887672652
H,0,-2.770885188,-1.5823320653,0.514042447
H,0,-4.2001225663,-1.4008566844,-1.4956054839
H,0,-1.9264977238,2.0150915103,-2.7966928798
H,0,-3.7848765575,0.3986476353,-3.167955954

E(RB3LYP) = -694.408413936 A.U.

Zero-point correction= 0.261761 (Hartree/Particle)
Thermal correction to Energy= 0.275430
Thermal correction to Enthalpy= 0.276374
Thermal correction to Gibbs Free Energy= 0.221008
Sum of electronic and zero-point Energies= -694.146653
Sum of electronic and thermal Energies= -694.132984
Sum of electronic and thermal Enthalpies= -694.132040
Sum of electronic and thermal Free Energies= -694.187406

2: *in silico*

Charge = 0 Multiplicity = 1
C,0,-1.1255961142,-0.3033857753,-0.6849615116
C,0,1.0460437578,0.4626679047,-2.3038218617
C,0,0.0500366111,0.2159169811,-0.1200494908
C,0,-1.194390943,-0.4326739417,-2.0828275471
C,0,-0.1153742844,-0.0516541618,-2.880978663
C,0,1.1445627976,0.6040510994,-0.9089088377
H,0,0.1146779277,0.3204645123,0.9587241945
H,0,-2.0832371282,-0.8552607738,-2.5414956659
H,0,-0.1800241707,-0.1562595135,-3.9604121735
H,0,1.8695243001,0.779406206,-2.9367197844
C,0,-2.2656418517,-0.7148641403,0.1775792465
C,0,-4.4317134468,-1.4974400361,1.8108847022
C,0,-3.5920770277,-0.4421521048,-0.2014266625
C,0,-2.0479760855,-1.3878280083,1.3929353411
C,0,-3.1186240105,-1.7746234518,2.2009090983
C,0,-4.6634267313,-0.8293138988,0.6054362779
H,0,-3.7835919278,0.0978397375,-1.1241609416

H,0,-1.0335712159,-1.6319643528,1.6946174336
H,0,-2.9265223243,-2.3014120356,3.1314438368
H,0,-5.6793839188,-0.6005993062,0.2958709521
H,0,-5.2648960751,-1.7988473382,2.4390374931
C,0,2.3738837545,1.1598093882,-0.2820860656
C,0,4.7089155975,2.2155395513,0.9032618877
C,0,2.2938723929,2.0557860341,0.7987469735
C,0,3.6491908474,0.8040233815,-0.7558424449
C,0,4.8039941833,1.3260981012,-0.1705288239
C,0,3.4481131818,2.5777163531,1.3852933964
H,0,1.319560412,2.3650744346,1.1657420003
H,0,3.7363310013,0.0950196587,-1.574028915
H,0,5.7787288254,1.0303989783,-0.5483707903
H,0,3.3614371217,3.2753365015,2.2136150843
H,0,5.6070752634,2.6219952958,1.3590240312

E(RB3LYP) = -694.409601581 A.U.

Zero-point correction= 0.262115 (Hartree/Particle)
Thermal correction to Energy= 0.275736
Thermal correction to Enthalpy= 0.276680
Thermal correction to Gibbs Free Energy= 0.220440
Sum of electronic and zero-point Energies= -694.147487
Sum of electronic and thermal Energies= -694.133865
Sum of electronic and thermal Enthalpies= -694.132921
Sum of electronic and thermal Free Energies= -694.189162

2: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,-1.1525689907,-0.3092664695,-0.7264139628
C,0,1.1188179357,0.3676796429,-2.2475450515
C,0,0.0443808842,0.0824538566,-0.1043680854
C,0,-1.1918125008,-0.3558333163,-2.1313982771
C,0,-0.0633101558,-0.0194330175,-2.8807939668
C,0,1.1885556991,0.424181343,-0.8440951979
H,0,0.0863937039,0.1222053881,0.9796787803
H,0,-2.0976305356,-0.6764037762,-2.6367880966
H,0,-0.1053580271,-0.0592059849,-3.9655068083
H,0,1.9818648244,0.647900822,-2.8436218541
C,0,-2.3466240033,-0.6746548324,0.08372449
C,0,-4.6160331682,-1.3709003835,1.6155407246
C,0,-3.6394194787,-0.3022079409,-0.3285984289
C,0,-2.215453656,-1.402883225,1.2804820213
C,0,-3.3372030213,-1.7470669861,2.0382272736
C,0,-4.7617245743,-0.6466706364,0.428144878
H,0,-3.7660833116,0.2785200274,-1.2375454592
H,0,-1.2310422499,-1.7223384126,1.6096052061
H,0,-3.2117838129,-2.3170380188,2.9544739988
H,0,-5.7491746927,-0.3416829474,0.0934322525

H,0,-5.4884534311,-1.6390326909,2.2041718758
C,0,2.4406230551,0.8445404908,-0.1576736366
C,0,4.8197010837,1.6447191565,1.1390349871
C,0,2.400296323,1.6583226345,0.9894616156
C,0,3.6987851824,0.4397433698,-0.6406212288
C,0,4.8752390488,0.8355279774,-0.0001572798
C,0,3.5762745829,2.0539425987,1.6309594357
H,0,1.4433621082,2.0034675928,1.3697047313
H,0,3.7565436359,-0.2060234965,-1.5118930725
H,0,5.8347331038,0.5044010099,-0.3872416842
H,0,3.5203763097,2.689470649,2.5102117962
H,0,5.7342468293,1.9527803254,1.6372341638

E(RB3LYP) = -694.414754186 A.U.

Zero-point correction= 0.262064 (Hartree/Particle)
Thermal correction to Energy= 0.275691
Thermal correction to Enthalpy= 0.276636
Thermal correction to Gibbs Free Energy= 0.220379
Sum of electronic and zero-point Energies= -694.152690
Sum of electronic and thermal Energies= -694.139063
Sum of electronic and thermal Enthalpies= -694.138119
Sum of electronic and thermal Free Energies= -694.194375

3: *in silico*

Charge = 0 Multiplicity = 1
C,0,1.3645388935,-0.3410939466,-1.015180213
C,0,-1.4674366693,-0.426774266,-0.695712328
C,0,0.5198072714,0.4863045277,-1.7755871037
C,0,0.7611870014,-1.2122342462,-0.0913415293
C,0,-0.622699455,-1.2540988928,0.0647613171
C,0,-0.8640858671,0.4444145128,-1.6195064979
H,0,0.9490414033,1.1465877424,-2.5235677173
H,0,1.3848012358,-1.8406191341,0.537884827
H,0,-1.0519565721,-1.9143063994,0.8127987227
H,0,-1.4876617038,1.0728891194,-2.2486790358
C,0,2.8400912919,-0.2963404287,-1.1815007837
C,0,5.6453720619,-0.2110319896,-1.4977507289
C,0,3.6094098589,-1.4730336416,-1.136716854
C,0,3.5081494537,0.9240559277,-1.3883981388
C,0,4.8943427292,0.9666485838,-1.5459084885
C,0,4.9958988899,-1.4313062346,-1.2917648709
H,0,3.1141868522,-2.4304942352,-1.0039488032
H,0,2.9392411226,1.8491389391,-1.4012872919
H,0,5.3888012371,1.9222047339,-1.6966956229
H,0,5.5679229388,-2.3544370775,-1.2612487498
H,0,6.7241242983,-0.178234364,-1.6193668804
C,0,-2.9429927399,-0.4714728077,-0.5293855019
C,0,-5.7483637955,-0.5563691499,-0.2136144322

C,0,-3.712146192,0.7053320911,-0.5743002127
C,0,-3.6113055749,-1.6917875823,-0.3228511613
C,0,-4.997521396,-1.7341796533,-0.1655327919
C,0,-5.098676843,0.6637980027,-0.4194815113
H,0,-3.2167955717,1.6627272248,-0.7070232179
H,0,-3.0425974803,-2.6169933601,-0.3100876687
H,0,-5.4921484391,-2.6896891405,-0.0150040421
H,0,-5.6705272836,1.5870360478,-0.4500773567
H,0,-6.8271410468,-0.5890326036,-0.0922043418

E(RB3LYP) = -694.409952849 A.U.

Zero-point correction= 0.262087 (Hartree/Particle)
Thermal correction to Energy= 0.275714
Thermal correction to Enthalpy= 0.276658
Thermal correction to Gibbs Free Energy= 0.220409
Sum of electronic and zero-point Energies= -694.147865
Sum of electronic and thermal Energies= -694.134239
Sum of electronic and thermal Enthalpies= -694.133295
Sum of electronic and thermal Free Energies= -694.189544

3: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,1.4262607162,0.,0.
C,0,-1.4262503445,0.,0.
C,0,0.6969706211,1.2026249999,0.0131176933
C,0,0.6969706211,-1.2026249999,-0.0131176933
C,0,-0.6969904145,-1.2026184051,-0.0134939094
C,0,-0.6969904145,1.2026184051,0.0134939094
H,0,1.2245662549,2.1515350382,0.0371825274
H,0,1.2245662549,-2.1515350382,-0.0371825274
H,0,-1.2246301541,-2.1518110306,-0.010431128
H,0,-1.2246301541,2.1518110306,0.010431128
C,0,2.9126998329,0.,0.
C,0,5.7384810493,0.,0.
C,0,3.6364004934,-0.9559561326,0.7371675953
C,0,3.6364004934,0.9559561326,-0.7371675953
C,0,5.0330060745,0.956475396,-0.7371006622
C,0,5.0330060745,-0.956475396,0.7371006622
H,0,3.1027976378,-1.6907413187,1.3327594128
H,0,3.1027976378,1.6907413187,-1.3327594128
H,0,5.5696286049,1.6993847364,-1.3204031015
H,0,5.5696286049,-1.6993847364,1.3204031015
H,0,6.8245053348,0.,0.
C,0,-2.91269882,0.,0.
C,0,-5.7384894455,0.,0.
C,0,-3.6363850402,0.9386597896,0.7590561943
C,0,-3.6363850402,-0.9386597896,-0.7590561943
C,0,-5.0330048475,-0.9391483034,-0.7590466378

C,0,-5.0330048475,0.9391483034,0.7590466378
H,0,-3.1027747697,1.6595077077,1.3714547206
H,0,-3.1027747697,-1.6595077077,-1.3714547206
H,0,-5.5695831524,-1.6683823064,-1.3593992968
H,0,-5.5695831524,1.6683823064,1.3593992968
H,0,-6.8245109395,0.,0.

E(RB3LYP) = -694.415193691 A.U.

Zero-point correction= 0.262023 (Hartree/Particle)
Thermal correction to Energy= 0.275683
Thermal correction to Enthalpy= 0.276627
Thermal correction to Gibbs Free Energy= 0.220809
Sum of electronic and zero-point Energies= -694.153171
Sum of electronic and thermal Energies= -694.139511
Sum of electronic and thermal Enthalpies= -694.138567
Sum of electronic and thermal Free Energies= -694.194385

1b: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.293137291,1.1944773095,0.6004856732
C,0,-0.1562668929,0.8945181391,3.4484004228
C,0,-0.8416067529,0.3388894946,1.106111673
C,0,1.1437281855,1.7865699832,1.5425979393
C,0,0.9292238737,1.6376890379,2.9103801503
C,0,-1.0218367049,0.2942403534,2.5859075843
H,0,1.9615748879,2.4182524669,1.2180435408
H,0,1.6112711459,2.1347335946,3.5957763067
H,0,-1.870709336,-0.2774065378,2.9498261931
H,0,-0.2860009609,0.8237732766,4.5227194058
C,0,0.4846238514,1.3850765739,-0.8251364244
C,0,0.8721365729,1.7622425857,-3.5912892058
C,0,-0.5778296633,1.1916939747,-1.7448410543
C,0,1.750696618,1.7697185037,-1.3409921524
C,0,1.940536155,1.9462577048,-2.7044819621
C,0,-0.3868278606,1.3871428944,-3.1059522406
H,0,-1.5664874752,0.9225011019,-1.3927359261
H,0,2.6003480708,1.8846328655,-0.6778340545
H,0,2.9198859223,2.2217932206,-3.08138869
H,0,-1.2172801831,1.2548434007,-3.7914528118
H,0,1.0195961127,1.9118223898,-4.6563390628
C,0,-0.7647481424,-1.1333315569,0.614774839
C,0,-0.6707087563,-3.8149763788,-0.1790376798
C,0,-1.9069586863,-1.7506494019,0.0921870527
C,0,0.4210864081,-1.8655195988,0.7557991319
C,0,0.4668733564,-3.2013262078,0.3525224848
C,0,-1.8570555905,-3.0888048194,-0.3068574616
H,0,-2.8358043565,-1.1947545082,-0.0094243045
H,0,1.3103388575,-1.4018208891,1.1736850624

H,0,1.3906876793,-3.7616016945,0.4571129779
H,0,-2.7449505392,-3.5593129506,-0.717367395
H,0,-0.6327793997,-4.8538962551,-0.4905132374
H,0,-1.7778939974,0.742531817,0.6893131952

E(RB3LYP) = -694.725219085 A.U.

Zero-point correction= 0.273424 (Hartree/Particle)
Thermal correction to Energy= 0.287536
Thermal correction to Enthalpy= 0.288481
Thermal correction to Gibbs Free Energy= 0.230851
Sum of electronic and zero-point Energies= -694.451795
Sum of electronic and thermal Energies= -694.437683
Sum of electronic and thermal Enthalpies= -694.436738
Sum of electronic and thermal Free Energies= -694.494368

1b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.2828932963,1.1982170318,0.6176434519
C,0,-0.1653542291,0.9221446235,3.4618014861
C,0,-0.8356221729,0.3272287774,1.126733005
C,0,1.1147293672,1.8242784445,1.5472606657
C,0,0.9004841402,1.6860295318,2.9185896748
C,0,-1.0106986171,0.2839228643,2.6059783161
H,0,1.9177572446,2.4706869517,1.2153960053
H,0,1.5683603765,2.2068283549,3.5988755989
H,0,-1.8444050516,-0.3053601091,2.9749687692
H,0,-0.2961930386,0.8622511594,4.5360499172
C,0,0.47759173,1.3738122756,-0.8144347216
C,0,0.8787274628,1.7228117776,-3.5807591274
C,0,-0.5922641909,1.2185329201,-1.7291232688
C,0,1.7560495705,1.7064933714,-1.3281851824
C,0,1.9524291437,1.8694597444,-2.6943010937
C,0,-0.3932041937,1.40032284,-3.0928120197
H,0,-1.5915780717,0.9963442849,-1.3744291114
H,0,2.6066901352,1.7921108887,-0.6619494849
H,0,2.9423026484,2.1050779983,-3.070826585
H,0,-1.2295641384,1.2974697264,-3.7762061626
H,0,1.0319882685,1.8601294657,-4.6465347724
C,0,-0.7587457968,-1.1340292687,0.6150332451
C,0,-0.6555798669,-3.8045653696,-0.2248637087
C,0,-1.9052436678,-1.755322726,0.1067981649
C,0,0.4372199823,-1.8570612038,0.7159092077
C,0,0.4875923809,-3.1865501102,0.2910060177
C,0,-1.8514958809,-3.087282865,-0.3140874828
H,0,-2.8395364261,-1.2054478512,0.0340482465
H,0,1.331046506,-1.3898936309,1.118532148
H,0,1.4203373218,-3.7371458906,0.3652286381
H,0,-2.7440617043,-3.5590479008,-0.7132994739

H,0,-0.6140133639,-4.8378686508,-0.5550514245
H,0,-1.7786394742,0.7354224344,0.7270110318

E(RB3LYP) = -694.784276053 A.U.

Zero-point correction= 0.273587 (Hartree/Particle)
Thermal correction to Energy= 0.287644
Thermal correction to Enthalpy= 0.288589
Thermal correction to Gibbs Free Energy= 0.231089
Sum of electronic and zero-point Energies= -694.510689
Sum of electronic and thermal Energies= -694.496632
Sum of electronic and thermal Enthalpies= -694.495687
Sum of electronic and thermal Free Energies= -694.553187

TS1-2: *in silico*

Charge = 1 Multiplicity = 1
C,0,-0.5458554948,2.9770056762,-0.5155143436
C,0,-0.3392750625,0.62965561,1.0251501986
C,0,-1.5850128225,2.6689744834,0.315293652
C,0,0.6011652971,2.1284312729,-0.6220507722
C,0,0.7402470861,0.9690374536,0.1172914191
C,0,-1.5246631035,1.456251985,1.107405495
H,0,-2.4440753629,3.3220949797,0.4220542912
H,0,1.3936749362,2.4214547619,-1.3029780748
C,0,-1.8811773992,-0.0171681996,0.3329468849
C,0,-3.3592911256,-2.0936848518,-0.8000662475
C,0,-2.4868036468,-0.9879591437,1.1607126959
C,0,-2.0094183217,-0.1020305404,-1.0682350604
C,0,-2.7498169681,-1.1354987004,-1.6242227761
C,0,-3.2264974267,-2.018375239,0.5906130823
H,0,-2.3864612942,-0.9261614968,2.2407314448
H,0,-1.5393035112,0.6342555446,-1.7100844155
H,0,-2.8546310475,-1.1987061265,-2.7022385921
H,0,-3.6988040505,-2.7580085744,1.2284709747
H,0,-3.9360999525,-2.898457694,-1.2448019938
H,0,-2.1133525182,1.435902463,2.0187264822
H,0,-0.1221611682,-0.0668987609,1.8257430037
H,0,-0.5701852838,3.8926466007,-1.0984719393
C,0,1.9394984531,0.1121253081,0.0668035616
C,0,4.2176366329,-1.5339724308,-0.0562849765
C,0,3.2102144011,0.662532753,-0.1921319913
C,0,1.834834658,-1.2773787564,0.2730812264
C,0,2.9641327752,-2.0926142373,0.2064102823
C,0,4.3369099285,-0.1541856969,-0.2525758698
H,0,3.3251312409,1.7354746628,-0.31141181
H,0,0.8654433002,-1.7325506735,0.4549498603
H,0,2.8648045954,-3.1632522417,0.3546678977
H,0,5.3105634394,0.2870305944,-0.4404106657
H,0,5.0973775464,-2.1680025953,-0.1021356441

E(RB3LYP) = -694.702507790 A.U.

Imaginary Frequency = -222.8882

Zero-point correction= 0.272651 (Hartree/Particle)
Thermal correction to Energy= 0.286139
Thermal correction to Enthalpy= 0.287083
Thermal correction to Gibbs Free Energy= 0.231848
Sum of electronic and zero-point Energies= -694.429856
Sum of electronic and thermal Energies= -694.416369
Sum of electronic and thermal Enthalpies= -694.415425
Sum of electronic and thermal Free Energies= -694.470660

TS1-2: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.550103303,2.9707040095,-0.5243449932
C,0,-0.3457033342,0.6305227842,1.0323618034
C,0,-1.5865449644,2.6671720995,0.3095907105
C,0,0.5985926315,2.1215585649,-0.6238764674
C,0,0.7339983297,0.9704322757,0.1231681556
C,0,-1.5249553351,1.4624774422,1.1130666357
H,0,-2.4476382184,3.3176152027,0.4111402725
H,0,1.3882860382,2.4102488921,-1.3092917799
C,0,-1.8684738784,-0.0215597322,0.3377667022
C,0,-3.3556532383,-2.0870334667,-0.797957615
C,0,-2.478023163,-0.9890300432,1.1654293334
C,0,-1.9985475999,-0.1007384568,-1.0633729333
C,0,-2.7431928762,-1.1298546699,-1.6210588876
C,0,-3.2218788156,-2.0150540259,0.5924140107
H,0,-2.3733197747,-0.9322528107,2.2443075205
H,0,-1.5273130069,0.6344592414,-1.7049991087
H,0,-2.8482245421,-1.1899006399,-2.6988961756
H,0,-3.6943114453,-2.7549617885,1.2292702361
H,0,-3.9349206062,-2.8890176104,-1.2439212202
H,0,-2.1219254463,1.4418962717,2.017827163
H,0,-0.1285571332,-0.0566513757,1.8405891416
H,0,-0.5759757009,3.878945415,-1.1174873071
C,0,1.9355470497,0.1115044716,0.0705250226
C,0,4.2168097705,-1.5356255817,-0.0607151578
C,0,3.2072083261,0.6630446442,-0.1795621677
C,0,1.8306446665,-1.2791687367,0.2637548524
C,0,2.9614085756,-2.0945216175,0.1942664176
C,0,4.3352447342,-0.1536406048,-0.2451867805
H,0,3.3201326477,1.7363794889,-0.2947820035
H,0,0.8614666261,-1.7344028956,0.4424242079
H,0,2.8593443324,-3.1662143442,0.3345895331
H,0,5.3087235872,0.2904080318,-0.4291868001
H,0,5.0966037966,-2.1697722451,-0.1104150415

E(RB3LYP) = -694.761729002 A.U.

Imaginary Frequency = -215.0678

Zero-point correction= 0.272728 (Hartree/Particle)
Thermal correction to Energy= 0.286209
Thermal correction to Enthalpy= 0.287153
Thermal correction to Gibbs Free Energy= 0.231993
Sum of electronic and zero-point Energies= -694.489001
Sum of electronic and thermal Energies= -694.475520
Sum of electronic and thermal Enthalpies= -694.474576
Sum of electronic and thermal Free Energies= -694.529736

2b: *in silico*

Charge = 1 Multiplicity = 1
C,0,-0.3899208019,1.1624033457,-0.7114609624
C,0,-1.1388317945,1.0358335014,2.0703964948
C,0,-0.6004637353,-0.0670795875,-0.1097286399
C,0,-0.5608232068,2.3080302757,0.1137924695
C,0,-0.9222583273,2.2539940928,1.4758777743
C,0,-1.0232074307,-0.2170164828,1.2982512043
H,0,-0.4620117802,-0.9842551381,-0.6757083685
H,0,-0.417141873,3.2863011107,-0.3386365481
H,0,-1.0287015228,3.1765982408,2.0368816721
H,0,-1.4262601334,0.9594909952,3.1152019004
C,0,0.0133670086,1.2927998701,-2.1323563101
C,0,0.7831048106,1.5317268167,-4.8200287925
C,0,0.9589637528,2.258652791,-2.5191587847
C,0,-0.5413888643,0.448072785,-3.1095856259
C,0,-0.1595025321,0.5701359498,-4.4451683002
C,0,1.342380551,2.3740835992,-3.8550393344
H,0,1.4240943389,2.9010510355,-1.7760793542
H,0,-1.2967026761,-0.2833173313,-2.8354530451
H,0,-0.6040985227,-0.078519268,-5.1930924674
H,0,2.0825291603,3.114768533,-4.1401969337
H,0,1.0804546032,1.6243013342,-5.8597348557
C,0,-0.3155790944,-1.3621974994,2.0491715247
C,0,1.0047278724,-3.4181430456,3.4049520827
C,0,-1.0199721735,-2.50551407,2.4399771258
C,0,1.0516777661,-1.2459393307,2.3366198787
C,0,1.7079017944,-2.2748307861,3.0139416663
C,0,-0.3571641648,-3.5325124767,3.1179364029
H,0,-2.0803333203,-2.6027829599,2.2209583883
H,0,1.6044907192,-0.3598400599,2.0346720527
H,0,2.7664928555,-2.1823040068,3.2352637031
H,0,-0.9071627777,-4.4180422266,3.4200247218
H,0,1.5173690256,-4.2165366935,3.9318003782
H,0,-2.0860295969,-0.5494132239,1.2057087123

E(RB3LYP) = -694.713620467 A.U.

Zero-point correction= 0.272160 (Hartree/Particle)
Thermal correction to Energy= 0.286418
Thermal correction to Enthalpy= 0.287362
Thermal correction to Gibbs Free Energy= 0.228483
Sum of electronic and zero-point Energies= -694.441460
Sum of electronic and thermal Energies= -694.427202
Sum of electronic and thermal Enthalpies= -694.426258
Sum of electronic and thermal Free Energies= -694.485138

2b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.384998835,1.1592248433,-0.7179924912
C,0,-1.1491454388,1.0034082223,2.0490997851
C,0,-0.5360519629,-0.0781757032,-0.1220820371
C,0,-0.6188244196,2.2991039202,0.0974481289
C,0,-0.9903665255,2.2295089984,1.4537930052
C,0,-0.9801818679,-0.2433782072,1.2765886043
H,0,-0.353358216,-0.9878030313,-0.6865018985
H,0,-0.5189904468,3.2823504342,-0.3539410175
H,0,-1.1456398992,3.1453458022,2.0125772746
H,0,-1.442219261,0.9168967251,3.0905586948
C,0,0.0229602419,1.3080729874,-2.1389172083
C,0,0.8008489883,1.58438078,-4.8237643737
C,0,0.9408591961,2.3033671135,-2.5156915509
C,0,-0.5005594517,0.4529383356,-3.1234319682
C,0,-0.1137825765,0.5923828204,-4.4572522438
C,0,1.3277001952,2.4383093216,-3.8499996009
H,0,1.3754489358,2.957909393,-1.7656200839
H,0,-1.2297057681,-0.3054141159,-2.8539411831
H,0,-0.5331369682,-0.0683775264,-5.2095605611
H,0,2.0449353383,3.2049440755,-4.1260928947
H,0,1.1009498012,1.6914455197,-5.8615917577
C,0,-0.2960994138,-1.3844866834,2.0415184717
C,0,0.9835064454,-3.4334645434,3.4556609451
C,0,-1.0425859184,-2.4424970273,2.5712493412
C,0,1.0940228288,-1.3518284142,2.2213491389
C,0,1.7299898934,-2.3759419019,2.9262221422
C,0,-0.4020098272,-3.4649471471,3.2776952585
H,0,-2.1199708477,-2.4745430183,2.4344387772
H,0,1.6788417241,-0.5319326072,1.8132227914
H,0,2.8068168424,-2.3459558468,3.0608528385
H,0,-0.9871601567,-4.283882115,3.684378029
H,0,1.4800900154,-4.2288491541,4.0027677591
H,0,-2.0421827154,-0.5681121597,1.1369597146

E(RB3LYP) = -694.776149786 A.U.

Zero-point correction= 0.272425 (Hartree/Particle)
Thermal correction to Energy= 0.286612
Thermal correction to Enthalpy= 0.287556
Thermal correction to Gibbs Free Energy= 0.229273
Sum of electronic and zero-point Energies= -694.503725
Sum of electronic and thermal Energies= -694.489538
Sum of electronic and thermal Enthalpies= -694.488593
Sum of electronic and thermal Free Energies= -694.546877

TS2-3: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.0119876661,0.6141387542,-0.1445581399
C,0,-1.5864744366,1.8273984341,-0.2216865649
C,0,0.156083833,0.3284447736,-1.1833188616
C,0,0.5526907333,1.5269189594,0.8848333801
C,0,-0.6840520481,2.107648094,0.8587147287
C,0,-1.1784077109,0.8903417522,-1.2438384091
H,0,0.4801331998,-0.2918088527,-2.0117750709
H,0,1.2272695302,1.7609185794,1.7020467248
H,0,-0.9883668331,2.8066545419,1.6302749224
C,0,2.3766330348,0.04709452,-0.0775920016
C,0,4.9749006183,-1.0237638345,0.0108252993
C,0,3.4477339634,0.8057008237,0.4313972271
C,0,2.6300770244,-1.2597168058,-0.5357282646
C,0,3.9180827659,-1.7904621832,-0.4886887237
C,0,4.7365711854,0.2754494923,0.4680446971
H,0,3.2873540204,1.8263607161,0.7659875338
H,0,1.8134721506,-1.8751940179,-0.9019233581
H,0,4.0954794123,-2.8041987713,-0.8336092336
H,0,5.5551219033,0.8784482436,0.8479230901
H,0,5.9778532505,-1.4372730911,0.0459278559
C,0,-2.3864079778,0.1797754198,-0.2653033767
C,0,-4.3320936618,-1.5947125443,0.6451897003
C,0,-3.6884782165,0.2259941701,-0.8046663526
C,0,-2.0657859391,-0.7478221405,0.7434737747
C,0,-3.039391622,-1.6311572822,1.1892577564
C,0,-4.6539930021,-0.6672295982,-0.3509105713
H,0,-3.9375631874,0.9470698519,-1.5780941668
H,0,-1.0694107101,-0.7789937042,1.1695655024
H,0,-2.7942278397,-2.3512266271,1.9629513253
H,0,-5.6531896085,-0.6380744398,-0.7725188569
H,0,-5.0865977506,-2.2889174149,1.001332202
H,0,-1.6310539531,0.9522230073,-2.22800175
H,0,-2.4260827743,2.490986164,-0.3889172382

E(RB3LYP) = -694.701279992 A.U.

Imaginary Frequency = -264.1478

Zero-point correction= 0.272573 (Hartree/Particle)
Thermal correction to Energy= 0.286087
Thermal correction to Enthalpy= 0.287031
Thermal correction to Gibbs Free Energy= 0.231583
Sum of electronic and zero-point Energies= -694.428707
Sum of electronic and thermal Energies= -694.415193
Sum of electronic and thermal Enthalpies= -694.414249
Sum of electronic and thermal Free Energies= -694.469697

TS2-3: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.0034052843,0.6147015186,-0.1432606616
C,0,-1.5898240585,1.8238797444,-0.2271589121
C,0,0.1554736819,0.3290770919,-1.1854968959
C,0,0.5456514311,1.5222974569,0.8901674216
C,0,-0.6898130505,2.1018186791,0.8595358859
C,0,-1.1753909441,0.896901795,-1.2526537665
H,0,0.4774318843,-0.2934636999,-2.0123925993
H,0,1.2153335214,1.7522551191,1.711965713
H,0,-1.0002224635,2.7968190997,1.6314010502
C,0,2.3715225066,0.0464470738,-0.077443127
C,0,4.9727409566,-1.0267041182,0.0118393322
C,0,3.4450049265,0.8079818667,0.4205552939
C,0,2.6229738521,-1.2643209176,-0.5233521082
C,0,3.9122584155,-1.7957678464,-0.4774380834
C,0,4.7348640011,0.2766297533,0.458984007
H,0,3.2828626373,1.8286403029,0.7531356205
H,0,1.804217764,-1.8796251401,-0.8835310549
H,0,4.0861992315,-2.8126481248,-0.8157500715
H,0,5.5538133118,0.8826905627,0.8340253536
H,0,5.9757816003,-1.4407280735,0.0473295114
C,0,-2.3859342138,0.1962522058,-0.2552964091
C,0,-4.3180873849,-1.5992671997,0.6380362033
C,0,-3.6871081196,0.2391678458,-0.7954454845
C,0,-2.0574319217,-0.7395277286,0.7432266886
C,0,-3.0248734791,-1.6332444204,1.1810247892
C,0,-4.6465593121,-0.6641524146,-0.3483886939
H,0,-3.9398864297,0.9673534194,-1.5593034928
H,0,-1.0615883584,-0.7698128016,1.169280827
H,0,-2.7739730895,-2.3587153549,1.9473642854
H,0,-5.6461696615,-0.6357192655,-0.7683395453
H,0,-5.0677072928,-2.3015828315,0.9879725377
H,0,-1.6336252472,0.9482015345,-2.2340202943
H,0,-2.4214729597,2.4951798579,-0.3999585401

E(RB3LYP) = -694.760614802 A.U.

Imaginary Frequency = -251.2929

Zero-point correction= 0.272765 (Hartree/Particle)
Thermal correction to Energy= 0.286253
Thermal correction to Enthalpy= 0.287197
Thermal correction to Gibbs Free Energy= 0.231875
Sum of electronic and zero-point Energies= -694.487850
Sum of electronic and thermal Energies= -694.474362
Sum of electronic and thermal Enthalpies= -694.473418
Sum of electronic and thermal Free Energies= -694.528740

3b: *in silico*

Charge = 1 Multiplicity = 1
C,0,-1.3334334672,-0.7946877265,0.6325804569
C,0,1.4707664582,-1.0262276037,-0.1231730926
C,0,-0.7720950171,0.0477160033,-0.3877236547
C,0,-0.4739973662,-1.7528376499,1.2713189216
C,0,0.8362413768,-1.8686353963,0.9227248633
C,0,0.5390279041,-0.0463961046,-0.7388982028
H,0,-1.3911901341,0.8056594887,-0.8516730937
H,0,-0.8835309553,-2.4199076965,2.0197433464
H,0,1.4645119022,-2.6113604982,1.4069849281
H,0,0.949684527,0.6202985178,-1.4924322524
C,0,-2.7296975115,-0.6797025558,1.0071770654
C,0,-5.4397228316,-0.4541547115,1.7346332347
C,0,-3.1862279926,-1.1390860516,2.2711195918
C,0,-3.677622112,-0.1042879213,0.1198542019
C,0,-5.0152734891,-0.0068028899,0.4767078487
C,0,-4.5204234981,-1.0139413319,2.6317008932
H,0,-2.4876853772,-1.5519066852,2.9895385044
H,0,-3.3757191858,0.2226328762,-0.8683445864
H,0,-5.731205989,0.4134038272,-0.2217399618
H,0,-4.8489944921,-1.3481961539,3.6101123839
H,0,-6.4849299674,-0.3675547516,2.0150999991
C,0,2.7908169398,-0.382162809,0.3515584701
C,0,5.1750984683,0.7946236882,1.2223439185
C,0,4.0055795125,-0.7350169059,-0.245895153
C,0,2.7707305878,0.5620323622,1.3874823041
C,0,3.9616301034,1.1479732823,1.8198544786
C,0,5.1957282827,-0.1462801329,0.1905825348
H,0,4.0300690224,-1.4661162819,-1.049927486
H,0,1.8312828497,0.8425258697,1.8571332585
H,0,3.9410185793,1.8790588859,2.6220219322
H,0,6.1349713154,-0.4241856119,-0.2771241291
H,0,6.099958237,1.2512645129,1.5601010066
H,0,1.7629115998,-1.7203475943,-0.9367602703

E(RB3LYP) = -694.730901051 A.U.

Zero-point correction= 0.273537 (Hartree/Particle)

Thermal correction to Energy= 0.287587
Thermal correction to Enthalpy= 0.288531
Thermal correction to Gibbs Free Energy= 0.230798
Sum of electronic and zero-point Energies= -694.457364
Sum of electronic and thermal Energies= -694.443314
Sum of electronic and thermal Enthalpies= -694.442370
Sum of electronic and thermal Free Energies= -694.500103

3b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.3331723316,-0.0536735469,-0.8953286509
C,0,1.3963675045,-0.4658195615,0.0127824959
C,0,-0.4862124957,-1.0188959426,-1.5345440696
C,0,-0.8009068295,0.7080592181,0.1980042758
C,0,0.4811596158,0.5343326261,0.6185800027
C,0,0.7944715878,-1.215285953,-1.1193894927
H,0,-0.8780725126,-1.6237514369,-2.3420493547
H,0,-1.4122495893,1.4680353019,0.6675966986
H,0,0.8729634413,1.1389209074,1.4310961652
H,0,1.4147338394,-1.9619441093,-1.6061470921
C,0,-2.7004540403,0.1498152614,-1.344319327
C,0,-5.3471178198,0.5503413207,-2.2134807588
C,0,-3.6707232883,0.720019401,-0.4811533467
C,0,-3.097689044,-0.215218112,-2.6560653174
C,0,-4.4015862439,-0.0040405452,-3.0855690906
C,0,-4.9791448902,0.904747745,-0.909538793
H,0,-3.4128833327,0.9783523508,0.5389557416
H,0,-2.3776773454,-0.6257435492,-3.3538136636
H,0,-4.6840643724,-0.2684411864,-4.0990253865
H,0,-5.7144048316,1.3220409882,-0.2297977297
H,0,-6.3679226834,0.7045033163,-2.5488218808
C,0,2.7856985651,0.1062780026,-0.3222451065
C,0,5.3074250423,1.1500135518,-0.9582042892
C,0,2.9025981399,1.1494421578,-1.2517653421
C,0,3.9345371857,-0.4115603947,0.2858387829
C,0,5.1925917983,0.1096048539,-0.0326418054
C,0,4.160028506,1.6688851905,-1.5670850284
H,0,2.0154741946,1.5577833979,-1.7282869821
H,0,3.8516874141,-1.2203399856,1.0064761904
H,0,6.0787106906,-0.2980712335,0.4442406267
H,0,4.2419993934,2.4777271932,-2.2867958965
H,0,6.284342787,1.5548452655,-1.2041789232
H,0,1.5680633949,-1.2218522332,0.8060653778

E(RB3LYP) = -694.789307476 A.U.

Zero-point correction= 0.273633 (Hartree/Particle)
Thermal correction to Energy= 0.287642
Thermal correction to Enthalpy= 0.288586

Thermal correction to Gibbs Free Energy= 0.231095
Sum of electronic and zero-point Energies= -694.515674
Sum of electronic and thermal Energies= -694.501666
Sum of electronic and thermal Enthalpies= -694.500721
Sum of electronic and thermal Free Energies= -694.558213

1a: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.8994449592,-1.0247539315,0.0004541479
C,0,-0.1191069153,-3.7243831468,-0.0733035319
C,0,-0.5368701575,-1.2435691738,-0.0102832737
C,0,1.782746656,-2.1590842292,0.0611198344
C,0,1.323946043,-3.4371580364,0.0088384774
C,0,-0.9942874067,-2.53683555,-0.0475963795
H,0,2.8509366966,-1.9782335984,0.0666526154
H,0,2.0208919245,-4.2705114157,-0.0017352261
H,0,-2.0668778994,-2.7104469564,-0.0276429278
C,0,1.5096950184,0.2952399703,-0.0763814232
C,0,2.785489517,2.7923408726,-0.3003638587
C,0,2.7305399353,0.5526690716,0.6014755119
C,0,0.94896483,1.3265022952,-0.8721537205
C,0,1.5968114363,2.5485892582,-0.9991182325
C,0,3.3435556989,1.7949874256,0.5099761165
H,0,3.1669670038,-0.2041294068,1.2447065569
H,0,0.0323383665,1.1514949599,-1.4204349731
H,0,1.1740614541,3.3161791072,-1.6388391402
H,0,4.2565850905,1.9887457264,1.0631756898
H,0,3.2764835665,3.7567784785,-0.3866794997
C,0,-1.5420186967,-0.141295257,0.0847125422
C,0,-3.5188986483,1.8370432726,0.3205287307
C,0,-1.543335248,0.7333467093,1.1838098273
C,0,-2.5448070343,-0.0188897529,-0.8900455086
C,0,-3.5250886047,0.970026064,-0.7744482784
C,0,-2.5292781919,1.7131124667,1.300951002
H,0,-0.7838773336,0.6411175594,1.9549538939
H,0,-2.5502686316,-0.6848515362,-1.7490911554
H,0,-4.2906445487,1.0602416082,-1.538729401
H,0,-2.5282287987,2.3760590501,2.1605328767
H,0,-4.2830697359,2.6023558299,0.4128173288
H,0,-0.3323350366,-4.3338518273,-0.9719540511
H,0,-0.4122701786,-4.4116037474,0.7421448698

E(RB3LYP) = -694.730651140 A.U.

Zero-point correction= 0.272789 (Hartree/Particle)
Thermal correction to Energy= 0.286905
Thermal correction to Enthalpy= 0.287849
Thermal correction to Gibbs Free Energy= 0.231113
Sum of electronic and zero-point Energies= -694.457862
Sum of electronic and thermal Energies= -694.443746

Sum of electronic and thermal Enthalpies= -694.442802
Sum of electronic and thermal Free Energies= -694.499538

1a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.8961854277,-1.0366685541,-0.0051564521
C,0,-0.1157106801,-3.7233068505,-0.0906633886
C,0,-0.535472005,-1.2517095919,-0.0163562495
C,0,1.7831827771,-2.1601890286,0.0547737555
C,0,1.3232432019,-3.4404064263,0.0003311558
C,0,-0.9951557756,-2.5445220472,-0.0644397158
H,0,2.8502604757,-1.9751363552,0.0685391285
H,0,2.0172332892,-4.2750997724,-0.0057124454
H,0,-2.0659468629,-2.7250589699,-0.0564552182
C,0,1.5027136986,0.2927809155,-0.0820273874
C,0,2.7617716629,2.7966236147,-0.3005509682
C,0,2.6832762338,0.5739068167,0.6462321884
C,0,0.9713193326,1.2947986246,-0.9270853077
C,0,1.6107447628,2.523770043,-1.0492261653
C,0,3.2897303707,1.8223108244,0.55468876
H,0,3.0973583112,-0.1693471602,1.3191011025
H,0,0.0846157357,1.0948644032,-1.5155386213
H,0,1.209431406,3.2722644082,-1.7244996374
H,0,4.1757703491,2.0347369031,1.1437805151
H,0,3.2462663653,3.7644133434,-0.3842989111
C,0,-1.5349744386,-0.1446182828,0.0891631843
C,0,-3.4966971525,1.8500727623,0.3474459697
C,0,-1.5147616131,0.735143751,1.1839984727
C,0,-2.552043798,-0.0187637016,-0.8698179537
C,0,-3.5250902016,0.9765308369,-0.7428361066
C,0,-2.491485056,1.7236287773,1.3122646778
H,0,-0.7420004753,0.6417971836,1.9411302498
H,0,-2.5738368269,-0.6892111418,-1.7244135017
H,0,-4.301353233,1.0679883396,-1.4964209303
H,0,-2.468835583,2.3926645169,2.1671144765
H,0,-4.2531850217,2.6224929477,0.4470463857
H,0,-0.3238260389,-4.32737673,-0.9942081376
H,0,-0.4145335082,-4.4221422395,0.7121465154

E(RB3LYP) = -694.789984429 A.U.

Zero-point correction= 0.272648 (Hartree/Particle)
Thermal correction to Energy= 0.286766
Thermal correction to Enthalpy= 0.287710
Thermal correction to Gibbs Free Energy= 0.231022
Sum of electronic and zero-point Energies= -694.517337
Sum of electronic and thermal Energies= -694.503218
Sum of electronic and thermal Enthalpies= -694.502274
Sum of electronic and thermal Free Energies= -694.558962

1c: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.5414162905,-1.2226701325,0.0101173538
C,0,-1.1457206643,-3.5647140317,-0.00115528
C,0,-0.8575532349,-1.0203448684,0.0195502781
C,0,1.0189617104,-2.5452134848,0.015194605
C,0,0.2065105807,-3.7099675949,0.0228013481
C,0,-1.7534941745,-2.220274147,0.0376397985
H,0,2.0971519747,-2.6787758942,-0.0261502026
H,0,0.6741026764,-4.6885741987,0.0115859374
H,0,-1.8104305822,-4.4232513229,-0.0333271788
C,0,1.5549721189,-0.1293589724,-0.082679369
C,0,3.5410142915,1.8406161789,-0.3022441
C,0,2.570655956,-0.0335254373,0.8824260167
C,0,1.5493796923,0.7658503601,-1.1649350849
C,0,2.5403026449,1.7414664943,-1.2740240714
C,0,3.5544009601,0.9524649164,0.7758912329
H,0,2.583626855,-0.7164121803,1.7282833346
H,0,0.7804779369,0.6923658816,-1.9283277265
H,0,2.534182125,2.4206314129,-2.1207771403
H,0,4.3288103843,1.0234891292,1.5331654966
H,0,4.3090966802,2.6026855616,-0.3884612322
C,0,-1.5053610727,0.2874528774,0.0682263268
C,0,-2.8450833902,2.7543751268,0.2808999077
C,0,-0.9839289253,1.327878295,0.8760520029
C,0,-2.7154799362,0.5205354871,-0.631092052
C,0,-3.3652413138,1.7459786032,-0.5388449684
C,0,-1.6602515563,2.5364261458,0.9934423369
H,0,-0.072945203,1.1702772458,1.4398297087
H,0,-3.1222614235,-0.2363581884,-1.2940140638
H,0,-4.2732273067,1.9186189728,-1.1072887241
H,0,-1.2624569953,3.312349224,1.6392983309
H,0,-3.3589116172,3.707301683,0.3601506549
H,0,-2.5340775532,-2.1385233408,-0.7359631435
H,0,-2.3547583784,-2.1582117217,0.9639310669

E(RB3LYP) = -694.727752958 A.U.

Zero-point correction= 0.272495 (Hartree/Particle)
Thermal correction to Energy= 0.286774
Thermal correction to Enthalpy= 0.287718
Thermal correction to Gibbs Free Energy= 0.230377
Sum of electronic and zero-point Energies= -694.455258
Sum of electronic and thermal Energies= -694.440979
Sum of electronic and thermal Enthalpies= -694.440034
Sum of electronic and thermal Free Energies= -694.497375

1c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.5387489013,-1.2333385774,0.013187282
C,0,-1.1480313904,-3.5653613852,0.0220188782
C,0,-0.8528282959,-1.0335953887,0.0306458609
C,0,1.0196144097,-2.5579016008,0.0239671958
C,0,0.2067831792,-3.7162061399,0.0385396241
C,0,-1.7500261544,-2.2238070551,0.0548204624
H,0,2.0968050277,-2.695297097,-0.0136093117
H,0,0.6708300928,-4.695666205,0.0313990431
H,0,-1.8157138928,-4.4208305608,0.000323422
C,0,1.5463181193,-0.1344540097,-0.0904901623
C,0,3.5115471838,1.8579366595,-0.3305562626
C,0,2.5758645819,-0.0330535599,0.8585297
C,0,1.5168118195,0.7664803744,-1.1674447592
C,0,2.4956293887,1.7541397167,-1.2865718536
C,0,3.5496890669,0.9622662913,0.7415656627
H,0,2.6071350095,-0.7211810744,1.6988219228
H,0,0.7351615417,0.6897099454,-1.9169669624
H,0,2.466086026,2.4401294598,-2.1276226679
H,0,4.3348522215,1.0358615688,1.487784855
H,0,4.2698513737,2.6294193157,-0.4232085165
C,0,-1.4969907884,0.2833474184,0.0797790514
C,0,-2.8142763635,2.7609419623,0.2752812857
C,0,-1.0138503985,1.2892815432,0.9465065142
C,0,-2.6549246414,0.546704217,-0.6852788371
C,0,-3.294975403,1.7807522515,-0.5989958117
C,0,-1.6786170091,2.5070248987,1.0530767397
H,0,-0.1412349196,1.1006312374,1.5603419602
H,0,-3.0297438375,-0.1926290472,-1.385179298
H,0,-4.1671048503,1.9772648017,-1.2140540762
H,0,-1.3095852147,3.2600712189,1.7418872839
H,0,-3.3202038747,3.7185117113,0.3488902125
H,0,-2.5336184603,-2.1440321142,-0.7166447915
H,0,-2.3561228988,-2.1585326969,0.9784577545

E(RB3LYP) = -694.787947935 A.U.

Zero-point correction= 0.272346 (Hartree/Particle)
Thermal correction to Energy= 0.286643
Thermal correction to Enthalpy= 0.287587
Thermal correction to Gibbs Free Energy= 0.230251
Sum of electronic and zero-point Energies= -694.515602
Sum of electronic and thermal Energies= -694.501305
Sum of electronic and thermal Enthalpies= -694.500361
Sum of electronic and thermal Free Energies= -694.557697

1d: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.6547731704,-1.0095968305,0.103337813
C,0,-0.3300717428,-3.6206982798,0.0380260195
C,0,-0.7397635835,-1.2165128052,0.0726446153
C,0,1.5396427857,-2.0955726041,0.1075128411
C,0,1.0485945656,-3.4009605565,0.0783019489
C,0,-1.2114100333,-2.5392972961,0.0325075451
H,0,2.6128006922,-1.9240117885,0.1201327203
H,0,1.7393724739,-4.2380023892,0.0790249799
H,0,-2.2827428545,-2.7135491438,0.0167894142
H,0,-0.7200110547,-4.6333435814,0.0151001304
C,0,1.2312298213,0.4170567881,0.0608454166
C,0,3.5321818374,2.0410001574,-0.3008064516
C,0,1.6574852593,0.8875939696,-1.2665339778
C,0,2.1087874807,0.7892303368,1.1780975511
C,0,3.2102875998,1.5942593695,0.9969539652
C,0,2.7583674003,1.6968215128,-1.4280570653
H,0,1.0465610146,0.6016567938,-2.1181848627
H,0,1.8422232423,0.4295660281,2.1681506046
H,0,3.8358948606,1.8772885955,1.8368636292
H,0,3.0455870816,2.0546154115,-2.4110909345
H,0,4.4066783059,2.6723844421,-0.4368547527
C,0,-1.7000713133,-0.0760220466,0.0678954816
C,0,-3.4949700522,2.0959149781,0.0449010275
C,0,-2.5491752444,0.1385088237,-1.0318751947
C,0,-1.7770750562,0.8095638064,1.1637773523
C,0,-2.667486617,1.8890172661,1.1493250933
C,0,-3.437912508,1.2146076022,-1.0419349827
H,0,-2.5077801605,-0.539512071,-1.879563632
H,0,-1.183599801,0.6154145502,2.0540993589
H,0,-2.7272442788,2.550103596,2.0084362357
H,0,-4.0880591524,1.3666038401,-1.8980714883
H,0,-4.1910674749,2.928620646,0.0335391004
H,0,0.306327906,1.0551672384,0.2479626182

E(RB3LYP) = -694.712404649 A.U.

Zero-point correction= 0.271794 (Hartree/Particle)
Thermal correction to Energy= 0.285951
Thermal correction to Enthalpy= 0.286895
Thermal correction to Gibbs Free Energy= 0.229286
Sum of electronic and zero-point Energies= -694.440611
Sum of electronic and thermal Energies= -694.426454
Sum of electronic and thermal Enthalpies= -694.425509
Sum of electronic and thermal Free Energies= -694.483119

1d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.652172396,-0.9660214376,0.0764345945

C,0,-0.3277862627,-3.5861862738,0.0374441428
C,0,-0.7417784105,-1.1795677073,0.0732432492
C,0,1.5360488484,-2.0538266231,0.0629176683
C,0,1.0510779835,-3.361480376,0.0478815894
C,0,-1.2095417961,-2.5052111251,0.0471664751
H,0,2.6080312811,-1.8767958341,0.0536481145
H,0,1.7457844924,-4.1954021694,0.0381731743
H,0,-2.2807494289,-2.6815987009,0.049244612
H,0,-0.7169139762,-4.5995652408,0.0250835832
C,0,1.2484536871,0.4491910814,0.0283009429
C,0,3.6176578255,1.9775500129,-0.2851097263
C,0,1.746076984,0.8648604532,-1.2974491746
C,0,2.1006478942,0.8186373068,1.17327921
C,0,3.2315328795,1.5812492395,1.0120565201
C,0,2.8793571775,1.6282535366,-1.4345500626
H,0,1.1594473112,0.5781999508,-2.1648292874
H,0,1.7879261239,0.4951736226,2.1614134285
H,0,3.8353313376,1.8673965053,1.8656182671
H,0,3.2189825933,1.9486106209,-2.4128846569
H,0,4.5181732124,2.5735498916,-0.403509975
C,0,-1.7256389821,-0.0562250405,0.0810150432
C,0,-3.6006898903,2.047325037,0.0834721462
C,0,-2.5875138256,0.1368171915,-1.0129462641
C,0,-1.8266009688,0.8161788822,1.1812110479
C,0,-2.7561504531,1.8612141632,1.1805115038
C,0,-3.5161900657,1.1797933168,-1.0113111539
H,0,-2.5224108527,-0.5296186305,-1.8680929147
H,0,-1.2001062393,0.6572084185,2.0545090976
H,0,-2.8251564745,2.5193622767,2.041391859
H,0,-4.172266641,1.3165129289,-1.8657649307
H,0,-4.3238181588,2.857209432,0.0826698851
H,0,0.3649649687,1.1351216506,0.1610141114

E(RB3LYP) = -694.774101612 A.U.

Zero-point correction= 0.272202 (Hartree/Particle)
Thermal correction to Energy= 0.286403
Thermal correction to Enthalpy= 0.287347
Thermal correction to Gibbs Free Energy= 0.229221
Sum of electronic and zero-point Energies= -694.501899
Sum of electronic and thermal Energies= -694.487698
Sum of electronic and thermal Enthalpies= -694.486754
Sum of electronic and thermal Free Energies= -694.544880

1e: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.725946023,-1.1637527926,0.0251012171
C,0,-0.5655895044,-3.6635557017,-0.0831629472
C,0,-0.7044244412,-1.22529585,-0.0311442101

C,0,1.4617109215,-2.377473168,0.0801581123
C,0,0.8294965908,-3.6097330984,0.0160758592
C,0,-1.3128469197,-2.4858337214,-0.0972504831
H,0,2.5456374602,-2.3545278896,0.0908586676
H,0,1.416730018,-4.5218500804,0.0245332709
H,0,-2.3965946159,-2.5392726477,-0.113867484
H,0,-1.071687615,-4.6227202299,-0.1318422791
C,0,1.4663481481,0.0861650153,-0.0711193942
C,0,3.1102752707,2.4462353182,-0.4017635174
C,0,2.7264608246,0.2704272799,0.7170406519
C,0,1.0696182072,1.1366995037,-0.9123506742
C,0,1.8710760795,2.2595814207,-1.0824046469
C,0,3.5407537208,1.4809790476,0.4534807981
H,0,0.1584683424,1.0478387107,-1.4901246941
H,0,1.5476372838,3.0203391783,-1.78816434
H,0,4.483689614,1.5772640198,0.9841076429
H,0,3.6972255818,3.3390732558,-0.5875863229
C,0,-1.5761057143,-0.0267141763,0.082532023
C,0,-3.2854774261,2.1942118174,0.3308049817
C,0,-1.4230021647,0.8815608951,1.1468878411
C,0,-2.6131718298,0.1856171459,-0.8442591857
C,0,-3.4536831576,1.2931876474,-0.7256615235
C,0,-2.2733328032,1.9805626152,1.2712900358
H,0,-0.6636278129,0.7026166967,1.9031209279
H,0,-2.7473224995,-0.5069399393,-1.6703872993
H,0,-4.2412807266,1.4510225787,-1.4559072806
H,0,-2.1564128489,2.6607056263,2.1094654584
H,0,-3.9472393084,3.0491184532,0.427871602
H,0,3.3593055995,-0.6275952867,0.71365312
H,0,2.4117660525,0.3206457658,1.7782339026

E(RB3LYP) = -694.729612158 A.U.

Zero-point correction= 0.272639 (Hartree/Particle)
Thermal correction to Energy= 0.286856
Thermal correction to Enthalpy= 0.287800
Thermal correction to Gibbs Free Energy= 0.230842
Sum of electronic and zero-point Energies= -694.456973
Sum of electronic and thermal Energies= -694.442756
Sum of electronic and thermal Enthalpies= -694.441812
Sum of electronic and thermal Free Energies= -694.498770

1e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.728046158,-1.1708184434,0.0029407074
C,0,-0.5723921037,-3.6668569574,-0.0645546545
C,0,-0.6988584121,-1.2263633952,-0.0183552169
C,0,1.4608671465,-2.3815900497,0.0356507742
C,0,0.8230127446,-3.6152957831,-0.0073441123

C,0,-1.3146543344,-2.4850968552,-0.0601897835
H,0,2.544448698,-2.3572658629,0.0249170333
H,0,1.4102268993,-4.5274785228,-0.0107056515
H,0,-2.3986922312,-2.5344675288,-0.0533987121
H,0,-1.0836997294,-4.6237757889,-0.0976713978
C,0,1.4766696863,0.0840061882,-0.0923935973
C,0,3.0966352031,2.4583613437,-0.3749680708
C,0,2.7160078486,0.2690846175,0.7159091836
C,0,1.0937399156,1.118670353,-0.9477373518
C,0,1.8865399191,2.2572472859,-1.0910827821
C,0,3.5139009009,1.491018182,0.4896238532
H,0,0.2015294221,1.0215922744,-1.5528297519
H,0,1.5704709809,3.0170098524,-1.8003210701
H,0,4.4370893461,1.5961907185,1.0508726963
H,0,3.6743904436,3.3611074201,-0.5360179447
C,0,-1.571272758,-0.0235675738,0.0924846172
C,0,-3.2894523356,2.1955231358,0.3292991543
C,0,-1.4163157698,0.8943976792,1.1468780713
C,0,-2.6114679464,0.1800914057,-0.8318399767
C,0,-3.458368109,1.2844881807,-0.7183106851
C,0,-2.2696069317,1.9931750056,1.264495914
H,0,-0.6428138798,0.7363319921,1.8925858416
H,0,-2.743742226,-0.518264852,-1.6531326566
H,0,-4.2481699756,1.4331127637,-1.4485268384
H,0,-2.1422530092,2.6858899024,2.0910298684
H,0,-3.950997646,3.0516549399,0.4202025317
H,0,3.366121013,-0.6176328217,0.691995319
H,0,2.4034074218,0.2781086039,1.7787145189

E(RB3LYP) = -694.789810967 A.U.

Zero-point correction= 0.272467 (Hartree/Particle)
Thermal correction to Energy= 0.286742
Thermal correction to Enthalpy= 0.287686
Thermal correction to Gibbs Free Energy= 0.230197
Sum of electronic and zero-point Energies= -694.517344
Sum of electronic and thermal Energies= -694.503069
Sum of electronic and thermal Enthalpies= -694.502125
Sum of electronic and thermal Free Energies= -694.559614

1f: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.6163772674,-1.3090034313,-0.0207979518
C,0,-0.9221943779,-3.6558640865,0.0074150396
C,0,-0.7976740411,-1.2163305404,0.0371656734
C,0,1.2294781005,-2.5736245893,-0.0544837055
C,0,0.4704122986,-3.74169903,-0.0397019757
C,0,-1.5419070047,-2.4067229973,0.0445940145
H,0,2.3106021684,-2.6449080386,-0.13425264

H,0,0.9622871076,-4.7081384984,-0.0779171332
H,0,-2.6237088287,-2.3453946095,0.1096083262
H,0,-1.5257511627,-4.5579007957,0.0199389643
C,0,1.478434677,-0.1001090237,-0.0866399976
C,0,3.0813053667,2.2836651209,-0.3617937459
C,0,2.6567991896,0.0127080627,0.6225800548
C,0,1.1349122208,0.9918340276,-0.9365450343
C,0,1.9090046603,2.1694078936,-1.059192584
C,0,3.5317314798,1.1954489417,0.5210664983
H,0,2.9676376908,-0.7830728099,1.2938827101
H,0,0.2474385017,0.8983370509,-1.5540108182
H,0,1.5749181293,2.9566259366,-1.7266166549
H,0,3.7068426027,3.167050205,-0.4556875511
C,0,-1.5203631577,0.0858310908,0.1193058909
C,0,-2.9419234828,2.5155472689,0.2900533546
C,0,-1.2127838704,1.0349593815,1.1155691009
C,0,-2.5592190287,0.3759409586,-0.7843842092
C,0,-3.2608472026,1.579529584,-0.7008775012
C,0,-1.9206677423,2.2373480637,1.2008838864
H,0,-0.4508614257,0.807660914,1.855623759
H,0,-2.8119883769,-0.3435689221,-1.5579197344
H,0,-4.0594598631,1.786209204,-1.4067611527
H,0,-1.6867945686,2.9454063512,1.9902416086
H,0,-3.4953125675,3.4469026738,0.3578678736
H,0,4.5531344754,0.8842105679,0.2249502227
H,0,3.7211821248,1.6004919856,1.5347294819

E(RB3LYP) = -694.719418730 A.U.

Zero-point correction= 0.272142 (Hartree/Particle)
Thermal correction to Energy= 0.286341
Thermal correction to Enthalpy= 0.287285
Thermal correction to Gibbs Free Energy= 0.230530
Sum of electronic and zero-point Energies= -694.447277
Sum of electronic and thermal Energies= -694.433078
Sum of electronic and thermal Enthalpies= -694.432134
Sum of electronic and thermal Free Energies= -694.488889

1f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.6112938292,-1.2880415953,-0.0371818064
C,0,-0.9161715029,-3.6463108103,-0.0062908633
C,0,-0.8013421753,-1.2043608494,0.0363599838
C,0,1.2289612198,-2.5497736785,-0.0814563041
C,0,0.4768278023,-3.7234744224,-0.0635814164
C,0,-1.540264567,-2.3995026314,0.0426351412
H,0,2.3100657474,-2.6107591925,-0.1635705969
H,0,0.9754751442,-4.6865624152,-0.1057968319
H,0,-2.622143077,-2.343639119,0.1134014667

H,0,-1.5159402869,-4.5511406003,0.0070568681
C,0,1.4820363168,-0.0805163508,-0.1081356182
C,0,3.139295267,2.2525046612,-0.4010176229
C,0,2.6201010408,0.0434911043,0.6614432807
C,0,1.2020131432,0.9747668911,-1.0199250471
C,0,2.0053111763,2.1251711887,-1.1616386445
C,0,3.5126235266,1.2050658479,0.5553829588
H,0,2.883060177,-0.724593468,1.3824522634
H,0,0.3302254164,0.8812448621,-1.6598517335
H,0,1.7236185909,2.885612347,-1.8808135722
H,0,3.7852631518,3.1197702422,-0.494780095
C,0,-1.5369387841,0.090802177,0.1362972687
C,0,-2.9915987541,2.4975183518,0.3444869653
C,0,-1.2377700765,1.0278349611,1.1426150272
C,0,-2.5836522589,0.3785171556,-0.7584042862
C,0,-3.3025279127,1.5715360189,-0.6567931494
C,0,-1.9599570023,2.2196324094,1.2459045059
H,0,-0.4544749818,0.8124753354,1.863149663
H,0,-2.8263077673,-0.3318102152,-1.5434746688
H,0,-4.1034184578,1.7779205243,-1.3605996145
H,0,-1.7215254885,2.925437501,2.0360676077
H,0,-3.5520578961,3.4240647321,0.4244117723
H,0,4.5444465084,0.8624045538,0.3417470687
H,0,3.6565142912,1.6534923934,1.5577940999

E(RB3LYP) = -694.783203930 A.U.

Zero-point correction= 0.271865 (Hartree/Particle)
Thermal correction to Energy= 0.286215
Thermal correction to Enthalpy= 0.287159
Thermal correction to Gibbs Free Energy= 0.229687
Sum of electronic and zero-point Energies= -694.511339
Sum of electronic and thermal Energies= -694.496989
Sum of electronic and thermal Enthalpies= -694.496045
Sum of electronic and thermal Free Energies= -694.553517

1g: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.6942164728,-1.1849520179,0.0577157693
C,0,-0.6407559354,-3.6536855365,-0.1150661998
C,0,-0.7359590112,-1.2154930749,-0.0375358875
C,0,1.4058964818,-2.4138550942,0.1382022881
C,0,0.7523741657,-3.6305834631,0.0352045277
C,0,-1.3665169828,-2.4629202109,-0.1377578906
H,0,2.488561372,-2.4041294762,0.1971219462
H,0,1.3186595332,-4.5555217473,0.0588294015
H,0,-2.4501592639,-2.4973208714,-0.1824825416
H,0,-1.1635936724,-4.6024295532,-0.1875236492
C,0,1.4782358999,0.0331425275,-0.0457406304

C,0,3.1588597927,2.3675161089,-0.3615316
C,0,2.7285643754,0.1453123433,0.6603566165
C,0,1.086400364,1.1084275566,-0.9165548672
C,0,1.8813541268,2.1981681513,-1.0894651764
C,0,3.5157111537,1.2466573118,0.5355203148
H,0,3.0155579135,-0.6437978599,1.3456857389
H,0,0.1646141336,1.0182401689,-1.4763603914
H,0,1.5900580954,2.9746196001,-1.7914375347
H,0,4.4324293932,1.3278275266,1.1134381217
C,0,-1.5778600685,-0.0006491509,0.0856207443
C,0,-3.2274284518,2.2611126754,0.3596770488
C,0,-1.3763734384,0.9111194345,1.1399367143
C,0,-2.6332403408,0.2296696069,-0.8174700935
C,0,-3.4430076588,1.3574667463,-0.6866678681
C,0,-2.1977121649,2.0303637887,1.2765385212
H,0,-0.6037912461,0.7176562157,1.8787071384
H,0,-2.8020305229,-0.4629931628,-1.6369935457
H,0,-4.2435653868,1.530441348,-1.3991397274
H,0,-2.045224245,2.7126487885,2.1071995995
H,0,-3.8670664678,3.1315258028,0.4670378359
H,0,3.9795016611,2.5416682071,-1.0817205191
H,0,3.1465391127,3.3141969302,0.2096016057

E(RB3LYP) = -694.734332618 A.U.

Zero-point correction= 0.272971 (Hartree/Particle)
Thermal correction to Energy= 0.287034
Thermal correction to Enthalpy= 0.287978
Thermal correction to Gibbs Free Energy= 0.231573
Sum of electronic and zero-point Energies= -694.461361
Sum of electronic and thermal Energies= -694.447299
Sum of electronic and thermal Enthalpies= -694.446355
Sum of electronic and thermal Free Energies= -694.502760

1g: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.6953497899,-1.1935556937,0.0315319511
C,0,-0.6454299262,-3.660611901,-0.0988984912
C,0,-0.7314804016,-1.2207190308,-0.0273706188
C,0,1.4078784207,-2.4174476447,0.084896504
C,0,0.7495387676,-3.6371008085,0.0042508784
C,0,-1.3686039999,-2.467118573,-0.1007786297
H,0,2.4916372015,-2.4042531434,0.1171379883
H,0,1.3177978817,-4.5610732,0.0125015021
H,0,-2.4530949104,-2.4989181193,-0.1193760551
H,0,-1.1723250413,-4.6079815023,-0.1551770082
C,0,1.4843770194,0.0328775412,-0.0648119086
C,0,3.1420011537,2.3680127129,-0.3412594101
C,0,2.7045169966,0.1511898079,0.6785948251

C,0,1.1050690783,1.0896988338,-0.9547413624
C,0,1.8935198925,2.1903141058,-1.1061790092
C,0,3.4879061107,1.2602277509,0.5680795262
H,0,2.9773339954,-0.6356733749,1.3715910506
H,0,0.2026960772,0.9846495365,-1.5428104899
H,0,1.6164930645,2.9651438583,-1.8144521385
H,0,4.3893764283,1.3530965034,1.1660987485
C,0,-1.5730986199,-0.0008854751,0.0954451013
C,0,-3.2209659546,2.266090662,0.3611886955
C,0,-1.3665459828,0.9172653059,1.1414192205
C,0,-2.6303739128,0.2259881943,-0.804619624
C,0,-3.4416934152,1.3544280526,-0.6769028362
C,0,-2.1852331284,2.0403846811,1.2730092477
H,0,-0.5814337016,0.7370792815,1.8698753465
H,0,-2.8009760985,-0.4712918576,-1.6195678554
H,0,-4.2441526505,1.522613338,-1.3887824557
H,0,-2.0190436525,2.733388428,2.0922985985
H,0,-3.8559294539,3.1409349317,0.4627255844
H,0,3.9824626669,2.5544368229,-1.0349785378
H,0,3.1056754954,3.318259596,0.2230074719

E(RB3LYP) = -694.793100507 A.U.

Zero-point correction= 0.272610 (Hartree/Particle)
Thermal correction to Energy= 0.286745
Thermal correction to Enthalpy= 0.287689
Thermal correction to Gibbs Free Energy= 0.231002
Sum of electronic and zero-point Energies= -694.520490
Sum of electronic and thermal Energies= -694.506355
Sum of electronic and thermal Enthalpies= -694.505411
Sum of electronic and thermal Free Energies= -694.562098

2a: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.2455709104,0.7207542877,0.1085337184
C,0,-1.2318553164,2.176863433,0.2855544091
C,0,0.0052767674,0.0437724029,0.0200898138
C,0,1.2538502632,2.1529048356,0.2859400251
C,0,0.091887882,2.8405910711,0.3699734523
C,0,-1.2186867882,0.6911161731,0.0928735909
H,0,0.0217702151,-1.0180892742,-0.1869241814
H,0,2.1988559824,2.6720698545,0.3873357545
H,0,0.1003086414,3.9168758746,0.518376268
C,0,2.5023716627,-0.0118940726,0.0074499774
C,0,4.9287393115,-1.4236739377,-0.199072383
C,0,3.6770946543,0.6271907455,-0.4597721038
C,0,2.5808687116,-1.3788382355,0.3715012422
C,0,3.7823962113,-2.0698569188,0.2801762855
C,0,4.8702576458,-0.0763823357,-0.5739015595
H,0,3.6469786403,1.6629593678,-0.7789502627

H,0,1.7113950136,-1.8874471119,0.7730612254
H,0,3.8316313069,-3.1096307274,0.5864093406
H,0,5.7551779178,0.4216147722,-0.9562138615
H,0,5.8646351189,-1.968053506,-0.2776110614
C,0,-2.4845317996,-0.032957846,-0.0130894449
C,0,-4.9238099281,-1.435099652,-0.1963849009
C,0,-2.5589441972,-1.4110244833,0.303238644
C,0,-3.6723211566,0.6220729067,-0.4147624505
C,0,-4.8729745389,-0.0729178235,-0.5120759053
C,0,-3.7634875456,-2.0992815189,0.2166885437
H,0,-1.6809291467,-1.9369736169,0.6613304457
H,0,-3.6594291959,1.6720780945,-0.6854235432
H,0,-5.7689364834,0.4442010971,-0.8396019288
H,0,-3.8024283308,-3.15133669,0.4797082287
H,0,-5.8626400966,-1.9750169102,-0.2691172954
H,0,-1.8079703257,2.4159353017,1.1948741838
H,0,-1.814641717,2.6638068528,-0.5127458167

E(RB3LYP) = -694.748445034 A.U.

Zero-point correction= 0.273529 (Hartree/Particle)
Thermal correction to Energy= 0.287675
Thermal correction to Enthalpy= 0.288620
Thermal correction to Gibbs Free Energy= 0.231245
Sum of electronic and zero-point Energies= -694.474916
Sum of electronic and thermal Energies= -694.460770
Sum of electronic and thermal Enthalpies= -694.459825
Sum of electronic and thermal Free Energies= -694.517200

2a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.2431090244,0.7287700538,0.1080414702
C,0,-1.2283956871,2.1788316955,0.2798224849
C,0,0.0051622953,0.0486682307,0.0117039654
C,0,1.2557176315,2.1548970726,0.2922060114
C,0,0.0904822521,2.8419813874,0.3739802907
C,0,-1.2157727884,0.697382669,0.0890791652
H,0,0.0240351253,-1.0131925809,-0.1929921683
H,0,2.1996586265,2.6746260812,0.3974292482
H,0,0.0952795423,3.9170952605,0.524859138
C,0,2.5012997253,-0.0100497934,0.0080081728
C,0,4.9229519626,-1.4295184948,-0.1959672824
C,0,3.6736752462,0.6232562198,-0.4672070876
C,0,2.5753242563,-1.3727213341,0.3817245152
C,0,3.7761143499,-2.0683563347,0.2905480871
C,0,4.86607986,-0.0846143289,-0.5790969571
H,0,3.6445000341,1.658037837,-0.7888352754
H,0,1.7044507793,-1.8770091914,0.7849573159
H,0,3.820971108,-3.1068828007,0.6016011672

H,0,5.7508320656,0.4102241909,-0.9660064751
H,0,5.8570242246,-1.9769956683,-0.2741234042
C,0,-2.4833680477,-0.031691844,-0.0141938601
C,0,-4.9191626337,-1.4411595134,-0.1961251211
C,0,-2.5503583953,-1.4107614789,0.2935472014
C,0,-3.6736179235,0.6227078835,-0.4047244812
C,0,-4.8735712195,-0.076411549,-0.500651501
C,0,-3.7539913639,-2.1033924827,0.2060881615
H,0,-1.668193311,-1.9376100332,0.6391479871
H,0,-3.6655669192,1.6755603439,-0.6622814356
H,0,-5.7725088268,0.4422282006,-0.8177543545
H,0,-3.7856863152,-3.1581406202,0.4593581119
H,0,-5.856363394,-1.9840188541,-0.2686869638
H,0,-1.8148401133,2.4266109435,1.1797889603
H,0,-1.799790881,2.6679812432,-0.5257766369

E(RB3LYP) = -694.805636261 A.U.

Zero-point correction= 0.273493 (Hartree/Particle)
Thermal correction to Energy= 0.287595
Thermal correction to Enthalpy= 0.288539
Thermal correction to Gibbs Free Energy= 0.231306
Sum of electronic and zero-point Energies= -694.532143
Sum of electronic and thermal Energies= -694.518041
Sum of electronic and thermal Enthalpies= -694.517097
Sum of electronic and thermal Free Energies= -694.574330

2c: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.0916541206,0.732872258,1.2944930403
C,0,0.2836304362,2.1052313549,-1.2369279467
C,0,-0.0788782011,-0.0092037127,0.
C,0,0.2836304362,2.1052313549,1.2369279467
C,0,0.370668531,2.7610978762,0.
C,0,0.0916541206,0.732872258,-1.2944930403
H,0,0.4221711333,2.6830520899,2.1425866995
H,0,0.5502978864,3.8331700088,0.
H,0,0.4221711333,2.6830520899,-2.1425866995
C,0,0.0099010189,0.0077032365,2.5586796967
C,0,-0.165932032,-1.3651032679,5.0147223651
C,0,-0.3926286825,0.6765774123,3.7409151084
C,0,0.3160775953,-1.3711133038,2.6453620839
C,0,0.235654713,-2.0446590806,3.8593077163
C,0,-0.4839196857,-0.0037498266,4.9492859593
H,0,-0.6778100663,1.7221864625,3.7048770755
H,0,0.6574781337,-1.9184159074,1.7735188722
H,0,0.4940074821,-3.0973898344,3.9088698514
H,0,-0.8104137323,0.5231122292,5.8399222655
H,0,-0.2307326383,-1.8936668488,5.960561424

C,0,0.0099010189,0.0077032365,-2.5586796967
C,0,-0.165932032,-1.3651032679,-5.0147223651
C,0,0.3160775953,-1.3711133038,-2.6453620839
C,0,-0.3926286825,0.6765774123,-3.7409151084
C,0,-0.4839196857,-0.0037498266,-4.9492859593
C,0,0.235654713,-2.0446590806,-3.8593077163
H,0,0.6574781337,-1.9184159074,-1.7735188722
H,0,-0.6778100663,1.7221864625,-3.7048770755
H,0,-0.8104137323,0.5231122292,-5.8399222655
H,0,0.4940074821,-3.0973898344,-3.9088698514
H,0,-0.2307326383,-1.8936668488,-5.960561424
H,0,-1.1080166227,-0.4074494508,0.
H,0,0.5352890344,-0.9169132792,0.

E(RB3LYP) = -694.745502857 A.U.

Zero-point correction= 0.273275 (Hartree/Particle)
Thermal correction to Energy= 0.287599
Thermal correction to Enthalpy= 0.288543
Thermal correction to Gibbs Free Energy= 0.230173
Sum of electronic and zero-point Energies= -694.472228
Sum of electronic and thermal Energies= -694.457904
Sum of electronic and thermal Enthalpies= -694.456960
Sum of electronic and thermal Free Energies= -694.515330

2c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.1028688881,0.7365952494,1.2900864204
C,0,0.2808161856,2.1093788525,-1.2368367028
C,0,-0.0224056774,-0.0140882242,0.
C,0,0.2808161856,2.1093788525,1.2368367028
C,0,0.3646923157,2.7658938427,0.
C,0,0.1028688881,0.7365952494,-1.2900864204
H,0,0.39822838,2.6925562232,2.1414371955
H,0,0.5278872859,3.8397832382,0.
H,0,0.39822838,2.6925562232,-2.1414371955
C,0,0.0113239199,0.0096979585,2.5571183667
C,0,-0.1835713296,-1.3669751762,5.0104293681
C,0,-0.392207967,0.6788142583,3.7370032695
C,0,0.3064445518,-1.3702979239,2.6407877384
C,0,0.2158601076,-2.046159699,3.8542408783
C,0,-0.4914856041,-0.0034319507,4.9452976756
H,0,-0.6664242768,1.7270595947,3.7032650545
H,0,0.6379027853,-1.9196116667,1.7670442662
H,0,0.4629708356,-3.101809345,3.8997223501
H,0,-0.8162846408,0.5259248846,5.8351829865
H,0,-0.2557615937,-1.8970158338,5.9549501176
C,0,0.0113239199,0.0096979585,-2.5571183667
C,0,-0.1835713296,-1.3669751762,-5.0104293681

C,0,0.3064445518,-1.3702979239,-2.6407877384
C,0,-0.392207967,0.6788142583,-3.7370032695
C,0,-0.4914856041,-0.0034319507,-4.9452976756
C,0,0.2158601076,-2.046159699,-3.8542408783
H,0,0.6379027853,-1.9196116667,-1.7670442662
H,0,-0.6664242768,1.7270595947,-3.7032650545
H,0,-0.8162846408,0.5259248846,-5.8351829865
H,0,0.4629708356,-3.101809345,-3.8997223501
H,0,-0.2557615937,-1.8970158338,-5.9549501176
H,0,-1.0056255565,-0.5110234661,0.
H,0,0.6817273685,-0.8560408527,0.

E(RB3LYP) = -694.803352910 A.U.

Zero-point correction= 0.273222 (Hartree/Particle)
Thermal correction to Energy= 0.287526
Thermal correction to Enthalpy= 0.288470
Thermal correction to Gibbs Free Energy= 0.230219
Sum of electronic and zero-point Energies= -694.530131
Sum of electronic and thermal Energies= -694.515827
Sum of electronic and thermal Enthalpies= -694.514883
Sum of electronic and thermal Free Energies= -694.573134

2d: *in silico*

Charge = 1 Multiplicity = 1
C,0,-0.1494514031,0.7521073426,1.2650183978
C,0,-0.4055636199,2.1109429122,-1.2558716758
C,0,-0.0162629936,0.1165373455,0.
C,0,-0.4055636199,2.1109429122,1.2558716758
C,0,-0.5307127431,2.8597584393,0.
C,0,-0.1494514031,0.7521073426,-1.2650183978
H,0,0.2363290987,-0.9408456696,0.
H,0,-0.5272548037,2.6555376185,2.1877286844
H,0,-0.5272548037,2.6555376185,-2.1877286844
C,0,0.0023770298,-0.0188392955,2.5231836322
C,0,0.2771694438,-1.4673640974,4.9107219758
C,0,0.6891586832,0.535526408,3.6173080849
C,0,-0.543029519,-1.3090419949,2.6400412205
C,0,-0.4086448841,-2.0261245135,3.8287255116
C,0,0.8266031948,-0.1867492809,4.8022265758
H,0,1.1469336365,1.5175610301,3.5354372276
H,0,-1.1037665256,-1.744447037,1.8172247397
H,0,-0.8454468372,-3.0160853153,3.9120870208
H,0,1.3700659339,0.2460665065,5.6359605549
H,0,0.3837465412,-2.0277518115,5.8340527062
C,0,0.0023770298,-0.0188392955,-2.5231836322
C,0,0.2771694438,-1.4673640974,-4.9107219758
C,0,-0.543029519,-1.3090419949,-2.6400412205
C,0,0.6891586832,0.535526408,-3.6173080849

C,0,0.8266031948,-0.1867492809,-4.8022265758
C,0,-0.4086448841,-2.0261245135,-3.8287255116
H,0,-1.1037665256,-1.744447037,-1.8172247397
H,0,1.1469336365,1.5175610301,-3.5354372276
H,0,1.3700659339,0.2460665065,-5.6359605549
H,0,-0.8454468372,-3.0160853153,-3.9120870208
H,0,0.3837465412,-2.0277518115,-5.8340527062
H,0,-1.4806121405,3.4298309592,0.
H,0,0.2040151475,3.6914926917,0.

E(RB3LYP) = -694.722981890 A.U.

Zero-point correction= 0.271702 (Hartree/Particle)
Thermal correction to Energy= 0.286039
Thermal correction to Enthalpy= 0.286983
Thermal correction to Gibbs Free Energy= 0.229196
Sum of electronic and zero-point Energies= -694.451280
Sum of electronic and thermal Energies= -694.436943
Sum of electronic and thermal Enthalpies= -694.435999
Sum of electronic and thermal Free Energies= -694.493786

2d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.1480042199,0.751383862,1.2599907583
C,0,-0.4091770903,2.1077993363,-1.2526878795
C,0,-0.0127560974,0.1125018408,0.
C,0,-0.4091770903,2.1077993363,1.2526878795
C,0,-0.5357608253,2.8538251152,0.
C,0,-0.1480042199,0.751383862,-1.2599907583
H,0,0.2388178711,-0.9446196641,0.
H,0,-0.5318774303,2.6561256449,2.1812208927
H,0,-0.5318774303,2.6561256449,-2.1812208927
C,0,0.0026966005,-0.0188201869,2.5223241597
C,0,0.2785974483,-1.4668541377,4.9142796951
C,0,0.6932942729,0.5339444603,3.6143566208
C,0,-0.5470836693,-1.3063469178,2.6434495134
C,0,-0.4106997592,-2.0239203666,3.8330048869
C,0,0.8301548494,-0.1869606367,4.8016007773
H,0,1.1475546329,1.5169027844,3.5307520438
H,0,-1.1053898181,-1.7409875989,1.8192604279
H,0,-0.8483941063,-3.0138336134,3.9159298623
H,0,1.3746449077,0.2481024689,5.6338952416
H,0,0.3860129876,-2.026745795,5.8381838262
C,0,0.0026966005,-0.0188201869,-2.5223241597
C,0,0.2785974483,-1.4668541377,-4.9142796951
C,0,-0.5470836693,-1.3063469178,-2.6434495134
C,0,0.6932942729,0.5339444603,-3.6143566208
C,0,0.8301548494,-0.1869606367,-4.8016007773
C,0,-0.4106997592,-2.0239203666,-3.8330048869

H,0,-1.1053898181,-1.7409875989,-1.8192604279
H,0,1.1475546329,1.5169027844,-3.5307520438
H,0,1.3746449077,0.2481024689,-5.6338952416
H,0,-0.8483941063,-3.0138336134,-3.9159298623
H,0,0.3860129876,-2.026745795,-5.8381838262
H,0,-1.4780059859,3.4346919255,0.
H,0,0.2015959352,3.6834728852,0.

E(RB3LYP) = -694.786528840 A.U.

Zero-point correction= 0.272053 (Hartree/Particle)
Thermal correction to Energy= 0.286302
Thermal correction to Enthalpy= 0.287246
Thermal correction to Gibbs Free Energy= 0.229839
Sum of electronic and zero-point Energies= -694.514476
Sum of electronic and thermal Energies= -694.500227
Sum of electronic and thermal Enthalpies= -694.499283
Sum of electronic and thermal Free Energies= -694.556689

2e: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.3374415818,1.1393712925,-0.0815226447
C,0,-1.1972939024,2.2754300282,-0.2203464672
C,0,0.2028392396,0.3211872386,-0.0372038456
C,0,1.2128067087,2.5264977178,-0.1935184336
C,0,-0.065420269,3.087479188,-0.2621789383
C,0,-1.086348609,0.8769853566,-0.1063965394
H,0,0.3081965818,-0.7545881189,0.0767650458
H,0,2.090304789,3.1663185145,-0.2278320252
H,0,-0.1744374148,4.1631000547,-0.3587589894
H,0,-2.1814575947,2.7258931339,-0.2978174958
C,0,2.7368608093,0.4816624285,0.0167537938
C,0,3.8601182929,-2.1157127438,0.2464191746
C,0,3.0952198019,-0.3303151264,-1.1655561811
C,0,2.9927810925,-0.1543863015,1.3260496601
C,0,3.5443618053,-1.4089173238,1.4268477247
C,0,3.6444843247,-1.5830635717,-1.0441872413
H,0,2.9135591548,0.1082009141,-2.1432265359
H,0,2.7328528414,0.4151694202,2.2143538925
H,0,3.7284333371,-1.8635068147,2.3944230813
H,0,3.904794414,-2.1678958577,-1.9199559718
H,0,4.2889745595,-3.1113959628,0.3341282562
C,0,-2.2901236215,0.0094781974,-0.0478025555
C,0,-4.5749287678,-1.6310229714,0.0703252202
C,0,-2.3353586631,-1.2103475658,-0.7458260994
C,0,-3.4105084798,0.3930661882,0.7103340423
C,0,-4.5417954913,-0.4213763212,0.76959169
C,0,-3.4688215621,-2.0221224743,-0.6891316205
H,0,-1.4949749264,-1.5094720691,-1.3663454876
H,0,-3.3879831284,1.3201881259,1.2755814983

H,0,-5.3949277677,-0.1134455822,1.3662650476
H,0,-3.4934568124,-2.9531856341,-1.247263531
H,0,-5.4569553552,-2.2622962987,0.1143073376
H,0,3.4449668313,1.341161549,-0.0167467421

E(RB3LYP) = -694.709998018 A.U.

Zero-point correction= 0.272246 (Hartree/Particle)
Thermal correction to Energy= 0.286506
Thermal correction to Enthalpy= 0.287451
Thermal correction to Gibbs Free Energy= 0.228900
Sum of electronic and zero-point Energies= -694.437752
Sum of electronic and thermal Energies= -694.423492
Sum of electronic and thermal Enthalpies= -694.422547
Sum of electronic and thermal Free Energies= -694.481098

2e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.3159970221,1.0986130987,-0.0567812066
C,0,-1.2101561777,2.2672655901,-0.2427332443
C,0,0.1670883057,0.3009135668,-0.0000466221
C,0,1.2029645268,2.4838620806,-0.2066332264
C,0,-0.0658518166,3.0622546002,-0.2986615957
C,0,-1.1133497387,0.8716775715,-0.0926976029
H,0,0.2628829293,-0.7721302277,0.1392207186
H,0,2.0908762066,3.107619197,-0.2508739229
H,0,-0.1595300569,4.136769705,-0.4212408225
H,0,-2.1874342821,2.7300380377,-0.3363673956
C,0,2.6956667002,0.4311656743,0.0501706805
C,0,4.0243685085,-2.0708785483,0.1873959551
C,0,3.1227513605,-0.3020660548,-1.162050651
C,0,2.9547672891,-0.2535259005,1.3345938477
C,0,3.6191286605,-1.4530521401,1.3894897343
C,0,3.7866113531,-1.5000928099,-1.0813100606
H,0,2.9209131212,0.161115237,-2.1232972677
H,0,2.6284001813,0.2464060775,2.2414794494
H,0,3.8225614839,-1.9349313474,2.3388299151
H,0,4.1140164921,-2.017768805,-1.9755201726
H,0,4.5405705959,-3.0254261046,0.2405861022
C,0,-2.3313569437,0.0200644936,-0.0307566896
C,0,-4.6448171687,-1.5910104168,0.0873006022
C,0,-2.3706969612,-1.232795296,-0.6692344566
C,0,-3.4741400715,0.450007944,0.6679752759
C,0,-4.6189275556,-0.3476566762,0.7267390989
C,0,-3.5158478254,-2.0300138453,-0.6112064592
H,0,-1.510179475,-1.5762769682,-1.2358806703
H,0,-3.4605644027,1.4041295017,1.1864028295
H,0,-5.4876520471,-0.0000807864,1.2781918792
H,0,-3.5285499155,-2.9896240156,-1.1198027345

H,0,-5.5354755788,-2.2106212357,0.1319890604
H,0,3.4291690803,1.2741874129,0.0852577722

E(RB3LYP) = -694.776794883 A.U.

Zero-point correction= 0.272706 (Hartree/Particle)
Thermal correction to Energy= 0.286847
Thermal correction to Enthalpy= 0.287791
Thermal correction to Gibbs Free Energy= 0.229819
Sum of electronic and zero-point Energies= -694.504089
Sum of electronic and thermal Energies= -694.489948
Sum of electronic and thermal Enthalpies= -694.489004
Sum of electronic and thermal Free Energies= -694.546976

2f: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.2139221923,0.7754970219,-0.0799985619
C,0,-1.2265066428,2.1579365714,-0.2520316938
C,0,-0.0247335305,0.0886951155,-0.0144542422
C,0,1.1890583442,2.1866111148,-0.2407215722
C,0,-0.0210845194,2.8604221169,-0.3237773217
C,0,-1.2498570056,0.7542207655,-0.0982321251
H,0,-0.0467960875,-0.9834204438,0.1406449964
H,0,2.1060279323,2.7562936069,-0.3235211088
H,0,-0.0310348732,3.9368622753,-0.4591888134
H,0,-2.1646350487,2.6971623059,-0.3381989053
C,0,2.4694590939,0.0571888778,0.0193288447
C,0,4.9599813972,-1.4322420214,0.1994009501
C,0,3.7125400628,0.7067204276,0.1172694017
C,0,2.4829686506,-1.4439239296,0.0219022474
C,0,3.7975145895,-2.1287189664,0.1148858611
C,0,4.9005190681,-0.0070167078,0.2023378397
H,0,3.7680337667,1.7870733262,0.1434362595
H,0,3.7908394997,-3.2150848553,0.1159390734
H,0,5.8303707702,0.5505452174,0.2803009144
H,0,5.9190788853,-1.9333630872,0.2686913269
C,0,-2.5345808642,0.0151492974,-0.0243612056
C,0,-4.9690624615,-1.3858550978,0.1248393748
C,0,-2.6948544115,-1.2157880332,-0.6848207722
C,0,-3.6160529789,0.5347985808,0.7086570454
C,0,-4.8217417094,-0.1628103298,0.784851231
C,0,-3.9031374299,-1.9093488088,-0.6120709572
H,0,-1.8859050403,-1.6147672786,-1.2908303257
H,0,-3.5073913284,1.4725524643,1.2460516237
H,0,-5.6436162724,0.2462835731,1.3641120842
H,0,-4.0167124757,-2.8505889274,-1.1410283483
H,0,-5.9094893171,-1.9250534492,0.1806307807
H,0,1.85041684,-1.8171923942,0.8445843631
H,0,1.9644089741,-1.8155810983,-0.8770745248

E(RB3LYP) = -694.734813628 A.U.

Zero-point correction= 0.272852 (Hartree/Particle)
Thermal correction to Energy= 0.287192
Thermal correction to Enthalpy= 0.288136
Thermal correction to Gibbs Free Energy= 0.228837
Sum of electronic and zero-point Energies= -694.461962
Sum of electronic and thermal Energies= -694.447622
Sum of electronic and thermal Enthalpies= -694.446678
Sum of electronic and thermal Free Energies= -694.505976

2f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.208623237,0.7636047182,-0.0896996173
C,0,-1.2248538439,2.1468544158,-0.3233043208
C,0,-0.0269096165,0.082263016,-0.0042091227
C,0,1.1928202775,2.1633828228,-0.3008238858
C,0,-0.0158715204,2.8392071295,-0.4178312922
C,0,-1.2489759261,0.7534477522,-0.1141208599
H,0,-0.0454880378,-0.9819609502,0.1977776659
H,0,2.1167353818,2.7176889474,-0.4111622356
H,0,-0.0193923556,3.9088290931,-0.5992974315
H,0,-2.1589942535,2.6883174923,-0.4325907516
C,0,2.4722440399,0.0448514883,0.0254606492
C,0,4.9660375025,-1.4149828083,0.2186392874
C,0,3.6762207713,0.6971093232,0.3093481656
C,0,2.5162315507,-1.4351556973,-0.1698069842
C,0,3.827410763,-2.1098045375,-0.0538870493
C,0,4.8740917294,-0.0087461394,0.4014744889
H,0,3.6964273233,1.7637767917,0.4914122796
H,0,3.8436849274,-3.1863248122,-0.192511797
H,0,5.7788814016,0.5455894006,0.6343910782
H,0,5.9264908173,-1.9095770754,0.3041506206
C,0,-2.5372939004,0.0186336622,-0.0059659042
C,0,-4.98000869,-1.3725310827,0.2042807646
C,0,-2.6950216475,-1.2501912661,-0.5918890262
C,0,-3.6264274295,0.5787309628,0.6855502159
C,0,-4.8357446651,-0.1112715643,0.7905155521
C,0,-3.9051804677,-1.939032216,-0.487825031
H,0,-1.8767726777,-1.6905813606,-1.1541823167
H,0,-3.5221137114,1.5478069991,1.1644499927
H,0,-5.6621536923,0.3341216721,1.3363605518
H,0,-4.0104027924,-2.9134842646,-0.9554962671
H,0,-5.9212061516,-1.9079740102,0.2846862468
H,0,1.8209685323,-1.9330422214,0.5268000058
H,0,2.0838911943,-1.6862984513,-1.1531399322

E(RB3LYP) = -694.796813235 A.U.

Zero-point correction= 0.273051 (Hartree/Particle)
Thermal correction to Energy= 0.287233
Thermal correction to Enthalpy= 0.288177
Thermal correction to Gibbs Free Energy= 0.230907
Sum of electronic and zero-point Energies= -694.523762
Sum of electronic and thermal Energies= -694.509580
Sum of electronic and thermal Enthalpies= -694.508636
Sum of electronic and thermal Free Energies= -694.565906

2g: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.1695544538,0.7487614346,0.1738377166
C,0,-1.2576417939,2.1077664468,0.4397662553
C,0,-0.0487790649,0.0624146749,0.044331188
C,0,1.1624018372,2.1290928814,0.437698976
C,0,-0.0530977791,2.7984031801,0.572726319
C,0,-1.2789166517,0.7265305588,0.1703994235
H,0,-0.0510110482,-0.9915061875,-0.219294352
H,0,2.0919663402,2.6741708806,0.5761886241
H,0,-0.0612620586,3.8596768668,0.7997985151
H,0,-2.1952758241,2.6391119795,0.5668358302
C,0,2.4515936288,0.0231798337,0.0212278692
C,0,5.0104683707,-1.2733219657,-0.3468601432
C,0,3.5631220566,0.6252405813,-0.6343218285
C,0,2.645033749,-1.2624191089,0.4983944739
C,0,3.9170006567,-1.9810654777,0.3328615067
C,0,4.818456978,0.003846252,-0.8089511185
H,0,3.4301048254,1.6258174304,-1.038472444
H,0,1.8451760396,-1.7732151809,1.0272144618
H,0,5.6109052071,0.5391626949,-1.3212190359
H,0,5.9599485843,-1.7846112177,-0.4776024737
C,0,-2.5614113103,-0.004944905,0.0078599479
C,0,-4.9948820305,-1.3862518619,-0.3054925198
C,0,-2.7347581088,-1.2882356106,0.5551701653
C,0,-3.6301873754,0.5747564504,-0.6979172355
C,0,-4.8351144159,-0.1111905704,-0.8545437808
C,0,-3.9413166691,-1.97215631,0.4013152776
H,0,-1.9351602426,-1.7401677619,1.1358163402
H,0,-3.5106816249,1.5553857296,-1.1492718636
H,0,-5.6465644371,0.3480739704,-1.4107312579
H,0,-4.0631565612,-2.9564356539,0.8433572669
H,0,-5.9338363879,-1.917847935,-0.4247195417
H,0,4.2660819727,-2.3482387755,1.3184625608
H,0,3.7268953345,-2.9435442534,-0.185058493

E(RB3LYP) = -694.719318409 A.U.

Zero-point correction= 0.271773 (Hartree/Particle)

Thermal correction to Energy= 0.286095
Thermal correction to Enthalpy= 0.287040
Thermal correction to Gibbs Free Energy= 0.229414
Sum of electronic and zero-point Energies= -694.447545
Sum of electronic and thermal Energies= -694.433223
Sum of electronic and thermal Enthalpies= -694.432279
Sum of electronic and thermal Free Energies= -694.489905

2g: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.172025687,0.7512387002,0.1722400071
C,0,-1.2599641887,2.1117317038,0.4451714071
C,0,-0.0459374691,0.0688984618,0.0326228489
C,0,1.1619776139,2.1281355855,0.4482758531
C,0,-0.0536954061,2.7989121707,0.5848587982
C,0,-1.2758811801,0.7334591305,0.1648750481
H,0,-0.0406112661,-0.9845548199,-0.2302422295
H,0,2.0929416974,2.6702417149,0.5837084259
H,0,-0.0603209867,3.8593496606,0.8166612869
H,0,-2.1965744574,2.644768894,0.5739999289
C,0,2.4579990061,0.0213350941,0.0212455565
C,0,4.998062481,-1.2829021007,-0.3462526274
C,0,3.5529445078,0.6074321366,-0.6706496835
C,0,2.6535096479,-1.2445101094,0.538820939
C,0,3.9219672253,-1.9637537095,0.379627721
C,0,4.8009501782,-0.0217062884,-0.8502086209
H,0,3.4177284585,1.5966879967,-1.0994070461
H,0,1.8646368853,-1.7407504739,1.0957979718
H,0,5.5837870014,0.4942900897,-1.3939662169
H,0,5.9434356738,-1.800157814,-0.4749328936
C,0,-2.5592482176,-0.000430096,-0.000508914
C,0,-4.9952251106,-1.3891543629,-0.317582458
C,0,-2.7179782139,-1.3029303976,0.5065575949
C,0,-3.6457709053,0.5928845302,-0.6687387645
C,0,-4.8511513446,-0.0944617832,-0.8258994542
C,0,-3.923461894,-1.9903848396,0.3496339915
H,0,-1.90247515,-1.7726832636,1.0486471376
H,0,-3.5411563409,1.5892744019,-1.0877294499
H,0,-5.6745927419,0.3792989182,-1.3522956773
H,0,-4.0276651122,-2.9919220344,0.7567454513
H,0,-5.9327378298,-1.9234390214,-0.4392384475
H,0,4.2901715996,-2.2874333048,1.3732231815
H,0,3.7279668018,-2.9505257004,-0.0862540362

E(RB3LYP) = -694.787342376 A.U.

Zero-point correction= 0.271948 (Hartree/Particle)
Thermal correction to Energy= 0.286234
Thermal correction to Enthalpy= 0.287178

Thermal correction to Gibbs Free Energy= 0.229596
Sum of electronic and zero-point Energies= -694.515395
Sum of electronic and thermal Energies= -694.501109
Sum of electronic and thermal Enthalpies= -694.500164
Sum of electronic and thermal Free Energies= -694.557747

2h: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.1970039251,0.7411163119,0.125873457
C,0,-1.2315800637,2.1239928262,0.3510826098
C,0,-0.0437438981,0.0576123985,0.0390447123
C,0,1.1838863872,2.1474463644,0.3280318884
C,0,-0.0224523789,2.8201774952,0.4499469375
C,0,-1.264888403,0.7291366266,0.136713825
H,0,-0.0625218775,-1.0037118385,-0.1780317673
H,0,2.1088081729,2.7001473859,0.440791516
H,0,-0.0297050964,3.8890159851,0.6362013838
H,0,-2.1667136134,2.6641238965,0.4613329899
C,0,2.4483697538,0.0243766339,0.0002495109
C,0,4.9532833228,-1.4083272403,-0.2494734981
C,0,3.6587199027,0.7092042116,-0.3701090492
C,0,2.5174738697,-1.3927067728,0.2417563842
C,0,3.6890687089,-2.0737112429,0.1335154404
C,0,4.8386599399,0.0455515022,-0.4956155889
H,0,3.6217135192,1.7680048125,-0.5931964955
H,0,1.6256346747,-1.9206023662,0.554744045
H,0,3.7182992293,-3.1395261415,0.3430276931
H,0,5.7336403529,0.5827016735,-0.7975247708
C,0,-2.5546451212,0.0048128462,0.0160236403
C,0,-4.9985177048,-1.3665946222,-0.2214623947
C,0,-2.7310622893,-1.2539333795,0.6169782507
C,0,-3.6239525106,0.5666623988,-0.7032950202
C,0,-4.8347156276,-0.1158905296,-0.8230039155
C,0,-3.9442383356,-1.9327909111,0.5004318667
H,0,-1.9309167172,-1.6884924101,1.2099029918
H,0,-3.5019250384,1.5268581808,-1.1964139161
H,0,-5.6471959729,0.3264647723,-1.3909220749
H,0,-4.0703166458,-2.8971105105,0.9828758366
H,0,-5.9424731879,-1.8948720285,-0.3114818741
H,0,5.7244504434,-1.5979625929,0.519801553
H,0,5.3841398197,-1.9061733658,-1.1377226468

E(RB3LYP) = -694.738408296 A.U.

Zero-point correction= 0.273042 (Hartree/Particle)
Thermal correction to Energy= 0.287182
Thermal correction to Enthalpy= 0.288126
Thermal correction to Gibbs Free Energy= 0.230969
Sum of electronic and zero-point Energies= -694.465367

Sum of electronic and thermal Energies= -694.451226
Sum of electronic and thermal Enthalpies= -694.450282
Sum of electronic and thermal Free Energies= -694.507439

2h: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.1952187023,0.7439269759,0.1280445426
C,0,-1.2320279377,2.1270453715,0.3659453138
C,0,-0.0406901097,0.0621660951,0.0334448692
C,0,1.1854049348,2.1433031778,0.3430416647
C,0,-0.0221205612,2.8180268145,0.4714215641
C,0,-1.2610717202,0.7366879718,0.1377304597
H,0,-0.0529706507,-0.9982785934,-0.1881927519
H,0,2.1124824821,2.6924962762,0.4555708928
H,0,-0.0260483301,3.8852510232,0.6660886808
H,0,-2.1651067287,2.6693746176,0.4803927995
C,0,2.4529533567,0.0199607138,0.000959854
C,0,4.9430515773,-1.4068549703,-0.241343778
C,0,3.6426193222,0.6970321909,-0.4249051837
C,0,2.5229089504,-1.3800324245,0.3016896421
C,0,3.6967737578,-2.0624916758,0.1950272561
C,0,4.8241882893,0.0305200562,-0.5465209054
H,0,3.5937015986,1.7456003927,-0.6896832492
H,0,1.6390234926,-1.894808567,0.6562545515
H,0,3.7374983518,-3.1179781423,0.4461826565
H,0,5.7117795038,0.5543116535,-0.888039851
C,0,-2.5515242218,0.0090327667,0.0090978792
C,0,-4.9977765155,-1.3684749793,-0.2398727589
C,0,-2.7189423021,-1.2668297577,0.5766271856
C,0,-3.6322896132,0.5831397037,-0.683888248
C,0,-4.8436159141,-0.1001505363,-0.8079794236
C,0,-3.9310998867,-1.9488709087,0.4533390924
H,0,-1.9071765618,-1.7183812441,1.1394310222
H,0,-3.5199052524,1.5580543747,-1.1489683247
H,0,-5.6636278188,0.3559703361,-1.3545786029
H,0,-4.0442179244,-2.9291631021,0.9066972817
H,0,-5.9404297542,-1.898880222,-0.3352161216
H,0,5.7331134308,-1.563832533,0.5160476871
H,0,5.3615115929,-1.9418724854,-1.1137721768

E(RB3LYP) = -694.799433541 A.U.

Zero-point correction= 0.272857 (Hartree/Particle)
Thermal correction to Energy= 0.287024
Thermal correction to Enthalpy= 0.287969
Thermal correction to Gibbs Free Energy= 0.230614
Sum of electronic and zero-point Energies= -694.526577
Sum of electronic and thermal Energies= -694.512409
Sum of electronic and thermal Enthalpies= -694.511465

Sum of electronic and thermal Free Energies= -694.568819

3a: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.4682303971,0.0588287407,-0.0192002012
C,0,-1.4697182463,-0.0070081508,0.0128327397
C,0,0.7609223552,1.1733065301,-0.3852493467
C,0,0.6884978514,-1.0831114826,0.3622915066
C,0,-0.7005457557,-1.1222990002,0.3723520479
C,0,-0.7202789465,1.2224740717,-0.3888736348
H,0,1.2783658233,2.0738701834,-0.7036011862
H,0,1.2211343207,-1.9723416352,0.6895895686
H,0,-1.1796566622,-2.0324611819,0.7116509768
C,0,2.9500371789,0.0083045689,0.0001751419
C,0,5.7568457241,-0.0775744973,0.0118606986
C,0,3.6302529802,-1.1450789148,-0.4278112629
C,0,3.6956873021,1.1162153482,0.4387742694
C,0,5.0895710185,1.071824505,0.4445602355
C,0,5.0246173354,-1.1848260066,-0.4248960087
H,0,3.0758966211,-2.0041748229,-0.7962461812
H,0,3.18771823,2.003582835,0.8061239758
H,0,5.653541173,1.9297516423,0.7966607943
H,0,5.5379355542,-2.0767922881,-0.7697099289
H,0,6.8417055061,-0.1110473982,0.0173678807
C,0,-2.9219916084,-0.0193841945,0.0197511247
C,0,-5.7409253683,-0.0550018055,0.0102779031
C,0,-3.6676144003,1.1862330951,-0.0211965278
C,0,-3.6381877257,-1.2441851647,0.0499752132
C,0,-5.0269193422,-1.2584346548,0.0404519328
C,0,-5.0556767557,1.1668334583,-0.0200488446
H,0,-3.1644874792,2.1467225604,-0.0272973812
H,0,-3.1093854615,-2.1900773181,0.0426767196
H,0,-5.5557374737,-2.2057207692,0.0502051696
H,0,-5.6081979813,2.1004312138,-0.036173616
H,0,-6.826359619,-0.0677520167,0.0096238424
H,0,-1.0532005294,1.5332240779,-1.3936319902
H,0,-1.030717556,2.073544201,0.2410777089

E(RB3LYP) = -694.736382036 A.U.

Zero-point correction= 0.272823 (Hartree/Particle)
Thermal correction to Energy= 0.287122
Thermal correction to Enthalpy= 0.288066
Thermal correction to Gibbs Free Energy= 0.230100
Sum of electronic and zero-point Energies= -694.463559
Sum of electronic and thermal Energies= -694.449260
Sum of electronic and thermal Enthalpies= -694.448316
Sum of electronic and thermal Free Energies= -694.506282

3a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.4624343235,0.057291163,-0.0023266476
C,0,-1.4652035793,-0.0060650392,0.0262014784
C,0,0.7581095784,1.176958939,-0.3564527628
C,0,0.6876150936,-1.085862748,0.3725321588
C,0,-0.7022955032,-1.1230809215,0.3837305972
C,0,-0.7186949436,1.226080432,-0.357588385
H,0,1.2710975931,2.0825981968,-0.6652023743
H,0,1.216146979,-1.9807251424,0.688513724
H,0,-1.1795752898,-2.0379196788,0.7104918648
C,0,2.9470456753,0.0074017293,0.0042893993
C,0,5.7581847541,-0.0772894898,-0.0077317588
C,0,3.625462182,-1.1397591745,-0.4424810296
C,0,3.6969323206,1.1098113591,0.4493904582
C,0,5.0920660325,1.0668850978,0.4423064921
C,0,5.0209693484,-1.1797909437,-0.4500347497
H,0,3.0668013525,-1.9954082084,-0.8108389076
H,0,3.1902559637,1.9941025858,0.8246164595
H,0,5.6573156467,1.9232082439,0.7971977964
H,0,5.530461083,-2.0693923326,-0.8074274882
H,0,6.8433748378,-0.1101814227,-0.0117554833
C,0,-2.9216084964,-0.0204978366,0.0205160517
C,0,-5.7405555769,-0.0571149315,-0.0089863747
C,0,-3.6650878497,1.1827277866,-0.0535919681
C,0,-3.6357470401,-1.2436085226,0.0721749092
C,0,-5.0256472355,-1.258488329,0.0539158459
C,0,-5.0545621459,1.1626776002,-0.0625803202
H,0,-3.1614028005,2.1417639867,-0.0844380173
H,0,-3.1072850134,-2.1888743702,0.0968326087
H,0,-5.5530002845,-2.206138852,0.0836379517
H,0,-5.6054295218,2.0962380088,-0.1072348472
H,0,-6.8258749528,-0.0703948051,-0.0176100545
H,0,-1.0495793027,1.5622094594,-1.3541887779
H,0,-1.0213647682,2.0685138901,0.288465491

E(RB3LYP) = -694.796501167 A.U.

Zero-point correction= 0.272844 (Hartree/Particle)
Thermal correction to Energy= 0.287152
Thermal correction to Enthalpy= 0.288096
Thermal correction to Gibbs Free Energy= 0.229727
Sum of electronic and zero-point Energies= -694.523657
Sum of electronic and thermal Energies= -694.509350
Sum of electronic and thermal Enthalpies= -694.508405
Sum of electronic and thermal Free Energies= -694.566774

3c: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.4199354483,0.4790982455,0.2197201038
C,0,-1.3807198994,0.1395243441,0.0679574633
C,0,0.8804104209,-0.6915533353,-0.3305685194
C,0,0.5637307759,1.4781593431,0.6930353385
C,0,-0.8178382739,1.3054986969,0.6185160975
C,0,-0.5009572004,-0.8529590402,-0.4054173947
H,0,1.5304900615,-1.4750252961,-0.7125725657
H,0,0.9637552613,2.3888401713,1.1318271342
H,0,-1.4673397909,2.0785016109,1.015958813
H,0,-0.9031694685,-1.7527142937,-0.8595487864
C,0,2.9554869734,0.6486284359,0.2950919593
C,0,5.2943409451,-0.8042679419,-0.3972263949
C,0,3.5989208428,0.7737308861,-1.0297773512
C,0,3.607065142,-0.29118212,1.2318747915
C,0,4.7427683996,-0.9845993527,0.8902782998
C,0,4.7344746593,0.0712101011,-1.3533836677
H,0,3.1390947664,1.4527858158,-1.7428645869
H,0,3.1531376577,-0.4096126132,2.2121869134
H,0,5.2112164499,-1.6712118944,1.5873074551
H,0,5.196700291,0.171882795,-2.3295717982
H,0,6.1892303345,-1.3624306316,-0.663202813
C,0,-2.8513947365,-0.0389262463,-0.0111231193
C,0,-5.6423660517,-0.376175674,-0.1553061189
C,0,-3.4363144295,-1.2948680618,0.2299790562
C,0,-3.690178836,1.0448233144,-0.3266722259
C,0,-5.0730307907,0.8763320339,-0.4004078099
C,0,-4.8197570178,-1.4607423611,0.161045176
H,0,-2.8107172281,-2.1397553779,0.5032012928
H,0,-3.25912763,2.0175639658,-0.5450386042
H,0,-5.7047746161,1.7212940671,-0.6567000478
H,0,-5.2554511213,-2.4345832569,0.3624491731
H,0,-6.7187425434,-0.5060103674,-0.210296826
H,0,3.0987086848,1.6487184975,0.7652646926

E(RB3LYP) = -694.710259650 A.U.

Zero-point correction= 0.272195 (Hartree/Particle)
Thermal correction to Energy= 0.286486
Thermal correction to Enthalpy= 0.287430
Thermal correction to Gibbs Free Energy= 0.228856
Sum of electronic and zero-point Energies= -694.438065
Sum of electronic and thermal Energies= -694.423774
Sum of electronic and thermal Enthalpies= -694.422830
Sum of electronic and thermal Free Energies= -694.481404

3c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.4085503532,0.4409209856,0.1537839483

C,0,-1.399621864,0.127091354,0.0477042495
C,0,0.8445845682,-0.6910438147,-0.4499664872
C,0,0.5671288682,1.4128092624,0.7037645821
C,0,-0.8182044685,1.2552947149,0.6519957013
C,0,-0.5400740482,-0.8419336519,-0.5019658186
H,0,1.4819821295,-1.4530769357,-0.8901748112
H,0,0.9862910335,2.2929580142,1.1829867329
H,0,-1.4509257188,2.0120646936,1.1045068623
H,0,-0.9563664794,-1.7141907543,-0.9958068224
C,0,2.9344407877,0.5898357429,0.2120386959
C,0,5.393964614,-0.7332631702,-0.2850131374
C,0,3.6029309846,0.6382105898,-1.1056159433
C,0,3.6005956413,-0.2464422274,1.2351802382
C,0,4.802755567,-0.8610550753,0.9900292939
C,0,4.804791029,0.0137182661,-1.3269399813
H,0,3.123256776,1.2190955524,-1.8875872043
H,0,3.1179044898,-0.3294078809,2.2042285256
H,0,5.2922238928,-1.453199559,1.7546612126
H,0,5.2964943705,0.0767795912,-2.2907766371
H,0,6.3410817804,-1.2315973992,-0.4722028093
C,0,-2.8762171748,-0.0369069977,-0.0099157593
C,0,-5.6788458287,-0.3473567633,-0.1137602024
C,0,-3.4685688378,-1.3008734929,0.1654092384
C,0,-3.716026363,1.0682569815,-0.2393375011
C,0,-5.1029640769,0.9145055107,-0.2911591293
C,0,-4.8556107184,-1.4544122944,0.1147347809
H,0,-2.8427804778,-2.1655771733,0.365623341
H,0,-3.2818788501,2.0505152887,-0.4005837663
H,0,-5.7325042712,1.779685512,-0.4777177848
H,0,-5.2928355758,-2.4377291854,0.2616370607
H,0,-6.7574579691,-0.4667079043,-0.1532599871
H,0,3.119493317,1.6230066799,0.5995144488

E(RB3LYP) = -694.777095403 A.U.

Zero-point correction= 0.272712 (Hartree/Particle)
Thermal correction to Energy= 0.286864
Thermal correction to Enthalpy= 0.287809
Thermal correction to Gibbs Free Energy= 0.229814
Sum of electronic and zero-point Energies= -694.504384
Sum of electronic and thermal Energies= -694.490231
Sum of electronic and thermal Enthalpies= -694.489287
Sum of electronic and thermal Free Energies= -694.547281

3d: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.3962310907,0.0438566694,0.0109973564
C,0,-1.4696639388,0.0159275022,0.005936536
C,0,0.6605834158,-1.1582180427,-0.1885071355

C,0,0.6358245262,1.232156592,0.2080317184
C,0,-0.7441199542,1.215978794,0.2032684422
C,0,-0.7190383139,-1.1712366884,-0.1884165447
H,0,1.1759378552,-2.09636783,-0.3595556346
H,0,1.12929165,2.1807750746,0.3800532502
H,0,-1.2790752867,2.1406850389,0.3874200548
H,0,-1.2351841675,-2.1062433834,-0.3744491769
C,0,2.8350347777,0.0512057745,0.0112436548
C,0,5.7431941157,0.0166087028,-0.0035672689
C,0,3.5932678356,1.2247758991,0.2091355448
C,0,3.6004632473,-1.2272352025,-0.2053450305
C,0,5.0871630629,-1.1530989925,-0.1994476509
C,0,4.9772659619,1.2067113772,0.2021042204
H,0,3.1007499744,2.1746308795,0.3710154081
H,0,5.6279442338,-2.0816639665,-0.3588516051
H,0,5.5059567807,2.143008217,0.3600216391
H,0,6.8264681968,0.0657152547,0.0003882963
C,0,-2.9384849302,0.0005123709,0.0007144075
C,0,-5.7536162413,-0.0276646938,-0.0076663834
C,0,-3.6512015333,-1.1433103224,0.422128412
C,0,-3.671353684,1.1297565408,-0.4253967887
C,0,-5.0629303765,1.1110900117,-0.43635314
C,0,-5.0429633452,-1.1524444495,0.4250426473
H,0,-3.1161445143,-2.014036263,0.7870342755
H,0,-3.1512733284,2.0107798413,-0.7871598613
H,0,-5.6104639136,1.9810563692,-0.7846326173
H,0,-5.5750597095,-2.0332257512,0.7700499545
H,0,-6.8390702766,-0.038492839,-0.0109437668
H,0,3.2970913924,-1.9705641007,0.5495678407
H,0,3.2881455169,-1.6875738142,-1.1566360445

E(RB3LYP) = -694.740831997 A.U.

Zero-point correction= 0.273293 (Hartree/Particle)
Thermal correction to Energy= 0.287567
Thermal correction to Enthalpy= 0.288511
Thermal correction to Gibbs Free Energy= 0.230367
Sum of electronic and zero-point Energies= -694.467539
Sum of electronic and thermal Energies= -694.453265
Sum of electronic and thermal Enthalpies= -694.452321
Sum of electronic and thermal Free Energies= -694.510465

3d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.3931141163,0.0454257443,0.0067539877
C,0,-1.4634207349,0.0151141174,0.0092895715
C,0,0.6647309316,-1.1459347836,-0.2418644272
C,0,0.6399492594,1.2208857781,0.2627804275
C,0,-0.7442508085,1.2027415478,0.2642478606

C,0,-0.7191057851,-1.1589791916,-0.2422976964
H,0,1.1820476319,-2.0728577724,-0.458479815
H,0,1.1346028159,2.1579951417,0.4857810968
H,0,-1.2790343103,2.1175566634,0.4938604035
H,0,-1.2342848469,-2.085614274,-0.4694462375
C,0,2.8427991633,0.0546210187,0.0024670777
C,0,5.7442854995,0.0170365421,0.0025541463
C,0,3.5921792808,1.2326322415,0.1470889548
C,0,3.6022379075,-1.2262657643,-0.1625103482
C,0,5.082769627,-1.1603474525,-0.1478789066
C,0,4.98148118,1.2110056075,0.1466872567
H,0,3.1018314075,2.1909273727,0.2538346125
H,0,5.6184402643,-2.0971445314,-0.2663186938
H,0,5.5092621652,2.153663803,0.2595359376
H,0,6.8270377096,0.0636678399,0.0114367021
C,0,-2.9412483261,0.000073627,0.0036214508
C,0,-5.7600808835,-0.0285368829,-0.0099638132
C,0,-3.653324255,-1.1404763649,0.4258519302
C,0,-3.6722126283,1.1260575171,-0.4254149547
C,0,-5.0666284386,1.1090469294,-0.4362520795
C,0,-5.0478518054,-1.1517610301,0.4233396199
H,0,-3.1161565442,-2.0120542324,0.7859505666
H,0,-3.1491345006,2.0081526651,-0.7806752265
H,0,-5.6116958258,1.9815064229,-0.7834399004
H,0,-5.5784156384,-2.035240529,0.7650906953
H,0,-6.8457507187,-0.0396523453,-0.0154746333
H,0,3.2863469482,-1.9483646723,0.6075936175
H,0,3.3004502619,-1.7210261828,-1.1005241734

E(RB3LYP) = -694.799696484 A.U.

Zero-point correction= 0.273091 (Hartree/Particle)
Thermal correction to Energy= 0.287360
Thermal correction to Enthalpy= 0.288304
Thermal correction to Gibbs Free Energy= 0.230197
Sum of electronic and zero-point Energies= -694.526605
Sum of electronic and thermal Energies= -694.512337
Sum of electronic and thermal Enthalpies= -694.511392

3e: *in silico*

Charge = 1 Multiplicity = 1
C,0,1.3637164418,0.0077683617,0.0098951915
C,0,-1.4779300881,0.0030285325,0.0038714414
C,0,0.6390451006,1.1070979179,0.5063082047
C,0,0.6450577837,-1.0938939156,-0.4895108606
C,0,-0.7452201433,-1.0911272115,-0.4973751217
C,0,-0.7508858909,1.0998864331,0.5076629132
H,0,1.1594253736,1.9560238535,0.9416755796
H,0,1.1679333059,-1.9429162649,-0.9221121196

H,0,-1.272465263,-1.9351430384,-0.9292560525
H,0,-1.2829544885,1.9420166956,0.9373890653
C,0,-2.9592371586,0.0002530262,0.0001064115
C,0,-5.7749139372,-0.0051184928,-0.006525803
C,0,-3.6800634191,1.1823708825,-0.2507964904
C,0,-3.6767413938,-1.1846815039,0.2472917751
C,0,-5.071286903,-1.1858843651,0.2471182022
C,0,-5.0745919774,1.1783154132,-0.2569279714
H,0,-3.1491729577,2.1032459364,-0.4732463858
H,0,-3.1434465856,-2.1035639207,0.4721951565
H,0,-5.6083549411,-2.1067593357,0.4525850209
H,0,-5.6142257838,2.097149869,-0.4648047699
H,0,-6.8604693322,-0.0071964844,-0.0091310696
C,0,2.840065288,0.0127662433,0.0076168893
C,0,5.73322789,-0.1186419866,0.004467301
C,0,3.5867947222,-1.1827346307,0.2238419322
C,0,3.5826970396,1.1627427715,-0.2089392092
C,0,5.0526953304,1.1657958297,-0.2083226363
C,0,4.9952550801,-1.2573176925,0.2096543086
H,0,3.0327511798,-2.0959355636,0.4256235419
H,0,3.0816436969,2.1072243336,-0.4017975197
H,0,5.4785203838,-2.21360961,0.3798868787
H,0,6.8191040911,-0.1404273307,0.0032861799
H,0,5.4221454948,1.6360883664,-1.141032622
H,0,5.4122896009,1.898383081,0.5432930983

E(RB3LYP) = -694.720641499 A.U.

Zero-point correction= 0.271822 (Hartree/Particle)
Thermal correction to Energy= 0.286135
Thermal correction to Enthalpy= 0.287079
Thermal correction to Gibbs Free Energy= 0.229509
Sum of electronic and zero-point Energies= -694.448820
Sum of electronic and thermal Energies= -694.434507
Sum of electronic and thermal Enthalpies= -694.433563
Sum of electronic and thermal Free Energies= -694.491132

3e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.3658117094,0.0041957994,-0.0001714918
C,0,-1.4735700891,0.0016057844,-0.0023040472
C,0,0.6446585157,1.0902550033,0.5238952655
C,0,0.6476164936,-1.0837773529,-0.5241576639
C,0,-0.7452073104,-1.0815758776,-0.5274560349
C,0,-0.7478480802,1.0862393344,0.5239219149
H,0,1.1699502821,1.9300331535,0.9692978211
H,0,1.1727564876,-1.9250029502,-0.9674317611
H,0,-1.2716356412,-1.9210235222,-0.970105971
H,0,-1.2765043287,1.924021755,0.9671009635

C,0,-2.9595021871,-0.0001837827,-0.0014325287
C,0,-5.7817761589,-0.0028673499,0.0022616375
C,0,-3.6825691509,1.1842609149,-0.2345806637
C,0,-3.679668042,-1.1860302378,0.2334242366
C,0,-5.0759423051,-1.1872455732,0.2357373995
C,0,-5.0788247837,1.1828379095,-0.2332206174
H,0,-3.1509533641,2.1083284291,-0.4409336882
H,0,-3.1457455134,-2.1090129438,0.4386632206
H,0,-5.6117232224,-2.1122388315,0.4279448803
H,0,-5.616874036,2.1068450966,-0.423842206
H,0,-6.867674003,-0.0038662528,0.0038646769
C,0,2.8496034754,0.0106421936,-0.0026789136
C,0,5.7277850762,-0.1125918884,0.0266489394
C,0,3.5872801367,-1.1777641563,0.2532516346
C,0,3.5833911625,1.1554180781,-0.2504989821
C,0,5.0500058018,1.1600328282,-0.2362337196
C,0,4.9943842997,-1.2487393437,0.2611529531
H,0,3.033436461,-2.087229719,0.4688178273
H,0,3.0850925968,2.0937131908,-0.473523959
H,0,5.478017613,-2.1970170831,0.465517663
H,0,6.8128469392,-0.12907513,0.0374806347
H,0,5.4309594937,1.6021585803,-1.1771523707
H,0,5.402829212,1.9198601441,0.4907334106

E(RB3LYP) = -694.787997892 A.U.

Zero-point correction= 0.271911 (Hartree/Particle)
Thermal correction to Energy= 0.286225
Thermal correction to Enthalpy= 0.287169
Thermal correction to Gibbs Free Energy= 0.229484
Sum of electronic and zero-point Energies= -694.516087
Sum of electronic and thermal Energies= -694.501773
Sum of electronic and thermal Enthalpies= -694.500829
Sum of electronic and thermal Free Energies= -694.558514

3f: *in silico*

Charge = 1 Multiplicity = 1
C,0,0.,0.,1.3873367505
C,0,0.,0.,-1.4768034458
C,0,0.3099005097,1.1733036302,0.6402342389
C,0,-0.3099005097,-1.1733036302,0.6402342389
C,0,-0.3175919227,-1.1681926796,-0.7389839689
C,0,0.3175919227,1.1681926796,-0.7389839689
H,0,0.6003705459,2.0852766115,1.1477222228
H,0,-0.6003705459,-2.0852766115,1.1477222228
H,0,-0.6103890281,-2.0698429793,-1.2645652713
H,0,0.6103890281,2.0698429793,-1.2645652713
C,0,0.,0.,2.8253560647
C,0,0.,0.,5.7334081923
C,0,0.0100029945,-1.2335871649,3.5732476454

C,0,-0.0100029945,1.2335871649,3.5732476454
C,0,-0.0152976798,1.2449192461,4.9307448653
C,0,0.0152976798,-1.2449192461,4.9307448653
H,0,0.050800642,-2.1764391738,3.0431553708
H,0,-0.050800642,2.1764391738,3.0431553708
H,0,-0.0429487016,2.1918487226,5.4628859477
H,0,0.0429487016,-2.1918487226,5.4628859477
C,0,0.,0.,-2.9452888465
C,0,0.,0.,-5.7606073412
C,0,-0.2959965839,1.176372152,-3.6683153669
C,0,0.2959965839,-1.176372152,-3.6683153669
C,0,0.3036929494,-1.1723395696,-5.0599644468
C,0,-0.3036929494,1.1723395696,-5.0599644468
H,0,-0.5602453695,2.0872990701,-3.1412768634
H,0,0.5602453695,-2.0872990701,-3.1412768634
H,0,0.5517727527,-2.0805972583,-5.5997902545
H,0,-0.5517727527,2.0805972583,-5.5997902545
H,0,0.,0.,-6.8461149516
H,0,0.8612326582,0.0105924401,6.4258467297
H,0,-0.8612326582,-0.0105924401,6.4258467297

E(RB3LYP) = -694.744779804 A.U.

Zero-point correction= 0.273417 (Hartree/Particle)
Thermal correction to Energy= 0.287558
Thermal correction to Enthalpy= 0.288503
Thermal correction to Gibbs Free Energy= 0.231929
Sum of electronic and zero-point Energies= -694.471363
Sum of electronic and thermal Energies= -694.457221
Sum of electronic and thermal Enthalpies= -694.456277
Sum of electronic and thermal Free Energies= -694.512851

3f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.,0.,1.3842317886
C,0,0.,0.,-1.4678951002
C,0,0.3565055077,1.15893428,0.6464224716
C,0,-0.3565055077,-1.15893428,0.6464224716
C,0,-0.3661641477,-1.152521578,-0.7371806451
C,0,0.3661641477,1.152521578,-0.7371806451
H,0,0.6784026949,2.0575256163,1.1586436732
H,0,-0.6784026949,-2.0575256163,1.1586436732
H,0,-0.6908912497,-2.0432068486,-1.2631995804
H,0,0.6908912497,2.0432068486,-1.2631995804
C,0,0.,0.,2.8325257076
C,0,0.,0.,5.722521236
C,0,0.0432827331,-1.2333039459,3.5683328932
C,0,-0.0432827331,1.2333039459,3.5683328932
C,0,-0.0483390855,1.2436565405,4.9285769904

C,0,0.0483390855,-1.2436565405,4.9285769904
H,0,0.1090026425,-2.17200374,3.0336119029
H,0,-0.1090026425,2.17200374,3.0336119029
H,0,-0.1003946225,2.1868999983,5.4638379114
H,0,0.1003946225,-2.1868999983,5.4638379114
C,0,0.,0.,-2.9455150039
C,0,0.,0.,-5.7640515246
C,0,-0.3111920847,1.1700643593,-3.6668959428
C,0,0.3111920847,-1.1700643593,-3.6668959428
C,0,0.3160727022,-1.1674633878,-5.061356919
C,0,-0.3160727022,1.1674633878,-5.061356919
H,0,-0.5803193706,2.0781420006,-3.1371111516
H,0,0.5803193706,-2.0781420006,-3.1371111516
H,0,0.5720628285,-2.0751369854,-5.5992874027
H,0,-0.5720628285,2.0751369854,-5.5992874027
H,0,0.,0.,-6.8497839286
H,0,0.8573081107,0.033767929,6.4191732715
H,0,-0.8573081107,-0.033767929,6.4191732715

E(RB3LYP) = -694.802596732 A.U.

Zero-point correction= 0.273052 (Hartree/Particle)
Thermal correction to Energy= 0.287215
Thermal correction to Enthalpy= 0.288160
Thermal correction to Gibbs Free Energy= 0.231538
Sum of electronic and zero-point Energies= -694.529545
Sum of electronic and thermal Energies= -694.515381
Sum of electronic and thermal Enthalpies= -694.514437
Sum of electronic and thermal Free Energies= -694.571059

V. Triphenylbenzene Rearrangement

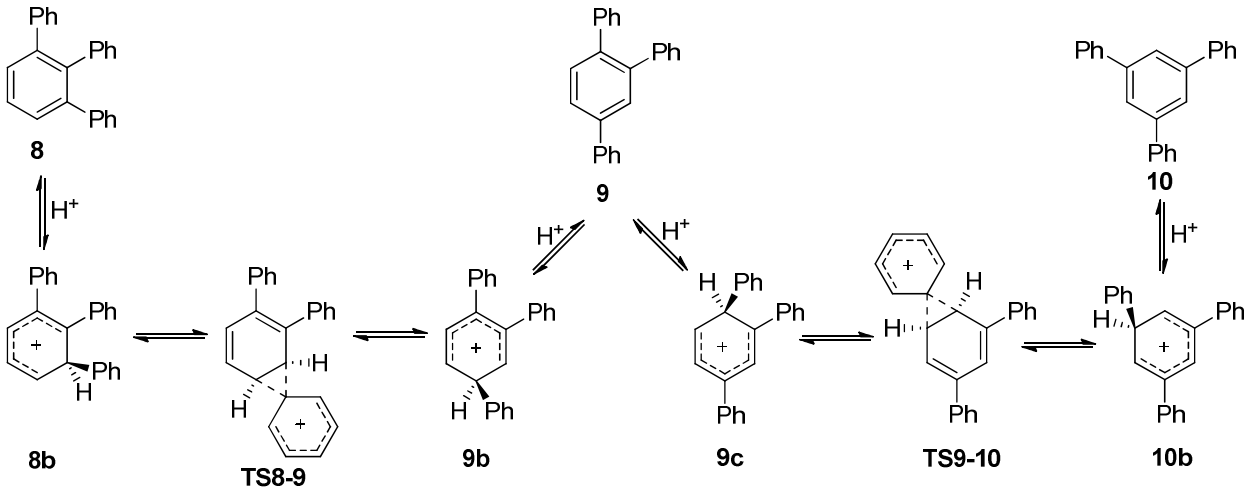

Figure S10. Rearrangement of triphenylbenzene isomers

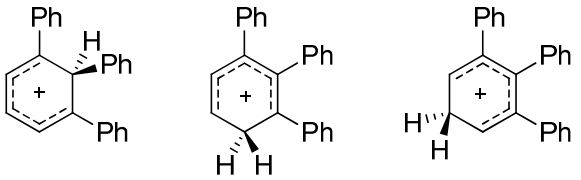

Figure S11. 1,2,3-Triphenylbenzene cations

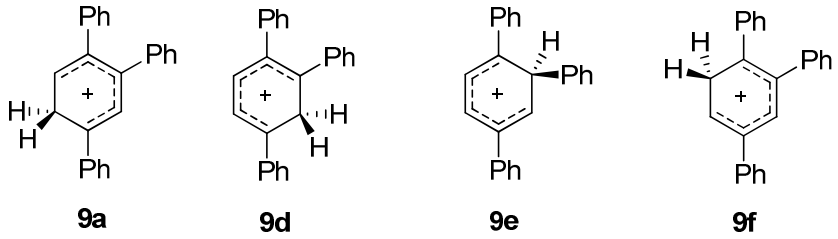

Figure S12. 1,2,4-Triphenylbenzene cations

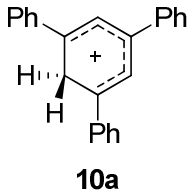

Figure S13. 1,3,5-Triphenylbenzene cation

8: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
H,0,2.145534583,0.0020190313,3.3235681215
C,0,1.2032636289,-0.0088229292,2.7838741596
C,0,-1.2234497093,-0.003157521,1.3793075536
C,0,1.2234497093,0.003157521,1.3793075536
C,0,0.,0.,3.4856664354
C,0,-1.2032636289,0.0088229292,2.7838741596
C,0,0.,0.,0.6614548906
H,0,0.,0.,4.5717014946
H,0,-2.145534583,-0.0020190313,3.3235681215
C,0,2.5605895497,0.0480049379,0.7097199481
C,0,5.132404066,0.1574282269,-0.4478822521
C,0,3.5200295584,-0.9399698395,0.9897264218
C,0,2.9165234866,1.0975844018,-0.1545347695
C,0,4.1895825387,1.1527152199,-0.7263952558
C,0,4.7928129089,-0.8895896927,0.4136591789

H,0,3.2623447186,-1.7602924754,1.6540005459
H,0,2.1952055712,1.8781541433,-0.3745526989
H,0,4.4456768912,1.9758024392,-1.387592605
H,0,5.5158249462,-1.6689330281,0.6374420751
H,0,6.1210309766,0.199623163,-0.8956930276
C,0,0.,0.,-0.8371948496
C,0,0.,0.,-3.6576431182
C,0,0.5263229185,-1.0854947342,-1.5557908511
C,0,-0.5263229185,1.0854947342,-1.5557908511
C,0,-0.5238547264,1.0884970315,-2.9530208919
C,0,0.5238547264,-1.0884970315,-2.9530208919
H,0,0.9369469978,-1.9345130033,-1.016965022
H,0,-0.9369469978,1.9345130033,-1.016965022
H,0,-0.9319955429,1.9402792425,-3.489806266
H,0,0.9319955429,-1.9402792425,-3.489806266
H,0,0.,0.,-4.7438076111
C,0,-2.5605895497,-0.0480049379,0.7097199481
C,0,-5.132404066,-0.1574282269,-0.4478822521
C,0,-2.9165234866,-1.0975844018,-0.1545347695
C,0,-3.5200295584,0.9399698395,0.9897264218
C,0,-4.7928129089,0.8895896927,0.4136591789
C,0,-4.1895825387,-1.1527152199,-0.7263952558
H,0,-2.1952055712,-1.8781541433,-0.3745526989
H,0,-3.2623447186,1.7602924754,1.6540005459
H,0,-5.5158249462,1.6689330281,0.6374420751
H,0,-4.4456768912,-1.9758024392,-1.387592605
H,0,-6.1210309766,-0.199623163,-0.8956930276

E(RB3LYP) = -925.473379418 A.U.

Zero-point correction= 0.342118 (Hartree/Particle)
Thermal correction to Energy= 0.360673
Thermal correction to Enthalpy= 0.361618
Thermal correction to Gibbs Free Energy= 0.294364
Sum of electronic and zero-point Energies= -925.131261
Sum of electronic and thermal Energies= -925.112706
Sum of electronic and thermal Enthalpies= -925.111762
Sum of electronic and thermal Free Energies= -925.179016

9: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,0.7684686139,-1.0627911085,-0.0456591011
C,0,-2.043821458,-0.5957542506,-0.0259368761
C,0,0.2666547396,0.2613493994,0.0175382351
C,0,-0.1560743171,-2.1217673877,-0.0737536385
C,0,-1.5310334013,-1.9027563012,-0.0631453495
C,0,-1.1231834348,0.4625583058,0.0176426718
H,0,0.2167337414,-3.1394934484,-0.1437975234
H,0,-2.2056554764,-2.7516110088,-0.1185333902

H,0,-1.4928676972,1.4796617634,0.1046398208
C,0,2.2220767244,-1.3916854352,-0.1259971754
C,0,4.9463020516,-2.1032972416,-0.3224737687
C,0,2.7868827158,-2.3325493023,0.7527335205
C,0,3.0470280837,-0.8188012753,-1.1101124018
C,0,4.3942593573,-1.1721694729,-1.2089065093
C,0,4.1368163969,-2.682801212,0.6589077985
H,0,2.1674846268,-2.7813894911,1.5242955179
H,0,2.6276328067,-0.100016632,-1.8071963328
H,0,5.0122076005,-0.7223045147,-1.9808645225
H,0,4.5545348654,-3.4054802028,1.3541889113
H,0,5.9951614844,-2.3751331005,-0.3977345836
C,0,1.1435382067,1.4649822242,0.1394380833
C,0,2.7168841684,3.7913443197,0.4172620158
C,0,2.105053616,1.5660593388,1.1600396162
C,0,0.9821944103,2.5531013761,-0.7355714979
C,0,1.7634010641,3.7044655894,-0.6012483622
C,0,2.882158214,2.7178691394,1.2991497108
H,0,2.237627698,0.7418450483,1.854055893
H,0,0.2494653044,2.490985644,-1.5353543527
H,0,1.6278925342,4.5301990543,-1.2940310884
H,0,3.6144615166,2.7781967825,2.0993072777
H,0,3.3238610404,4.6856544968,0.5242371969
C,0,-3.5083830439,-0.3390282383,-0.0209017469
C,0,-6.2922753475,0.1451434294,-0.0150270307
C,0,-4.0540929621,0.7550235605,-0.7179444173
C,0,-4.3884675681,-1.1850447873,0.6793260528
C,0,-5.7645291876,-0.9463732757,0.6819934228
C,0,-5.429887745,0.9951210259,-0.714651002
H,0,-3.3998435904,1.4110058652,-1.284579117
H,0,-3.9920216499,-2.0238609124,1.2438151962
H,0,-6.4231185309,-1.6091425802,1.2361342404
H,0,-5.8282239443,1.8418582925,-1.2664147261
H,0,-7.3622631269,0.3310525136,-0.0129930377

E(RB3LYP) = -925.480623290 A.U.

Zero-point correction= 0.342531 (Hartree/Particle)
Thermal correction to Energy= 0.360974
Thermal correction to Enthalpy= 0.361918
Thermal correction to Gibbs Free Energy= 0.294283
Sum of electronic and zero-point Energies= -925.138092
Sum of electronic and thermal Energies= -925.119650
Sum of electronic and thermal Enthalpies= -925.118706
Sum of electronic and thermal Free Energies= -925.186341

10: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
H,0,0.,0.,2.4807921994

C,0,0.,0.,1.3955319452
C,0,0.,0.,-1.4117395835
C,0,-1.2239141217,0.0111469318,0.7083272681
C,0,1.2239141217,-0.0111469318,0.7083272681
C,0,1.20726064,-0.0102036893,-0.6954331819
C,0,-1.20726064,0.0102036893,-0.6954331819
H,0,2.1458741498,-0.0634745487,-1.2377383023
H,0,-2.1458741498,0.0634745487,-1.2377383023
C,0,-2.5131256028,0.0436113812,1.452181678
C,0,-4.9614445995,0.1070876129,2.8597367848
C,0,-2.6550424389,0.813669847,2.6211482423
C,0,-3.6239850183,-0.6944576045,1.0039820757
C,0,-4.8348410033,-0.6631002019,1.6994225262
C,0,-3.865416005,0.8451321558,3.3174744915
H,0,-1.81983729,1.4102249128,2.975991847
H,0,-3.5340294036,-1.3133873942,0.1161557007
H,0,-5.6766174382,-1.247083147,1.3382922387
H,0,-3.9538747952,1.4536833943,4.2129542685
H,0,-5.9028642794,0.1318943835,3.4006431997
C,0,2.5131256028,-0.0436113812,1.452181678
C,0,4.9614445995,-0.1070876129,2.8597367848
C,0,3.6239850183,0.6944576045,1.0039820757
C,0,2.6550424389,-0.813669847,2.6211482423
C,0,3.865416005,-0.8451321558,3.3174744915
C,0,4.8348410033,0.6631002019,1.6994225262
H,0,3.5340294036,1.3133873942,0.1161557007
H,0,1.81983729,-1.4102249128,2.975991847
H,0,3.9538747952,-1.4536833943,4.2129542685
H,0,5.6766174382,1.247083147,1.3382922387
H,0,5.9028642794,-0.1318943835,3.4006431997
C,0,0.,0.,-2.90012568
C,0,0.,0.,-5.7246884737
C,0,-0.9345837014,-0.7640542592,-3.6227872829
C,0,0.9345837014,0.7640542592,-3.6227872829
C,0,0.9348358559,0.7644787937,-5.0195102694
C,0,-0.9348358559,-0.7644787937,-5.0195102694
H,0,-1.6522299955,-1.3795564457,-3.0884111569
H,0,1.6522299955,1.3795564457,-3.0884111569
H,0,1.6607278728,1.3687518947,-5.556143664
H,0,-1.6607278728,-1.3687518947,-5.556143664
H,0,0.,0.,-6.8107110421

E(RB3LYP) = -925.486530110 A.U.

Zero-point correction= 0.342700 (Hartree/Particle)
Thermal correction to Energy= 0.361150
Thermal correction to Enthalpy= 0.362094
Thermal correction to Gibbs Free Energy= 0.294753
Sum of electronic and zero-point Energies= -925.143830
Sum of electronic and thermal Energies= -925.125380
Sum of electronic and thermal Enthalpies= -925.124436

Sum of electronic and thermal Free Energies= -925.191777

8b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-1.3664962776,3.177442462,0.9837922892
C,0,-0.6115000468,2.4065225035,1.1112343661
C,0,1.4417308712,0.4833631348,1.2293392357
C,0,-0.9033005624,1.1265126293,0.6003588548
C,0,0.5885925726,2.7588498828,1.7714213149
C,0,1.589744264,1.8384229795,1.8241719298
C,0,0.0599846268,0.107247977,0.750583474
H,0,0.712723331,3.7595755021,2.1685622105
H,0,2.5631351671,2.0827689938,2.2374990197
C,0,-2.2146402491,0.9545748517,-0.0952557968
C,0,-4.6702216535,0.7490621126,-1.4486013685
C,0,-2.2689786212,0.4299888847,-1.3976966366
C,0,-3.404458293,1.3827000641,0.5164390387
C,0,-4.6251037055,1.2747372902,-0.1544639856
C,0,-3.4881416854,0.3310595323,-2.0689474526
H,0,-1.3570135241,0.1077881986,-1.890559127
H,0,-3.3816440012,1.7813643214,1.5270232419
H,0,-5.5377267382,1.5995283571,0.3357939421
H,0,-3.5138124927,-0.0686296661,-3.0780951565
H,0,-5.6182754708,0.667905676,-1.971398497
C,0,-0.2352542596,-1.3120438544,0.5370351894
C,0,-0.8057126477,-4.0644803197,0.2979111516
C,0,0.7426607235,-2.2186884166,0.0634309356
C,0,-1.5022830167,-1.829218727,0.9040207287
C,0,-1.7745919821,-3.1889539395,0.7999078101
C,0,0.450822276,-3.5721953869,-0.0727537585
H,0,1.7202614299,-1.8617965613,-0.2327810825
H,0,-2.2595803483,-1.1698364594,1.3082150271
H,0,-2.7437631864,-3.5658898227,1.1101629118
H,0,1.206308458,-4.245187492,-0.4650781458
H,0,-1.0255848761,-5.1231741433,0.2020013888
C,0,2.5484984821,0.4237191485,0.1253736775
C,0,4.6001816597,0.4050644099,-1.7791016052
C,0,2.3420025748,1.0038427086,-1.1320030839
C,0,3.7880696314,-0.1490121269,0.4356045649
C,0,4.8096066419,-0.15965272,-0.5178787421
C,0,3.3657257678,0.9863318044,-2.0827239923
H,0,1.390838468,1.4644870962,-1.3796933911
H,0,3.9554669973,-0.5938397461,1.4122542129
H,0,5.7649108908,-0.6133902654,-0.2726896623
H,0,3.195608725,1.4301130694,-3.058730617
H,0,5.3934517897,0.3929454447,-2.5199806478
H,0,1.7393447196,-0.2512656681,1.9886897737

E(RB3LYP) = -925.842840752 A.U.

Zero-point correction= 0.353958 (Hartree/Particle)
Thermal correction to Energy= 0.372802
Thermal correction to Enthalpy= 0.373747
Thermal correction to Gibbs Free Energy= 0.305091
Sum of electronic and zero-point Energies= -925.488883
Sum of electronic and thermal Energies= -925.470038
Sum of electronic and thermal Enthalpies= -925.469094
Sum of electronic and thermal Free Energies= -925.537750

TS8-9: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-0.6734584025,3.2200431858,0.8499385485
C,0,-0.0833139216,2.3194639117,0.9844225224
C,0,1.3831314945,-0.0403419861,1.3024048625
C,0,-0.6709842462,1.0662388325,0.5658596903
C,0,1.1601112987,2.414602712,1.5355567535
C,0,1.9497202707,1.2239155718,1.7042769159
C,0,0.0330215904,-0.1158146218,0.757093939
H,0,1.5615963439,3.3662097912,1.8643796189
C,0,-2.0178740812,1.1345700651,-0.0655783865
C,0,-4.5342275539,1.3560445368,-1.3025918355
C,0,-2.2590963247,0.5242774237,-1.3088817484
C,0,-3.0522082683,1.865880601,0.5437479981
C,0,-4.3045940546,1.9664142793,-0.0659692094
C,0,-3.5057762053,0.6402657829,-1.9243898164
H,0,-1.4666326669,-0.0325954978,-1.798409262
H,0,-2.8862575247,2.339330448,1.507277892
H,0,-5.0979793079,2.5219424821,0.4247131026
H,0,-3.6734498711,0.1722911654,-2.8897260066
H,0,-5.5056804112,1.4402133142,-1.7801885202
C,0,-0.5048984806,-1.4811807299,0.5287123652
C,0,-1.4635995079,-4.1044431402,0.1693814046
C,0,0.2855889372,-2.4535425351,-0.1110291779
C,0,-1.7785978048,-1.8501476907,0.9999262977
C,0,-2.2502322066,-3.1505694017,0.8245423152
C,0,-0.1947459025,-3.7514318418,-0.2979989006
H,0,1.2713774848,-2.1933730819,-0.4848965485
H,0,-2.3940809667,-1.1216683013,1.5165392366
H,0,-3.2314740881,-3.4199970769,1.2033112247
H,0,0.423576038,-4.4844839237,-0.8070877925
H,0,-1.8349082597,-5.115157719,0.0299725283
C,0,2.6697179493,0.5153606731,0.2595717639
C,0,4.5551342003,0.3326029911,-1.7844349387
C,0,2.3771276993,1.0517895858,-1.0100387874
C,0,3.9129127087,-0.1066250674,0.50150442
C,0,4.8490232594,-0.1961737486,-0.523642221
C,0,3.3203683112,0.9552460521,-2.0228353008
H,0,1.4273908393,1.5375298805,-1.2016932837

H,0,4.1415525885,-0.5130827781,1.481795873
H,0,5.8038745111,-0.675540156,-0.3371140084
H,0,3.0969393353,1.3661846788,-3.0014994784
H,0,5.28612242,0.2631940359,-2.5834771806
H,0,1.7756441913,-0.9498148056,1.7410950619
H,0,2.7696040052,1.2434854929,2.4119027488

E(RB3LYP) = -925.827445549 A.U.

Imaginary Frequency = -243.2180

Zero-point correction= 0.353149 (Hartree/Particle)
Thermal correction to Energy= 0.371463
Thermal correction to Enthalpy= 0.372407
Thermal correction to Gibbs Free Energy= 0.305688
Sum of electronic and zero-point Energies= -925.474297
Sum of electronic and thermal Energies= -925.455983
Sum of electronic and thermal Enthalpies= -925.455039
Sum of electronic and thermal Free Energies= -925.521757

9b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.6870118787,-1.0243859264,0.3857493628
C,0,-2.0820722835,-0.4788513262,1.0411320537
C,0,0.236781725,0.3487433107,0.4754521321
C,0,-0.2249052103,-2.0874929726,0.6917844395
C,0,-1.5353327583,-1.8520044718,0.9705171132
C,0,-1.0816175861,0.5806460984,0.7749277475
H,0,0.1272154301,-3.1091316489,0.6144580852
H,0,-2.2180340345,-2.6789656533,1.1407161937
H,0,-1.4292652227,1.6055242525,0.8673708069
C,0,2.0368880258,-1.3970275419,-0.0299660802
C,0,4.590459353,-2.2156673255,-0.8745712309
C,0,2.6753007117,-2.5102099335,0.5695532306
C,0,2.7080829998,-0.707726236,-1.0679773693
C,0,3.9605816582,-1.13161495,-1.497867951
C,0,3.9487668655,-2.8966339709,0.1667314623
H,0,2.1935375533,-3.0389375062,1.3848201915
H,0,2.2313141451,0.1292077313,-1.5624008505
H,0,4.4501655268,-0.6136102274,-2.3159040045
H,0,4.4392877192,-3.7299272059,0.6588176068
H,0,5.5774771523,-2.5290600207,-1.2000608159
C,0,1.1442280907,1.5272400851,0.3195288591
C,0,2.763691309,3.8122880831,0.1049978625
C,0,2.2566501891,1.6911429776,1.1611124085
C,0,0.8473483723,2.5230869887,-0.6237878221
C,0,1.6562820928,3.6575643867,-0.7330495267
C,0,3.0585638429,2.8284809634,1.0550272407
H,0,2.4895904097,0.9363201321,1.9062509063

H,0,-0.008511302,2.4036942001,-1.2820348913
H,0,1.420182075,4.4164967446,-1.4727324832
H,0,3.9116246409,2.9472469515,1.7161295058
H,0,3.3915546917,4.6941124715,0.0212278722
C,0,-3.3906931902,-0.2928559935,0.2502640289
C,0,-5.7632747381,0.0370553808,-1.203061462
C,0,-4.592950221,-0.0330170671,0.9171912823
C,0,-3.3781649007,-0.3861762597,-1.1488300438
C,0,-4.5620241297,-0.2219760203,-1.8712158091
C,0,-5.7765720931,0.1313409179,0.1908423851
H,0,-4.6098606272,0.0417069371,2.0009552417
H,0,-2.4492854592,-0.5865377473,-1.6761465517
H,0,-4.5444723985,-0.2960283152,-2.9542776058
H,0,-6.7050360676,0.3324680038,0.7164423003
H,0,-6.6825334065,0.1647325501,-1.7663937986
H,0,-2.3592923792,-0.3366762467,2.1066922075

E(RB3LYP) = -925.851115070 A.U.

Zero-point correction= 0.353897 (Hartree/Particle)
Thermal correction to Energy= 0.372662
Thermal correction to Enthalpy= 0.373606
Thermal correction to Gibbs Free Energy= 0.304874
Sum of electronic and zero-point Energies= -925.497218
Sum of electronic and thermal Energies= -925.478453
Sum of electronic and thermal Enthalpies= -925.477509
Sum of electronic and thermal Free Energies= -925.546242

9c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.8547364673,-0.7464543759,1.1171784315
C,0,1.9342252753,-0.2878688129,0.4733318621
C,0,-0.3891206049,0.5210640271,0.4494725955
C,0,0.2344745377,-1.7045310495,1.4583170591
C,0,1.5347482736,-1.4975432221,1.137986017
C,0,0.9518185251,0.6854926539,0.1614880495
H,0,-0.0632781236,-2.6053419368,1.9863614393
H,0,2.2819794467,-2.2267284574,1.4245332818
H,0,1.271158111,1.599070652,-0.3223771633
C,0,-1.9449068226,-1.4985837827,0.3214384067
C,0,-3.8878373429,-2.9367041167,-1.0993674576
C,0,-1.7393936683,-1.8186521809,-1.0274524668
C,0,-3.1212977714,-1.911225372,0.9576758241
C,0,-4.0903419751,-2.6269360056,0.2480338442
C,0,-2.7101301922,-2.5309703624,-1.73506763
H,0,-0.8272030373,-1.5106815149,-1.5305181864
H,0,-3.2879536673,-1.673297874,2.0047280398
H,0,-5.0018883145,-2.9374691774,0.7495256104
H,0,-2.5443426537,-2.768929452,-2.7813822529

H,0,-4.641840873,-3.4899247831,-1.6508210665
C,0,-1.3658421073,1.5601131436,0.1105943064
C,0,-3.2273888385,3.5737612406,-0.5368928878
C,0,-1.1546106037,2.4139581406,-0.9966209613
C,0,-2.5375473229,1.7378208191,0.8795932347
C,0,-3.4507862791,2.7399484882,0.564048738
C,0,-2.0791313672,3.4030064691,-1.3185582524
H,0,-0.287379413,2.2749477226,-1.6328711742
H,0,-2.7214539564,1.1180458684,1.7495282213
H,0,-4.3353364117,2.8727771736,1.1785311008
H,0,-1.9086828525,4.0361673536,-2.1833478257
H,0,-3.9441973384,4.3501731211,-0.7853909013
C,0,3.3383538952,-0.0577712142,0.1439968046
C,0,6.0424558487,0.3705106536,-0.5091935342
C,0,3.853888978,1.2546160587,0.0168502699
C,0,4.2160887903,-1.1493337069,-0.0610983782
C,0,5.548285212,-0.9343260491,-0.3975019962
C,0,5.1930282721,1.462611823,-0.294000615
H,0,3.2192732448,2.1130139598,0.2048292113
H,0,3.847846265,-2.1668939448,-0.0000092782
H,0,6.2019983418,-1.7821707915,-0.573638237
H,0,5.5774753328,2.4746886149,-0.3655543465
H,0,7.0854190502,0.53593556,-0.7606233626
H,0,-1.3181187353,-0.4637838009,2.0769442759

E(RB3LYP) = -925.865209803 A.U.

Zero-point correction= 0.354491 (Hartree/Particle)
Thermal correction to Energy= 0.373275
Thermal correction to Enthalpy= 0.374219
Thermal correction to Gibbs Free Energy= 0.305318
Sum of electronic and zero-point Energies= -925.510719
Sum of electronic and thermal Energies= -925.491935
Sum of electronic and thermal Enthalpies= -925.490991
Sum of electronic and thermal Free Energies= -925.559892

TS9-10: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.1248786694,-0.3886481752,1.2875046078
C,0,1.6005821703,-0.0411208184,0.5310039369
C,0,-0.7529737,0.7662102653,0.506841376
C,0,-0.1352075852,-1.3835158401,1.6280452175
C,0,1.246637122,-1.1494591438,1.2608525463
C,0,0.5737374561,0.9000268435,0.1556905331
H,0,1.9905771899,-1.85653984,1.6092125539
H,0,0.868125646,1.7516011169,-0.4477618975
C,0,-1.1512500938,-2.0356865564,0.4459568371
C,0,-2.4237884427,-3.8221515465,-1.2721305352
C,0,-0.7809918668,-2.080453256,-0.9113065899
C,0,-2.1747891345,-2.8726475851,0.9349740858

C,0,-2.8012295053,-3.7681402696,0.0733873482
C,0,-1.4154506649,-2.9773969678,-1.7597085211
H,0,-0.0062141555,-1.4279539768,-1.2966418939
H,0,-2.4650562313,-2.828756158,1.9799379851
H,0,-3.5809643001,-4.4199011669,0.4524078499
H,0,-1.12676744,-3.0189422126,-2.8044631563
H,0,-2.9151022884,-4.5183358686,-1.9441088077
C,0,-1.7829816777,1.7652648589,0.1451383396
C,0,-3.7434817319,3.6570524502,-0.5686776828
C,0,-1.4612505326,3.1326942706,0.0511254667
C,0,-3.1070258979,1.3648800107,-0.1150615216
C,0,-4.0768983517,2.303237661,-0.4720027185
C,0,-2.4325075803,4.0680550076,-0.3041664058
H,0,-0.4563651136,3.4718149147,0.2827553845
H,0,-3.3806030376,0.315316819,-0.0659617398
H,0,-5.0906202877,1.9743387397,-0.6790145454
H,0,-2.1683630587,5.1194619038,-0.3627030539
H,0,-4.49905294,4.386929091,-0.8426060901
C,0,3.0095601968,0.2090064893,0.1351345362
C,0,5.6892484366,0.6697420932,-0.5951707785
C,0,3.5321077826,1.5149069572,0.1120576711
C,0,3.8512685651,-0.861295172,-0.2187341984
C,0,5.1790594398,-0.6320712438,-0.5817088237
C,0,4.8619568034,1.7415437254,-0.2458201283
H,0,2.9095382291,2.3567944217,0.399112428
H,0,3.4604497363,-1.8740488446,-0.2354031162
H,0,5.8113051064,-1.4690663183,-0.8618918385
H,0,5.251932647,2.7547829932,-0.2472179517
H,0,6.7221254919,0.8479829042,-0.8783796818
H,0,-2.0751412349,-0.3831092448,1.8058940934
H,0,-0.302104597,-1.9987959814,2.5060131294

E(RB3LYP) = -925.834147641 A.U.

Imaginary Frequency = -228.1594

Zero-point correction= 0.353500 (Hartree/Particle)
Thermal correction to Energy= 0.371738
Thermal correction to Enthalpy= 0.372682
Thermal correction to Gibbs Free Energy= 0.305936
Sum of electronic and zero-point Energies= -925.480647
Sum of electronic and thermal Energies= -925.462409
Sum of electronic and thermal Enthalpies= -925.461465
Sum of electronic and thermal Free Energies= -925.528212

10b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,0.697838524,-1.2317072556,-2.1794448616
C,0,0.5808130745,-0.6823020156,-1.2507488758

C,0,0.251309793,0.6591429256,1.257957155
C,0,0.251309793,0.6591429256,-1.257957155
C,0,0.8280502157,-1.4220536199,0.
C,0,0.5808130745,-0.6823020156,1.2507488758
C,0,0.1049196257,1.2972980027,0.
H,0,0.697838524,-1.2317072556,2.1794448616
H,0,-0.1122225019,2.361732673,0.
C,0,0.0477518139,1.4140921351,-2.522164699
C,0,-0.3462297647,2.8286714156,-4.9177422315
C,0,0.8866491751,1.1915597562,-3.6274859832
C,0,-0.9903477074,2.3551887392,-2.6318736236
C,0,-1.1856298946,3.0561214726,-3.8230264678
C,0,0.6900870278,1.8955694471,-4.8164991045
H,0,1.7099691493,0.4871497759,-3.5536760571
H,0,-1.665403647,2.5246002971,-1.7978753001
H,0,-1.997373652,3.7730944926,-3.8968459588
H,0,1.3513839227,1.7204416055,-5.6593781663
H,0,-0.4981710725,3.3754537468,-5.8432421122
C,0,0.0477518139,1.4140921351,2.522164699
C,0,-0.3462297647,2.8286714156,4.9177422315
C,0,-0.9903477074,2.3551887392,2.6318736236
C,0,0.8866491751,1.1915597562,3.6274859832
C,0,0.6900870278,1.8955694471,4.8164991045
C,0,-1.1856298946,3.0561214726,3.8230264678
H,0,-1.665403647,2.5246002971,1.7978753001
H,0,1.7099691493,0.4871497759,3.5536760571
H,0,1.3513839227,1.7204416055,5.6593781663
H,0,-1.997373652,3.7730944926,3.8968459588
H,0,-0.4981710725,3.3754537468,5.8432421122
C,0,0.3197578938,-2.86947379,0.
C,0,-0.6585267246,-5.4922969662,0.
C,0,-1.0625908674,-3.1041802425,0.
C,0,1.2094266519,-3.948817714,0.
C,0,0.718871386,-5.2584520106,0.
C,0,-1.5484220413,-4.4131732972,0.
H,0,-1.7573767881,-2.268742822,0.
H,0,2.2819186112,-3.7750217918,0.
H,0,1.4146511677,-6.0917441276,0.
H,0,-2.6198915828,-4.5879951047,0.
H,0,-1.0376117001,-6.5095651446,0.
H,0,1.9462185582,-1.4889084251,0.

E(RB3LYP) = -925.847029186 A.U.

Zero-point correction= 0.352941 (Hartree/Particle)
Thermal correction to Energy= 0.371893
Thermal correction to Enthalpy= 0.372837
Thermal correction to Gibbs Free Energy= 0.303329
Sum of electronic and zero-point Energies= -925.494088
Sum of electronic and thermal Energies= -925.475136
Sum of electronic and thermal Enthalpies= -925.474192

Sum of electronic and thermal Free Energies= -925.543700

8a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.4874786162,1.1402544947,1.2855188994
C,0,-1.5979541753,1.9647779582,-1.2353312057
C,0,0.043980152,0.5558378634,0.
C,0,-1.5979541753,1.9647779582,1.2353312057
C,0,-2.1424508496,2.3484260681,0.
C,0,-0.4874786162,1.1402544947,-1.2855188994
H,0,-2.0209448833,2.3786750379,2.1428333041
H,0,-2.9948435897,3.0219649102,0.
H,0,-2.0209448833,2.3786750379,-2.1428333041
C,0,0.1470208746,0.7856044476,2.5544667644
C,0,1.3458100783,0.1232348226,5.0156697881
C,0,-0.6262112842,0.6920093336,3.7355046553
C,0,1.5358326987,0.5390945524,2.6402894702
C,0,2.1272361974,0.2199860735,3.8594487285
C,0,-0.0329503123,0.3566590228,4.9480984138
H,0,-1.6997551036,0.8401643956,3.6937746982
H,0,2.1673499177,0.639173569,1.7646309998
H,0,3.1983768541,0.053457142,3.9092245193
H,0,-0.6450289944,0.2702817863,5.8400125301
H,0,1.8083017456,-0.1313320471,5.9641799085
C,0,-0.242981485,-0.978087313,0.
C,0,-0.7384861734,-3.7369208613,0.
C,0,-1.5590838444,-1.4567549404,0.
C,0,0.822990276,-1.8837885153,0.
C,0,0.5740660445,-3.2598825931,0.
C,0,-1.8043008932,-2.8315790876,0.
H,0,-2.3975917967,-0.7667995799,0.
H,0,1.8483853343,-1.5273953703,0.
H,0,1.4092373391,-3.953601802,0.
H,0,-2.8282888505,-3.1923048113,0.
H,0,-0.9306814315,-4.8053574007,0.
C,0,0.1470208746,0.7856044476,-2.5544667644
C,0,1.3458100783,0.1232348226,-5.0156697881
C,0,-0.6262112842,0.6920093336,-3.7355046553
C,0,1.5358326987,0.5390945524,-2.6402894702
C,0,2.1272361974,0.2199860735,-3.8594487285
C,0,-0.0329503123,0.3566590228,-4.9480984138
H,0,-1.6997551036,0.8401643956,-3.6937746982
H,0,2.1673499177,0.639173569,-1.7646309998
H,0,3.1983768541,0.053457142,-3.9092245193
H,0,-0.6450289944,0.2702817863,-5.8400125301
H,0,1.8083017456,-0.1313320471,-5.9641799085
H,0,1.134720487,0.6454809806,0.

E(RB3LYP) = -925.860636104 A.U.

Zero-point correction= 0.354669 (Hartree/Particle)
Thermal correction to Energy= 0.373449
Thermal correction to Enthalpy= 0.374393
Thermal correction to Gibbs Free Energy= 0.305863
Sum of electronic and zero-point Energies= -925.505967
Sum of electronic and thermal Energies= -925.487187
Sum of electronic and thermal Enthalpies= -925.486243
Sum of electronic and thermal Free Energies= -925.554773

8c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.2404798361,-1.3352248073,0.0033754326
C,0,-1.1991665972,-2.80980522,0.0563109299
C,0,0.0002915144,-0.6086796324,0.0071916611
C,0,1.2572148221,-2.76859832,-0.0359526124
C,0,0.1061453074,-3.4825686075,0.0245297241
C,0,-1.2008273499,-1.3200048806,0.0258403779
H,0,2.2141836337,-3.2758429644,-0.0336466378
H,0,0.1236914839,-4.5673150593,0.0621219887
C,0,2.5562726952,-0.6776426754,0.0603320457
C,0,5.1232963269,0.4631527228,0.1869704177
C,0,3.5987599345,-1.153010136,-0.7667503431
C,0,2.8314431086,0.3720845633,0.9630371004
C,0,4.1092266939,0.9195540163,1.036660024
C,0,4.8619580394,-0.5689236224,-0.7205250057
H,0,3.406858226,-1.9520730312,-1.4754946653
H,0,2.0579452917,0.7332367826,1.6289520892
H,0,4.3130937984,1.7073780262,1.7546598878
H,0,5.6427722474,-0.9234309163,-1.3855736256
H,0,6.1128974737,0.906847655,0.2351392261
C,0,0.0008280889,0.8907796511,-0.0145272985
C,0,-0.0126218963,3.6993488376,-0.0648095255
C,0,0.5018905885,1.584041467,-1.1269067079
C,0,-0.5069710132,1.618475205,1.0722225972
C,0,-0.5093590811,3.0148008964,1.0486430496
C,0,0.4906358426,2.9801542461,-1.1533876843
H,0,0.8948905993,1.032377664,-1.9761049803
H,0,-0.8947136531,1.0928333409,1.9399545449
H,0,-0.9002702901,3.5658111029,1.8986699058
H,0,0.8754465898,3.5041230508,-2.0230771293
H,0,-0.0177542366,4.7849418406,-0.0842813427
C,0,-2.5366879333,-0.6895702419,-0.026741024
C,0,-5.1270506689,0.3985087485,-0.1878439108
C,0,-2.8520301409,0.2709081367,-1.0092079771
C,0,-3.547057102,-1.1006006244,0.8666036161
C,0,-4.8249927574,-0.54679151,0.7965296833
C,0,-4.1392988167,0.7966511912,-1.0952241237

H,0,-2.0977246107,0.5843181336,-1.7208825607
H,0,-3.3275757089,-1.8238688008,1.6452057321
H,0,-5.5828075702,-0.8555187709,1.5096097938
H,0,-4.3704297329,1.5201783581,-1.8706644549
H,0,-6.1248104449,0.8219756363,-0.2484727827
H,0,-1.7984231939,-3.1714123379,-0.7977468256
H,0,-1.787245224,-3.1803471345,0.9134333799

E(RB3LYP) = -925.858447479 A.U.

Zero-point correction= 0.353431 (Hartree/Particle)
Thermal correction to Energy= 0.372296
Thermal correction to Enthalpy= 0.373240
Thermal correction to Gibbs Free Energy= 0.305430
Sum of electronic and zero-point Energies= -925.505017
Sum of electronic and thermal Energies= -925.486152
Sum of electronic and thermal Enthalpies= -925.485208
Sum of electronic and thermal Free Energies= -925.553017

8d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.257033828,-0.0066600982,1.3483116497
C,0,-1.2401364329,-0.0028200365,2.7208849227
C,0,0.,0.,0.6326565187
C,0,1.2401364329,0.0028200365,2.7208849227
C,0,0.,0.,3.5002813065
C,0,-1.257033828,0.0066600982,1.3483116497
H,0,2.1778991125,0.0481176309,3.2661227257
H,0,-2.1778991125,-0.0481176309,3.2661227257
C,0,2.5894559963,0.0534595894,0.6670361116
C,0,5.1513400551,0.2052020651,-0.4761212835
C,0,3.5330211791,-0.9589498239,0.898793534
C,0,2.9451547068,1.1490268317,-0.1360112423
C,0,4.2191255041,1.223824242,-0.701185795
C,0,4.8057959546,-0.8856163348,0.3256119194
H,0,3.2679820025,-1.811880869,1.5173309182
H,0,2.2312874014,1.947418133,-0.3137497827
H,0,4.4839546761,2.079332381,-1.3150900046
H,0,5.5230540078,-1.6803273404,0.5068425972
H,0,6.1403219374,0.2641043818,-0.9202917378
C,0,0.,0.,-0.8391802804
C,0,0.,0.,-3.6469358319
C,0,0.7608253703,-0.9483998641,-1.5554016785
C,0,-0.7608253703,0.9483998641,-1.5554016785
C,0,-0.7351325389,0.9634243836,-2.9473199292
C,0,0.7351325389,-0.9634243836,-2.9473199292
H,0,1.3414409397,-1.6924649295,-1.0228570251
H,0,-1.3414409397,1.6924649295,-1.0228570251
H,0,-1.298240963,1.7186195347,-3.4860217532
H,0,1.298240963,-1.7186195347,-3.4860217532

H,0,0.,0.,-4.7325091606
C,0,-2.5894559963,-0.0534595894,0.6670361116
C,0,-5.1513400551,-0.2052020651,-0.4761212835
C,0,-2.9451547068,-1.1490268317,-0.1360112423
C,0,-3.5330211791,0.9589498239,0.898793534
C,0,-4.8057959546,0.8856163348,0.3256119194
C,0,-4.2191255041,-1.223824242,-0.701185795
H,0,-2.2312874014,-1.947418133,-0.3137497827
H,0,-3.2679820025,1.811880869,1.5173309182
H,0,-5.5230540078,1.6803273404,0.5068425972
H,0,-4.4839546761,-2.079332381,-1.3150900046
H,0,-6.1403219374,-0.2641043818,-0.9202917378
H,0,-0.0032419198,-0.8544888191,4.2037310027
H,0,0.0032419198,0.8544888191,4.2037310027

E(RB3LYP) = -925.851291742 A.U.

Zero-point correction= 0.352320 (Hartree/Particle)
Thermal correction to Energy= 0.371454
Thermal correction to Enthalpy= 0.372398
Thermal correction to Gibbs Free Energy= 0.303563
Sum of electronic and zero-point Energies= -925.498972
Sum of electronic and thermal Energies= -925.479838
Sum of electronic and thermal Enthalpies= -925.478894
Sum of electronic and thermal Free Energies= -925.547729

9a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.8286854772,-1.0688068174,-0.0105603473
C,0,-2.0473771835,-0.5854066323,0.0037655247
C,0,0.2657027807,0.2698544371,0.0246311916
C,0,-0.0440366042,-2.1181742235,0.0135246661
C,0,-1.5128151712,-1.9737134775,0.0527315663
C,0,-1.1351540164,0.4572502725,-0.0100013544
H,0,0.3397531028,-3.1334150954,-0.0228996204
H,0,-1.4967378949,1.4755168626,0.0491086738
C,0,2.2921472555,-1.3459219424,-0.1305249505
C,0,5.0148502114,-1.9851148815,-0.4155138508
C,0,2.9271882863,-2.1886134288,0.7952859086
C,0,3.0361145144,-0.8297108328,-1.2045653809
C,0,4.3870178168,-1.1504481123,-1.3464783259
C,0,4.2816880663,-2.5034270162,0.6551542729
H,0,2.3650736315,-2.5863002084,1.6355311276
H,0,2.557203507,-0.1859986078,-1.9362645645
H,0,4.9481940079,-0.7504563723,-2.1855726105
H,0,4.7610686244,-3.1502604276,1.3836988764
H,0,6.0669507549,-2.2297707025,-0.5256037058
C,0,1.102863507,1.4735203141,0.1344382552
C,0,2.6174862029,3.8256927526,0.4146266167

C,0,2.2085010781,1.5157430755,1.0116589644
C,0,0.7704285605,2.6361139989,-0.5959985233
C,0,1.5346790716,3.7932842076,-0.4710063155
C,0,2.9431717276,2.6885335973,1.1625897533
H,0,2.4693974029,0.6434384376,1.5986971913
H,0,-0.0607050771,2.619740172,-1.2934475404
H,0,1.2844277386,4.6693052406,-1.0606236524
H,0,3.7740585754,2.7144194848,1.8602417158
H,0,3.2046248736,4.7324687234,0.5218556261
C,0,-3.4923767122,-0.3544169829,-0.0035912495
C,0,-6.2755525873,0.0899077348,-0.0470042358
C,0,-4.0267352782,0.8603350902,-0.4937262004
C,0,-4.39234734,-1.3434534135,0.4550992589
C,0,-5.7657542073,-1.1193452023,0.4390272639
C,0,-5.4009796764,1.0757314651,-0.5175623516
H,0,-3.370293232,1.6255584047,-0.8918733616
H,0,-4.0240712626,-2.2827388882,0.851945307
H,0,-6.4390791163,-1.8853703906,0.8096041679
H,0,-5.7913805674,2.0091968065,-0.9098071746
H,0,-7.3472645203,0.2617432743,-0.061090303
H,0,-1.9438154417,-2.5684082689,-0.7687391561
H,0,-1.8840893162,-2.4960468568,0.9509129167

E(RB3LYP) = -925.868210429 A.U.

Zero-point correction= 0.353604 (Hartree/Particle)
Thermal correction to Energy= 0.372582
Thermal correction to Enthalpy= 0.373527
Thermal correction to Gibbs Free Energy= 0.304616
Sum of electronic and zero-point Energies= -925.514607
Sum of electronic and thermal Energies= -925.495628
Sum of electronic and thermal Enthalpies= -925.494684
Sum of electronic and thermal Free Energies= -925.563594

9d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.8044733153,-1.0060094234,0.0229243121
C,0,-2.0871312251,-0.5972899923,0.0430328668
C,0,0.3328085392,0.3023582179,0.0785831474
C,0,-0.1561754306,-2.0508270446,0.0221084974
C,0,-1.5418286914,-1.8732696412,0.0318743602
C,0,-1.1404032357,0.5449122778,0.1658639632
H,0,0.2184645952,-3.0687241863,-0.0402423221
H,0,-2.1735023162,-2.7499785787,-0.0422235067
C,0,2.2421215103,-1.3900793914,-0.106582823
C,0,4.9166392005,-2.2081374468,-0.38555558
C,0,2.8104390742,-2.2929072529,0.8065272661
C,0,3.0259337564,-0.9098998413,-1.1684480125
C,0,4.3533085376,-1.3188996635,-1.3068640013

C,0,4.1419155587,-2.6943337054,0.6711979362
H,0,2.2164282865,-2.6702595375,1.6345158663
H,0,2.595176884,-0.2240795562,-1.8913594912
H,0,4.9461672389,-0.9449694484,-2.1361333349
H,0,4.5707438567,-3.3848419665,1.391050919
H,0,5.9504097188,-2.5220843426,-0.4932692134
C,0,1.1922958069,1.4965279488,0.1405157926
C,0,2.7720554689,3.8172471029,0.3349068877
C,0,2.3012237606,1.5407483753,1.0122445966
C,0,0.8896262406,2.64062691,-0.6276379829
C,0,1.6831649453,3.7837452994,-0.5410911836
C,0,3.0724254165,2.6952999259,1.1161960856
H,0,2.5385222449,0.6800968084,1.6269196045
H,0,0.0613116891,2.6276262759,-1.3288937491
H,0,1.4507179319,4.6460975741,-1.1577534143
H,0,3.9098008656,2.7199824606,1.806372831
H,0,3.3838738507,4.7109492553,0.4086180491
C,0,-3.5273712296,-0.3575780457,-0.0066653527
C,0,-6.3093765499,0.0824377366,-0.0814413956
C,0,-4.056389329,0.8541247097,-0.5073860341
C,0,-4.4311926273,-1.342828728,0.4579149112
C,0,-5.8036654169,-1.1206246569,0.425058426
C,0,-5.4314090301,1.0662614467,-0.5489144434
H,0,-3.4007679369,1.6227249625,-0.9000582049
H,0,-4.0579405728,-2.2677606128,0.8829193418
H,0,-6.4801047564,-1.8814591677,0.8006343126
H,0,-5.8190409512,1.9960367862,-0.9523634296
H,0,-7.3811319603,0.2518142408,-0.1116264181
H,0,-1.4275516434,1.3892606332,-0.4712392761
H,0,-1.3067083306,0.9573950221,1.1790784762

E(RB3LYP) = -925.866927321 A.U.

Zero-point correction= 0.353614 (Hartree/Particle)
Thermal correction to Energy= 0.372603
Thermal correction to Enthalpy= 0.373548
Thermal correction to Gibbs Free Energy= 0.304786
Sum of electronic and zero-point Energies= -925.513313
Sum of electronic and thermal Energies= -925.494324
Sum of electronic and thermal Enthalpies= -925.493380
Sum of electronic and thermal Free Energies= -925.562141

9e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.9791052431,-1.0858082326,-0.0246147934
C,0,-1.9129966245,-0.6661147872,0.0745806411
C,0,0.4032719614,0.0697084388,0.7455517578
C,0,0.0923426874,-1.9243128291,-0.701763011
C,0,-1.2835497371,-1.7160048076,-0.6615948968

C,0,-1.0821000018,0.1730048463,0.7691582029
H,0,0.4598341919,-2.7794155484,-1.2554065176
H,0,-1.9137632214,-2.4020533829,-1.2205373252
H,0,-1.488695715,0.9750556834,1.3777103443
C,0,2.4160326241,-1.3115925681,-0.0489645631
C,0,5.1965813697,-1.7635979252,-0.1077026089
C,0,3.2589469703,-0.7937254982,0.9646350843
C,0,3.0106395492,-2.0589344495,-1.0969450954
C,0,4.3832168879,-2.273741716,-1.1267213844
C,0,4.6289342662,-1.0258121473,0.9381452388
H,0,2.8410071171,-0.2380420248,1.7953318249
H,0,2.4042066484,-2.4359042938,-1.9121232997
H,0,4.821839765,-2.833613901,-1.9460151365
H,0,5.2555037472,-0.6371236808,1.73398387
H,0,6.267357178,-1.9402341525,-0.1280570239
C,0,0.9621296664,1.449437465,0.313945526
C,0,1.8843711884,3.9836190149,-0.4458395668
C,0,1.3403057344,2.3811676402,1.2877781774
C,0,1.0336372988,1.7941207973,-1.0422731224
C,0,1.4987041257,3.0563463402,-1.4184945127
C,0,1.802749842,3.6440428622,0.9073008104
H,0,1.2812336093,2.1247492936,2.3420182697
H,0,0.7363819646,1.0833622278,-1.8075501074
H,0,1.5578616274,3.3125060669,-2.471856173
H,0,2.1014801902,4.3570328021,1.6695542429
H,0,2.2468947149,4.9634306927,-0.7409277916
C,0,-3.3914328519,-0.5186183596,0.0822907974
C,0,-6.1884845124,-0.2343067437,0.1144979942
C,0,-3.9801971833,0.7553637023,0.009845322
C,0,-4.2229091151,-1.6487255016,0.1679586084
C,0,-5.6115154936,-1.5059104817,0.1861673529
C,0,-5.3690734436,0.8952064785,0.0260358737
H,0,-3.3531448834,1.6371124716,-0.0835494174
H,0,-3.7884659076,-2.6412260427,0.247333972
H,0,-6.2407772183,-2.3873436064,0.2625845561
H,0,-5.8098484215,1.885244383,-0.0397221316
H,0,-7.2685775684,-0.124640539,0.1258710463
H,0,0.7062061802,-0.062743757,1.7981650555

E(RB3LYP) = -925.855511727 A.U.

Zero-point correction= 0.354066 (Hartree/Particle)
Thermal correction to Energy= 0.372921
Thermal correction to Enthalpy= 0.373866
Thermal correction to Gibbs Free Energy= 0.304754
Sum of electronic and zero-point Energies= -925.501446
Sum of electronic and thermal Energies= -925.482590
Sum of electronic and thermal Enthalpies= -925.481646
Sum of electronic and thermal Free Energies= -925.550757

9f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.843182515,-1.0506880605,-0.0364104444
C,0,-2.0491403119,-0.6675579585,-0.0370910433
C,0,0.3036880943,0.2475069608,-0.0003188545
C,0,-0.099039705,-2.201259027,-0.0696500057
C,0,-1.5450790395,-1.9427695658,-0.045722592
C,0,-1.0953094837,0.3907290082,0.0011637434
H,0,-2.201522312,-2.8071104057,-0.0623240422
H,0,-1.479083636,1.4040987164,0.0791593727
C,0,2.2758072006,-1.3555995959,-0.0865537723
C,0,5.0016461363,-2.0281091649,-0.2826679551
C,0,2.8033287922,-2.4520605565,0.6326805963
C,0,3.1464459969,-0.6055643199,-0.9095537104
C,0,4.4900069415,-0.9515618435,-1.016221935
C,0,4.1556116918,-2.7723668099,0.5461746088
H,0,2.1693721471,-3.0291093679,1.297622302
H,0,2.7610497932,0.2233221131,-1.4906936641
H,0,5.1397013157,-0.3795816093,-1.6707428971
H,0,4.549207116,-3.6002314516,1.1269415455
H,0,6.0541160675,-2.2838776671,-0.3549650218
C,0,1.1165674828,1.4964635416,0.1200957807
C,0,2.5501818426,3.8964559245,0.3876517564
C,0,1.9852185097,1.6870437853,1.2068516134
C,0,0.9662845054,2.5236282187,-0.8249913751
C,0,1.684456302,3.7151852018,-0.6942619197
C,0,2.6947542644,2.8815682438,1.3396316721
H,0,2.0984437081,0.9064415047,1.9528752962
H,0,0.3005018028,2.3858780592,-1.6726741936
H,0,1.5665884905,4.4978830805,-1.437372145
H,0,3.3577863461,3.0204050523,2.1881165556
H,0,3.1062014733,4.8232443605,0.491229932
C,0,-3.5063363073,-0.3763942147,-0.0340870953
C,0,-6.2671451071,0.1573497263,-0.0479656252
C,0,-4.0224169324,0.6970052739,-0.7803448614
C,0,-4.3920658247,-1.176253283,0.708221981
C,0,-5.7622612817,-0.9106546039,0.7002570971
C,0,-5.393594395,0.9598157251,-0.7877728835
H,0,-3.3593864506,1.3157428512,-1.3783298908
H,0,-4.009024945,-1.9932721791,1.3125407471
H,0,-6.4328628707,-1.5323037572,1.2855080031
H,0,-5.778188884,1.786892462,-1.3765420564
H,0,-7.3330182669,0.3637190563,-0.0528821911
H,0,0.1174362911,-2.783232045,-0.9850653275
H,0,0.1547724164,-2.936958519,0.7121014489

E(RB3LYP) = -925.858957029 A.U.

Zero-point correction= 0.353091 (Hartree/Particle)
Thermal correction to Energy= 0.372071

Thermal correction to Enthalpy= 0.373015
Thermal correction to Gibbs Free Energy= 0.304449
Sum of electronic and zero-point Energies= -925.505866
Sum of electronic and thermal Energies= -925.486886
Sum of electronic and thermal Enthalpies= -925.485942
Sum of electronic and thermal Free Energies= -925.554508

10a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-2.1480811925,0.1323387801,-1.2529070701
C,0,-1.2304783206,0.0394343031,-0.687310748
C,0,1.279181053,-0.0359055504,0.6876688157
C,0,0.,0.,-1.3974377457
C,0,-1.279181053,0.0359055504,0.6876688157
C,0,0.,0.,1.4634828629
C,0,1.2304783206,-0.0394343031,-0.687310748
H,0,2.1480811925,-0.1323387801,-1.2529070701
C,0,-2.5545694285,0.0637992609,1.4165334383
C,0,-5.0125649602,0.0980574362,2.7992251945
C,0,-2.6429390199,0.5865967684,2.7253368251
C,0,-3.7291647187,-0.4515957169,0.8230093959
C,0,-4.9409375045,-0.4361212739,1.5079952238
C,0,-3.8594997924,0.6091967735,3.4036794721
H,0,-1.7700735004,1.0067602013,3.2120934198
H,0,-3.6884447994,-0.9008298347,-0.1630556843
H,0,-5.8280853068,-0.8488409952,1.0382978021
H,0,-3.9081478484,1.0304339173,4.4027003781
H,0,-5.9587761115,0.1131147987,3.3310622696
C,0,0.,0.,-2.8642986791
C,0,0.,0.,-5.6793082535
C,0,-1.0843089696,-0.5472748858,-3.5874437898
C,0,1.0843089696,0.5472748858,-3.5874437898
C,0,1.0765639388,0.5561639663,-4.9791371384
C,0,-1.0765639388,-0.5561639663,-4.9791371384
H,0,-1.9162420266,-1.0033377538,-3.0624669082
H,0,1.9162420266,1.0033377538,-3.0624669082
H,0,1.9075458575,0.9989394886,-5.5185678476
H,0,-1.9075458575,-0.9989394886,-5.5185678476
H,0,0.,0.,-6.7648495194
C,0,2.5545694285,-0.0637992609,1.4165334383
C,0,5.0125649602,-0.0980574362,2.7992251945
C,0,3.7291647187,0.4515957169,0.8230093959
C,0,2.6429390199,-0.5865967684,2.7253368251
C,0,3.8594997924,-0.6091967735,3.4036794721
C,0,4.9409375045,0.4361212739,1.5079952238
H,0,3.6884447994,0.9008298347,-0.1630556843
H,0,1.7700735004,-1.0067602013,3.2120934198
H,0,3.9081478484,-1.0304339173,4.4027003781
H,0,5.8280853068,0.8488409952,1.0382978021

H,0,5.9587761115,-0.1131147987,3.3310622696
H,0,0.0419066962,0.8627795577,2.1436983986
H,0,-0.0419066962,-0.8627795577,2.1436983986

E(RB3LYP) = -925.881953842 A.U.

Zero-point correction= 0.354447 (Hartree/Particle)
Thermal correction to Energy= 0.373375
Thermal correction to Enthalpy= 0.374319
Thermal correction to Gibbs Free Energy= 0.306007
Sum of electronic and zero-point Energies= -925.527507
Sum of electronic and thermal Energies= -925.508579
Sum of electronic and thermal Enthalpies= -925.507634
Sum of electronic and thermal Free Energies= -925.575947

VI. Tetraphenylbenzene Rearrangement

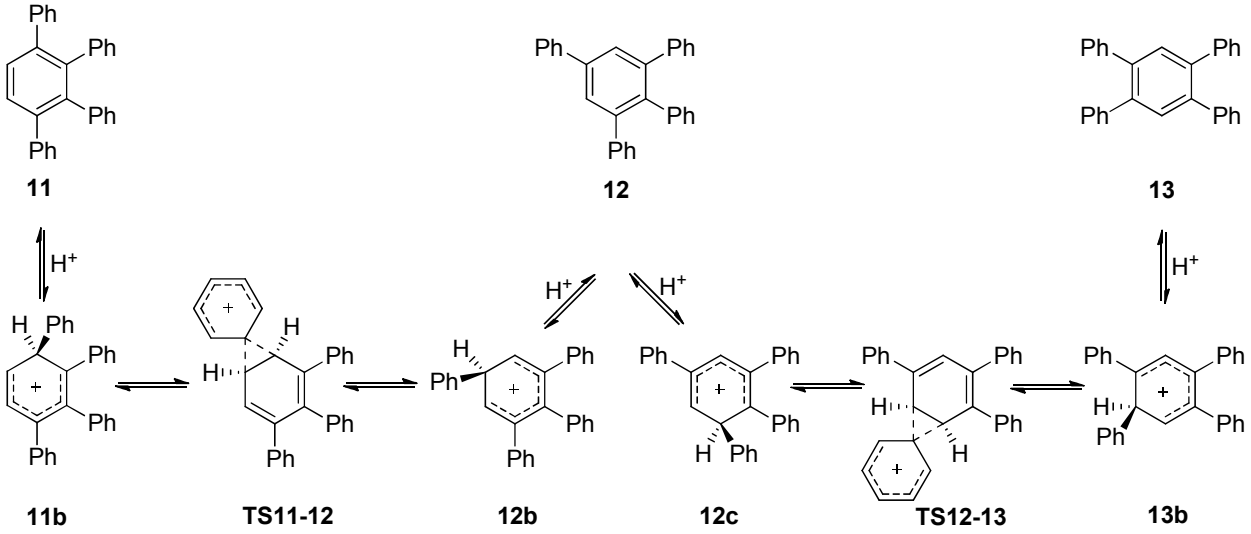

Figure S14. Rearrangement of tetraphenylbenzene isomers

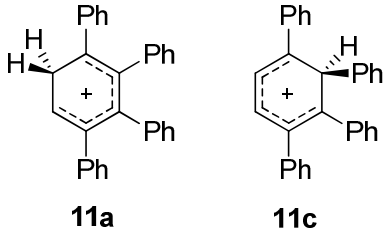

Figure S15. 1,2,3,4-Tetraphenylbenzene cations

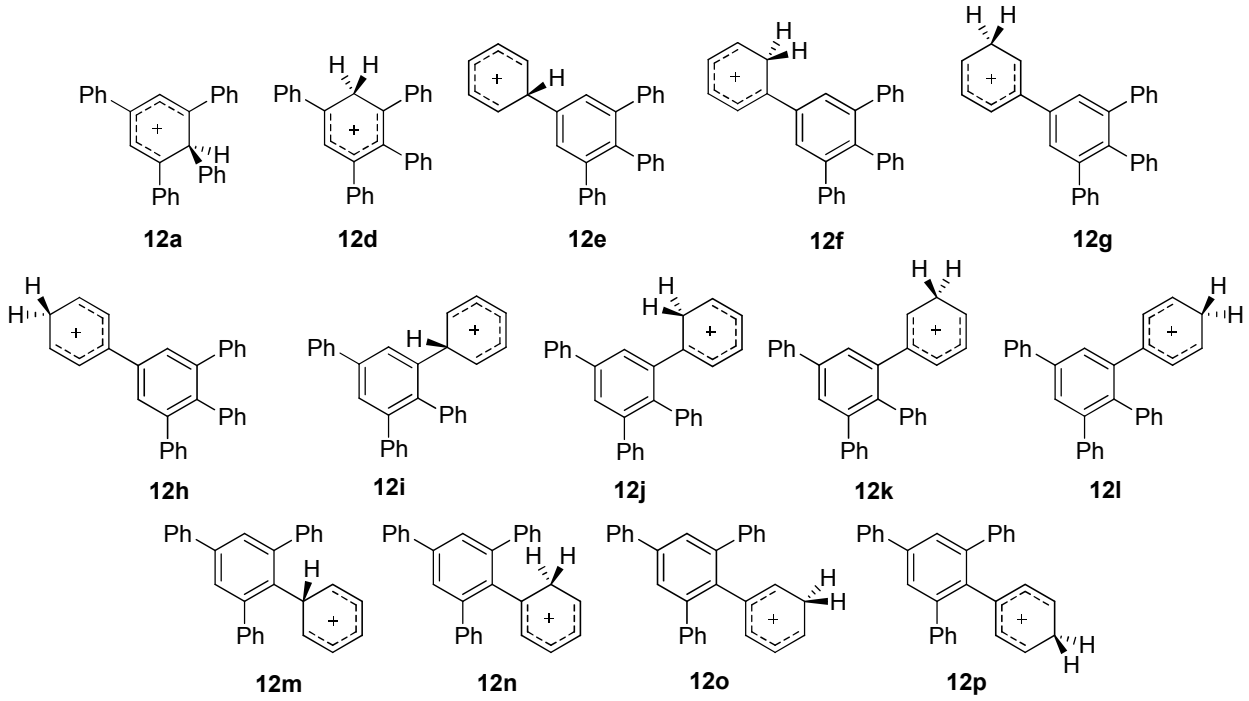

Figure S16. 1,2,3,5-Tetraphenylbenzene cations

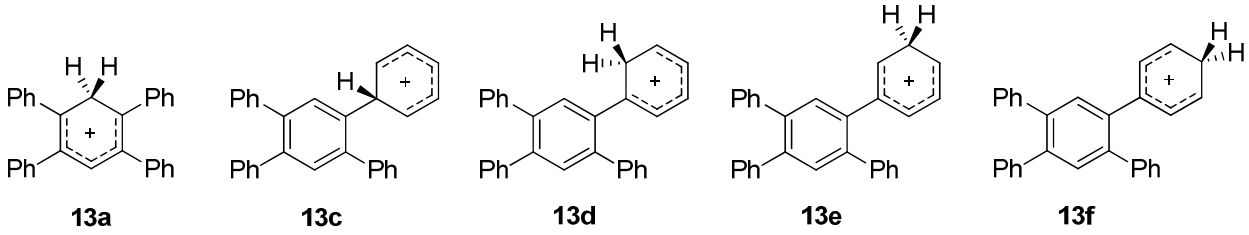

Figure S17. 1,2,4,5-Tetraphenylbenzene cations

11: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,-1.4183533792,-1.4225345396,-0.0119233723
C,0,1.4183544903,-1.4225333464,0.0119232136
C,0,-0.7096539224,-0.1964320049,-0.0068666099
C,0,-0.6946321691,-2.6238087694,-0.0024468037
C,0,0.6946342869,-2.6238081826,0.0024465245
C,0,0.7096539964,-0.1964314009,0.0068665641
H,0,-1.2323152306,-3.567224766,-0.0160717209
C,0,-2.9106684545,-1.5097485209,-0.0483690053
C,0,-5.7172425906,-1.7949031915,-0.1370637397
C,0,-3.5941410126,-2.2311345966,0.945593205
C,0,-3.6589174929,-0.9404941062,-1.0929673979
C,0,-5.0476352789,-1.0827611723,-1.1378617046
C,0,-4.9846266544,-2.3693771866,0.9055100919

H,0,-3.032862942,-2.6760444412,1.7626626649
H,0,-3.1503884583,-0.3911029272,-1.8786283305
H,0,-5.6062853032,-0.6396057649,-1.9574650621
H,0,-5.4929492738,-2.9237987549,1.6893885266
H,0,-6.7975501079,-1.9020164341,-0.1713050533
C,0,-1.4646011474,1.1002557356,-0.0038340488
C,0,-2.9058536527,3.5239715809,0.0109832853
C,0,-2.2394253534,1.4685644688,1.1074382284
C,0,-1.4247630261,1.9658068185,-1.1083147518
C,0,-2.1407815908,3.1656378272,-1.1035393324
C,0,-2.9514917832,2.6707670467,1.1178774628
H,0,-2.282469801,0.8102205654,1.9704019942
H,0,-0.8333370872,1.6958229673,-1.9781910047
H,0,-2.1004414129,3.8194532003,-1.9702467468
H,0,-3.5418207202,2.9390315111,1.9895537411
H,0,-3.4612033187,4.4574401095,0.016217113
C,0,1.4646001138,1.1002569825,0.0038340501
C,0,2.9058505227,3.5239740713,-0.0109832328
C,0,1.4247612597,1.965807994,1.1083147809
C,0,2.2394239799,1.46856642,-1.1074382306
C,0,2.9514893705,2.6707696138,-1.1178774426
C,0,2.1407787933,3.1656396229,1.1035393851
H,0,0.833335571,1.6958236112,1.9781910379
H,0,2.2824689812,0.8102225833,-1.9704020212
H,0,3.5418180588,2.9390346219,-1.9895537201
H,0,2.1004380668,3.8194549337,1.9702468212
H,0,3.4611993833,4.4574430806,-0.0162170514
C,0,2.9106696332,-1.5097460848,0.0483688325
C,0,5.7172440167,-1.7948984481,0.137063486
C,0,3.6589182364,-0.9404910589,1.0929671918
C,0,3.594142771,-2.2311316035,-0.9455934026
C,0,4.984628516,-2.3693730456,-0.9055103289
C,0,5.0476361467,-1.082756979,1.1378614579
H,0,3.1503887855,-0.3911003068,1.8786281533
H,0,3.0328650363,-2.6760418956,-1.7626628481
H,0,5.4929515721,-2.9237941963,-1.6893887742
H,0,5.6062858059,-0.6396011026,1.9574648115
H,0,6.7975516263,-1.9020108094,0.1713047629
H,0,1.232318143,-3.5672237298,0.0160713506

E(RB3LYP) = -1156.53861763 A.U.

Zero-point correction= 0.422406 (Hartree/Particle)
Thermal correction to Energy= 0.445855
Thermal correction to Enthalpy= 0.446799
Thermal correction to Gibbs Free Energy= 0.367203
Sum of electronic and zero-point Energies= -1156.116212
Sum of electronic and thermal Energies= -1156.092763
Sum of electronic and thermal Enthalpies= -1156.091818
Sum of electronic and thermal Free Energies= -1156.171415

12: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,2.2154980074,-0.000027608,0.0000046409
C,0,-0.6346799964,0.0000064115,0.0000080435
C,0,1.4899962535,1.1982955891,0.0155325189
C,0,1.4899676071,-1.1983335158,-0.0155212554
C,0,0.0881139276,-1.2191340681,-0.0052070672
C,0,0.0881431961,1.219128424,0.0052231356
H,0,2.0209914302,2.1450501145,0.0318657222
C,0,3.7029994752,-0.0000454187,0.0000027736
C,0,6.5276092042,-0.0000798018,-0.0000010366
C,0,4.4257290478,-0.9526888229,0.7417129268
C,0,4.4257502109,0.9525803877,-0.7417093689
C,0,5.8224285689,0.9529785213,-0.7416474625
C,0,5.8224073795,-0.9531209617,0.7416472805
H,0,3.8919220101,-1.6850099699,1.3401322677
H,0,3.8919593979,1.6849144197,-1.3401274272
H,0,6.3590335278,1.6932910381,-1.3282012845
H,0,6.3589958874,-1.6934465803,1.3281996169
H,0,7.6136432277,-0.0000930316,-0.0000025215
C,0,-0.578211113,2.5587957372,-0.021587237
C,0,-1.7362187706,5.1306583336,-0.0989528103
C,0,-1.4365930937,2.929645836,-1.0706900253
C,0,-0.3043087784,3.5024768554,0.9828204628
C,0,-0.8808917757,4.7755669769,0.9480479425
C,0,-2.0087173464,4.2031662781,-1.1100684974
H,0,-1.6514353092,2.2201311316,-1.8635343733
H,0,0.3551184725,3.2322594224,1.8029890147
H,0,-0.6620878108,5.4868714718,1.7394812266
H,0,-2.6652448238,4.47147646,-1.9329689917
H,0,-2.1839019219,6.1198001259,-0.1286063991
C,0,-2.1324528219,0.0000291136,-0.0000005507
C,0,-4.952691193,0.0000776112,-0.0000184096
C,0,-2.8509704952,-0.5206351227,-1.088403838
C,0,-2.8509663488,0.5207218114,1.0883918262
C,0,-4.2481466812,0.5184777732,1.0911718174
C,0,-4.2481506749,-0.5183445872,-1.0912007683
H,0,-2.3119544023,-0.9253633152,-1.9400988847
H,0,-2.3119470828,0.9254336775,1.9400926644
H,0,-4.7849503123,0.921895763,1.9451804321
H,0,-4.7849573764,-0.9217434853,-1.945216472
H,0,-6.0388629887,0.0000959103,-0.0000251025
C,0,-0.5782680388,-2.5587881311,0.0215995024
C,0,-1.7363185734,-5.1306321683,0.0989583185
C,0,-0.3043955013,-3.5024655127,-0.9828198515
C,0,-1.4366389719,-2.9296346042,1.0707128103
C,0,-2.0087845614,-4.2031455331,1.1100877309
C,0,-0.8810007578,-4.7755457041,-0.9480514943
H,0,0.3550250023,-3.2322521994,-1.8029951832

H,0,-1.6514553988,-2.2201250751,1.8635684937
H,0,-2.6653032785,-4.4714526548,1.932996212
H,0,-0.6622207654,-5.4868464616,-1.7394947654
H,0,-2.184018514,-6.1197664536,0.1286090812
H,0,2.0209406445,-2.1451004079,-0.0318563939

E(RB3LYP) = -1156.54553147 A.U.

Zero-point correction= 0.422726 (Hartree/Particle)
Thermal correction to Energy= 0.446154
Thermal correction to Enthalpy= 0.447098
Thermal correction to Gibbs Free Energy= 0.367244
Sum of electronic and zero-point Energies= -1156.122805
Sum of electronic and thermal Energies= -1156.099378
Sum of electronic and thermal Enthalpies= -1156.098434
Sum of electronic and thermal Free Energies= -1156.178288

13: *1,2-dichloroethane*

Charge = 0 Multiplicity = 1
C,0,1.2359325924,-0.7074735617,0.0099930827
C,0,-1.2359326175,0.7074736086,0.0099931676
C,0,1.2359326872,0.7074734902,-0.0099929377
C,0,-0.0000001044,-1.370579417,-0.0000001024
C,0,-1.2359327398,-0.7074734808,-0.0099932059
C,0,0.0000000232,1.3705794575,0.0000002109
H,0,-0.0000001038,-2.4565359395,-0.0000002011
C,0,2.4770800418,-1.5351147024,0.0712460032
C,0,4.7653963704,-3.1793554733,0.2292411261
C,0,2.6814464017,-2.5769120144,-0.8501735662
C,0,3.4388588933,-1.3353306361,1.0770564845
C,0,4.5701758628,-2.1501381069,1.1566125027
C,0,3.8159563269,-3.3897310617,-0.7749664954
H,0,1.9532491983,-2.7426743213,-1.6392690845
H,0,3.2945117616,-0.5437894058,1.8059036365
H,0,5.2979780201,-1.9826363322,1.9455213368
H,0,3.9576861142,-4.1838980408,-1.5025178321
H,0,5.6471232254,-3.8105961289,0.2901485787
C,0,2.4770801979,1.5351145102,-0.0712457237
C,0,4.7653966868,3.1793551329,-0.2292406008
C,0,3.4388592713,1.3353302465,-1.0770559866
C,0,2.681446457,2.5769119264,0.8501737261
C,0,3.8159564582,3.3897309206,0.7749667696
C,0,4.5701762955,2.1501376184,-1.1566118723
H,0,3.2945122335,0.5437889127,-1.8059030466
H,0,1.9532491484,2.7426744109,1.6392691004
H,0,3.957686076,4.1838979589,1.5025180721
H,0,5.2979786204,1.982635698,-1.9455205164
H,0,5.6471236114,3.8105956893,-0.2901480033
C,0,-2.4770802498,-1.5351144886,-0.0712461452

C,0,-4.7653966744,-3.1793551437,-0.2292413922
C,0,-3.438859277,-1.3353300851,-1.0770564307
C,0,-2.681446518,-2.5769120511,0.85017313
C,0,-3.8159564876,-3.3897310697,0.7749659861
C,0,-4.5701762708,-2.1501374889,-1.1566125004
H,0,-3.2945122289,-0.5437886323,-1.8059033529
H,0,-1.9532492238,-2.74267463,1.6392685077
H,0,-3.9576861225,-4.1838982337,1.5025171491
H,0,-5.2979785571,-1.9826354616,-1.9455211561
H,0,-5.6471235677,-3.8105957312,-0.2901489212
C,0,-2.4770801324,1.5351146714,0.0712461973
C,0,-4.7653965959,3.1793551756,0.2292416097
C,0,-2.6814465797,2.5769120611,-0.8501731938
C,0,-3.4388589503,1.3353303448,1.07705671
C,0,-4.5701759862,2.1501376619,1.1566128514
C,0,-3.8159566156,3.3897310104,-0.7749659755
H,0,-1.9532493977,2.7426746113,-1.639268681
H,0,-3.2945116469,0.5437889974,1.8059036985
H,0,-5.2979781347,1.9826357479,1.9455216588
H,0,-3.9576864709,4.18389809,-1.5025171943
H,0,-5.6471235221,3.8105957079,0.2901492045
H,0,0.0000000845,2.4565359774,0.0000003205

E(RB3LYP) = -1156.54647965 A.U.

Zero-point correction= 0.422745 (Hartree/Particle)
Thermal correction to Energy= 0.446113
Thermal correction to Enthalpy= 0.447057
Thermal correction to Gibbs Free Energy= 0.367593
Sum of electronic and zero-point Energies= -1156.123735
Sum of electronic and thermal Energies= -1156.100367
Sum of electronic and thermal Enthalpies= -1156.099422
Sum of electronic and thermal Free Energies= -1156.178887

11b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.39554641,-1.242168565,-0.505498204
C,0,0.7235753304,-0.0283102669,-0.5885771337
C,0,-0.746320521,-2.4560009301,-0.9022723459
C,0,-0.6459509893,-0.0274517767,-0.325595152
H,0,-1.3469087643,-3.351337878,-1.0398820207
C,0,1.5845116015,1.1606846477,-0.4263069261
C,0,3.3155338023,3.3579326923,-0.1200924655
C,0,2.4612002601,1.536602557,-1.4647534474
C,0,1.5980942154,1.9014268371,0.7734136397
C,0,2.4680635894,2.9786097361,0.9272425003
C,0,3.30447868,2.6374986466,-1.3183125886
H,0,2.4551697809,0.9949508665,-2.4088440119
H,0,0.9517458922,1.615908073,1.5958373629

H,0,2.482115512,3.5260370063,1.8678593694
H,0,3.9550115368,2.9300565986,-2.1403585076
H,0,3.981429379,4.2109559144,-0.0015562813
C,0,-1.335718531,1.2187050859,0.1456523422
C,0,-2.6176899254,3.5528475519,1.0408326892
C,0,-1.8930601115,1.2741722799,1.4322488401
C,0,-1.4262302719,2.3435566963,-0.6880906882
C,0,-2.0680205643,3.5022210697,-0.2443384766
C,0,-2.5260202447,2.4367161851,1.8786291831
H,0,-1.8269986218,0.4110760371,2.0927321203
H,0,-1.0003321886,2.3115467186,-1.6895912746
H,0,-2.1364592536,4.3658447304,-0.9034725647
H,0,-2.9476294396,2.4687874259,2.8817268257
H,0,-3.1141539479,4.4573199309,1.3879158161
C,0,-2.8550320762,-1.3162502012,-0.3350538361
C,0,-5.6418898308,-1.5779025707,-0.0659509948
C,0,-3.4124529965,-2.4202558802,0.3488399804
C,0,-3.7237216493,-0.3545770884,-0.8960199472
C,0,-5.1033696133,-0.5000143236,-0.7789079155
C,0,-4.7921553646,-2.5324584625,0.5045946355
H,0,-2.7620184187,-3.169439574,0.7964228652
H,0,-3.3223494743,0.4816970356,-1.456501512
H,0,-5.7614733375,0.2329072204,-1.2416962542
H,0,-5.2049038107,-3.3699613507,1.063685318
H,0,-6.7210634343,-1.6762075843,0.0395400467
C,0,2.6491083113,-1.6379823898,-0.177267626
C,0,4.8441153399,-2.3522776436,1.4128767633
C,0,3.9288417797,-1.7090739327,-0.7377088519
C,0,2.4682055511,-1.9369944966,1.1804821039
C,0,3.5636040752,-2.2883875715,1.972910644
C,0,5.0236405933,-2.0640981628,0.0572252044
H,0,4.0768673292,-1.4823285294,-1.7925359421
H,0,1.4768206162,-1.8962254712,1.6269011205
H,0,3.4144615173,-2.5142270715,3.0273247948
H,0,6.0165713923,-2.1117804755,-0.3864397324
H,0,5.69706092,-2.6267793081,2.0309195555
C,0,0.5758582915,-2.4725499297,-1.2040578975
H,0,1.0515488238,-3.3802106066,-1.5756396552
C,0,1.4285879121,-1.2733884073,-1.0542160974
H,0,1.8350337584,-1.0533860948,-2.0637233701

E(RB3LYP) = -1156.93055880 A.U.

Zero-point correction= 0.430973 (Hartree/Particle)
Thermal correction to Energy= 0.454686
Thermal correction to Enthalpy= 0.455630
Thermal correction to Gibbs Free Energy= 0.374965
Sum of electronic and zero-point Energies= -1156.499586
Sum of electronic and thermal Energies= -1156.475873
Sum of electronic and thermal Enthalpies= -1156.474929
Sum of electronic and thermal Free Energies= -1156.555594

TS11-12: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.0257788661,-1.0957024644,-0.6978523456
C,0,0.9623162208,0.3744875826,-0.7193877199
C,0,-0.3142158913,-2.1190618671,-1.2717226041
C,0,-0.3809492705,0.1897191625,-0.4193406725
H,0,-0.7958841504,-3.0649266632,-1.4913672977
C,0,1.6986410794,1.6622575693,-0.5855599415
C,0,3.1719467692,4.0532532583,-0.3853473017
C,0,1.1992949036,2.8584449593,-1.1307738529
C,0,2.956475951,1.6800935538,0.0432832384
C,0,3.6817816983,2.8686177429,0.152773241
C,0,1.9322652828,4.041542369,-1.0334879298
H,0,0.2428284231,2.8610404472,-1.6416418621
H,0,3.3641939015,0.7679160752,0.4685787942
H,0,4.643736648,2.8661763471,0.6563366206
H,0,1.5354429455,4.9544134263,-1.4672643565
H,0,3.737580426,4.9766589849,-0.3061383305
C,0,-1.1894252909,1.3004315941,0.1678275481
C,0,-2.6987801589,3.3889248803,1.2897311487
C,0,-0.8490127913,1.8317122666,1.4218670684
C,0,-2.2959895488,1.8268325209,-0.5177490202
C,0,-3.0389635529,2.8710293717,0.0358424827
C,0,-1.6046996861,2.8628374704,1.9832278116
H,0,0.0043390069,1.4326963327,1.9616932397
H,0,-2.5696835836,1.4288475385,-1.4899554456
H,0,-3.8847728172,3.2767686148,-0.5109187548
H,0,-1.3350995691,3.2570767621,2.9584095645
H,0,-3.2820563874,4.1959163998,1.7227951942
C,0,-2.4630644732,-1.3430589711,-0.3772727361
C,0,-5.1425170033,-1.9508424979,0.2225506071
C,0,-2.9457728331,-1.2174731845,0.9363680445
C,0,-3.3387418233,-1.7801349151,-1.3846533385
C,0,-4.6718485509,-2.074821192,-1.0874178356
C,0,-4.273911591,-1.5262489172,1.2335856352
H,0,-2.2815111937,-0.8898151489,1.7297636433
H,0,-2.9799762404,-1.872965231,-2.4057007878
H,0,-5.3395065978,-2.3998400976,-1.8796673708
H,0,-4.6299359788,-1.4342536543,2.2552555352
H,0,-6.1774874321,-2.1829725795,0.4547897389
C,0,3.7324598567,-3.2844604351,1.7473503527
C,0,3.4473931938,-2.6237984926,-0.55812208
C,0,2.4767046775,-2.7466229503,2.0675622974
C,0,4.2146414466,-3.2228924346,0.4360451051
H,0,3.8194072954,-2.57257401,-1.5764194144
H,0,2.104070832,-2.7989605544,3.0848862127
H,0,5.184800417,-3.6388591271,0.1868197367
H,0,4.3316859635,-3.7516511078,2.5221103797

C,0,1.7218934248,-0.7239794193,-1.2872757782
H,0,2.6487698326,-0.4718168902,-1.7867368052
C,0,1.0852791388,-1.9808970451,-1.5743470579
H,0,1.5127397612,-2.645260326,-2.3163334872
C,0,1.6998844193,-2.1482468092,1.0856666839
H,0,0.727633644,-1.7417362901,1.3379845021
C,0,2.1851071228,-2.085384955,-0.2344862996

E(RB3LYP) = -1156.89165440 A.U.

Imaginary Frequency = -263.4538

Zero-point correction= 0.433362 (Hartree/Particle)
Thermal correction to Energy= 0.456564
Thermal correction to Enthalpy= 0.457508
Thermal correction to Gibbs Free Energy= 0.379289
Sum of electronic and zero-point Energies= -1156.458292
Sum of electronic and thermal Energies= -1156.435091
Sum of electronic and thermal Enthalpies= -1156.434146
Sum of electronic and thermal Free Energies= -1156.512365

12b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.1337011362,1.2474206199,-0.4451350624
C,0,-1.4606239432,1.2014482485,-0.7880597575
C,0,0.5867067971,0.0056637947,-0.2631846026
H,0,-1.9969699732,2.127294166,-0.9726516627
C,0,0.5901188012,-2.5856333339,-0.2226752786
C,0,1.7067634464,-5.1280755343,0.2045929869
C,0,0.6268966558,-3.5300094273,-1.2598650414
C,0,1.1114280703,-2.9304648114,1.034823357
C,0,1.6634132007,-4.1947388338,1.2458963272
C,0,1.1871807882,-4.7929908981,-1.048265488
H,0,0.2280720322,-3.2736346628,-2.2373567421
H,0,1.0797511217,-2.2156542564,1.8512631399
H,0,2.0569518113,-4.451186351,2.2248226743
H,0,1.2159080898,-5.5110224941,-1.8621743872
H,0,2.1399729525,-6.1096946733,0.3706731421
C,0,2.0065647441,0.0360220376,0.1132506908
C,0,4.7182156085,0.0946628866,0.835505345
C,0,2.4387757598,0.8128155199,1.2099955036
C,0,2.95780641,-0.7108046889,-0.6148283774
C,0,4.3056522733,-0.654703688,-0.2721210347
C,0,3.7796302191,0.8150418978,1.583193968
H,0,1.7201890545,1.3813667909,1.7888615815
H,0,2.6456732912,-1.3016794956,-1.4679778032
H,0,5.0322290494,-1.205392033,-0.8606224801
H,0,4.0946964546,1.3888082355,2.4486988952
H,0,5.7669925146,0.1175486772,1.1148050345

C,0,0.516590863,2.5926685519,-0.346245135
C,0,1.6205826515,5.1738142219,-0.2363653514
C,0,0.0156326536,3.5428149913,0.5566952175
C,0,1.5709472107,2.9515245896,-1.2017024056
C,0,2.1168372028,4.234746816,-1.1470040075
C,0,0.5683576246,4.8253526966,0.6141697703
H,0,-0.7986058095,3.2758582491,1.2245234887
H,0,1.960385318,2.232163254,-1.9155375627
H,0,2.9279163585,4.5013387004,-1.8177889679
H,0,0.1760690558,5.5479209405,1.3232902601
H,0,2.0498052073,6.1701615799,-0.1930394072
C,0,-1.4136407932,-1.274866738,-0.7693559087
H,0,-1.935227023,-2.2239569516,-0.8491327901
C,0,-3.5690998339,-0.0694842974,-0.2617645088
C,0,-6.0261730215,-0.0736298874,1.0822122936
C,0,-4.7625896426,0.0523162319,-0.9812828111
C,0,-3.606816549,-0.1923669518,1.134558813
C,0,-4.8332891164,-0.1951992249,1.8024236078
C,0,-5.9887870492,0.0505019564,-0.3089430865
H,0,-4.7400128499,0.1485505231,-2.0631452129
H,0,-2.6840553135,-0.287920748,1.701118733
H,0,-4.8555973948,-0.2924465002,2.8835185929
H,0,-6.9107824892,0.1442496346,-0.8744689999
H,0,-6.9787072533,-0.0764944611,1.6030668809
C,0,-0.0798487645,-1.2650325126,-0.4498798039
C,0,-2.2106572152,-0.0537671595,-0.9890597402
H,0,-2.4550261206,-0.0611801971,-2.0730848865

E(RB3LYP) = -1156.91225537 A.U.

Zero-point correction= 0.433693 (Hartree/Particle)
Thermal correction to Energy= 0.457475
Thermal correction to Enthalpy= 0.458420
Thermal correction to Gibbs Free Energy= 0.376794
Sum of electronic and zero-point Energies= -1156.478562
Sum of electronic and thermal Energies= -1156.454780
Sum of electronic and thermal Enthalpies= -1156.453836
Sum of electronic and thermal Free Energies= -1156.535461

12c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.1019888099,1.2977502673,-0.8497578796
C,0,1.54953076,0.9641730827,-0.8866687419
C,0,-0.8461549041,0.1614652965,-0.5723704924
H,0,2.2119995611,1.766180814,-1.1974229494
C,0,-1.1284493943,-2.1201667719,0.5788511176
C,0,-2.5706031821,-4.194287432,1.8122757945
C,0,-2.0753838463,-1.8343198777,1.5769927373
C,0,-0.9077819825,-3.4581224188,0.2128708254

C,0,-1.6291358158,-4.4878729254,0.8220699522
C,0,-2.7881725631,-2.8650813093,2.1903073475
H,0,-2.2484476916,-0.806725471,1.8812532921
H,0,-0.1850910654,-3.6957888244,-0.562897249
H,0,-1.4553606011,-5.5163468256,0.5207451292
H,0,-3.51056541,-2.629832986,2.9659309657
H,0,-3.1289365052,-4.9945581856,2.2882279098
C,0,-2.2534896934,0.323854526,-0.9366547086
C,0,-4.9230897194,0.6252952604,-1.7993898283
C,0,-2.9945551203,-0.7836374433,-1.4195967022
C,0,-2.8860713826,1.5906175654,-0.9185238287
C,0,-4.2084659767,1.7316763374,-1.3253535154
C,0,-4.3050625207,-0.6284802891,-1.8577662423
H,0,-2.5291266896,-1.7584081529,-1.487304217
H,0,-2.3563888418,2.4609793171,-0.5535961517
H,0,-4.6820822435,2.7068079435,-1.2771285328
H,0,-4.844966181,-1.4865162785,-2.244772644
H,0,-5.9514883931,0.7413672426,-2.1269743942
C,0,0.0128026397,2.4695406629,0.1880022168
C,0,-0.0376640737,4.5983059334,2.0061846854
C,0,-0.005349218,3.7899256195,-0.2780710525
C,0,0.025841721,2.2154667727,1.5650815599
C,0,-0.0069450443,3.279690142,2.4693842275
C,0,-0.0336097129,4.8505531223,0.6316856043
H,0,-0.0075870079,3.9936546681,-1.3449520587
H,0,0.0603446448,1.1978521811,1.9406710809
H,0,-0.005188646,3.0742423759,3.5353466921
H,0,-0.0562683464,5.8709476919,0.261755221
H,0,-0.063120253,5.4230206509,2.711534576
C,0,1.0855522573,-1.1819313715,0.0041608114
C,0,3.4945190759,-0.5668761181,-0.4759121689
C,0,6.2395616547,-1.1771780083,-0.4977197807
C,0,4.4454337654,0.4077144398,-0.1275457684
C,0,3.9378131457,-1.8525797546,-0.8308451346
C,0,5.3008545229,-2.1541287917,-0.8427450102
C,0,5.8076403373,0.1037210046,-0.139666352
H,0,4.1210637994,1.3984998364,0.1762792668
H,0,3.2209282322,-2.6154299004,-1.1212315164
H,0,5.6281624293,-3.1493566055,-1.1275284917
H,0,6.5298266247,0.8647644946,0.1396095094
H,0,7.2993796134,-1.4126341162,-0.5058574683
C,0,-0.3111126762,-1.0240694489,-0.0255340891
C,0,2.0441133199,-0.2455994994,-0.480181102
H,0,1.4631782905,-2.0964861118,0.4531029359
H,0,-0.1680875029,1.7359096688,-1.8177443877

E(RB3LYP) = -1156.91413764 A.U.

Zero-point correction= 0.434633 (Hartree/Particle)
Thermal correction to Energy= 0.458310
Thermal correction to Enthalpy= 0.459254

Thermal correction to Gibbs Free Energy= 0.379144
Sum of electronic and zero-point Energies= -1156.479504
Sum of electronic and thermal Energies= -1156.455828
Sum of electronic and thermal Enthalpies= -1156.454884
Sum of electronic and thermal Free Energies= -1156.534993

TS12-13: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-1.0027454592,0.3293655255,-0.6335966166
C,0,-1.6381249285,-1.8764779119,0.4533412937
C,0,-3.419718265,-3.7228641253,1.6050033848
C,0,-2.5288585328,-1.4743987044,1.4632555227
C,0,-1.6453002797,-3.2180895001,0.0358606635
C,0,-2.5369980685,-4.132488715,0.6013073381
C,0,-3.4086736913,-2.3926658574,2.0376654405
H,0,-2.5256839892,-0.4443679252,1.8057684387
H,0,-0.966558832,-3.5447216997,-0.7469679597
H,0,-2.5402941828,-5.1625601518,0.2579663527
H,0,-4.0846706551,-2.0692821839,2.8234711555
H,0,-4.1088906724,-4.4347445779,2.0490650777
C,0,-2.3857908001,0.8149839637,-0.8548960947
C,0,-4.9797322779,1.7950012088,-1.3525653182
C,0,-3.3674811323,-0.012278171,-1.4332608431
C,0,-2.724094534,2.1460868118,-0.5452415776
C,0,-4.0128797969,2.6277692499,-0.7825540978
C,0,-4.6493885834,0.4758545513,-1.6825757422
H,0,-3.1216020942,-1.0334700047,-1.7031464751
H,0,-1.9866373437,2.804465487,-0.0961744921
H,0,-4.2587540475,3.6529318846,-0.5227387337
H,0,-5.3902167813,-0.1734875865,-2.1390782809
H,0,-5.9801036751,2.1711845631,-1.5438220818
C,0,0.7261489996,-1.3146472645,-0.09120754
C,0,3.1788294429,-1.0006165394,-0.5373947048
C,0,5.8600405258,-1.8678671417,-0.512826695
C,0,4.2337121721,-0.0769424493,-0.4080921275
C,0,3.4945011529,-2.3679556576,-0.661882828
C,0,4.821161335,-2.7956258468,-0.6479652334
C,0,5.5610738561,-0.507864665,-0.3933796389
H,0,4.0218921468,0.9811761609,-0.2920031256
H,0,2.7027930512,-3.098120671,-0.7959298195
H,0,5.0447519466,-3.8527548392,-0.7536370557
H,0,6.3597788763,0.2192102879,-0.283417792
H,0,6.8927584373,-2.2026690887,-0.5048792788
C,0,-0.6539085129,-0.9133541423,-0.118457399
C,0,1.7750337092,-0.5409093416,-0.5390467458
H,0,0.9399618904,-2.2915777725,0.3285584299
C,0,0.9828517381,2.0339828497,0.142801361
C,0,0.8773270954,1.6831317298,1.5043378981
H,0,0.5578154982,0.6896155794,1.7964974607

C,0,1.1846515711,2.6235229946,2.47688403
H,0,1.0999463097,2.3551624367,3.5244038804
C,0,1.6059273832,3.9106855204,2.1100791616
H,0,1.8465854329,4.6381622834,2.8784696986
C,0,1.719716733,4.2592342674,0.760428294
H,0,2.0457020257,5.2535786502,0.4750825511
C,0,1.4136204865,3.3271040532,-0.2256676992
H,0,1.498273352,3.5997396381,-1.2729236015
C,0,1.4481977256,0.7724982886,-1.0414553386
H,0,2.1680454249,1.2768042791,-1.6738900324
C,0,0.0746752292,1.2158211578,-1.0590206666
H,0,-0.197737412,1.9886711117,-1.7683457972

E(RB3LYP) = -1156.90165735 A.U.

Imaginary Frequency = -239.9640

Zero-point correction= 0.433965 (Hartree/Particle)
Thermal correction to Energy= 0.457090
Thermal correction to Enthalpy= 0.458034
Thermal correction to Gibbs Free Energy= 0.379856
Sum of electronic and zero-point Energies= -1156.467693
Sum of electronic and thermal Energies= -1156.444567
Sum of electronic and thermal Enthalpies= -1156.443623
Sum of electronic and thermal Free Energies= -1156.521801

13b: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.2184658745,-0.609630443,-0.4953658687
C,0,-0.2457131035,1.3723821763,-0.1943660761
C,0,0.101604048,-1.3231631272,-0.8216402445
C,0,1.0392482672,0.7816429509,-0.1239029989
H,0,0.203790326,-2.3584118387,-1.133543369
C,0,2.1466537297,1.6271157511,0.337765037
C,0,4.1898920055,3.2964183336,1.3100536763
C,0,2.2159525604,2.9844970283,-0.0511830225
C,0,3.1232863408,1.125343367,1.2270601991
C,0,4.1200466631,1.9608179418,1.7224172208
C,0,3.2406514971,3.802949888,0.4150194623
H,0,1.4938620185,3.3853252416,-0.7546919441
H,0,3.0787357174,0.094583764,1.5567627172
H,0,4.8469875725,1.5689549011,2.4264064466
H,0,3.2978077847,4.834631222,0.083567016
H,0,4.9806453241,3.9392377621,1.6841230911
C,0,2.5542364078,-1.27009823,-0.6107614185
C,0,5.0137543993,-2.5949252031,-0.9177840409
C,0,3.5359791932,-0.7570698728,-1.4746066649
C,0,2.8166956384,-2.4560978492,0.0925312408
C,0,4.0415004431,-3.1125540838,-0.0578625063

C,0,4.7558825511,-1.4173347738,-1.6280338578
H,0,3.342074852,0.1525442986,-2.0353184855
H,0,2.067796435,-2.8583952719,0.7689929473
H,0,4.2337359758,-4.0250141212,0.4984278573
H,0,5.5032812968,-1.0138777398,-2.3045172436
H,0,5.9649332344,-3.1051007831,-1.0356585993
C,0,-2.7015944294,1.3368281797,-0.5464061317
C,0,-5.2045869224,2.6289977917,-0.6338629338
C,0,-2.9530428664,2.4862538725,0.2391894124
C,0,-3.7420156729,0.8480965312,-1.3690355468
C,0,-4.9738909756,1.4937077485,-1.4183109508
C,0,-4.1916866611,3.1184007787,0.1989242958
H,0,-2.1931271257,2.860911519,0.9157440091
H,0,-3.5808082207,-0.016943127,-2.0014937452
H,0,-5.7530657112,1.1139220904,-2.0711176567
H,0,-4.3708226376,3.9886038056,0.8220556767
H,0,-6.1680373505,3.1278180518,-0.6694027701
C,0,-1.3960378287,0.6764215788,-0.511669123
H,0,-0.3197267671,2.4252425558,0.0466062541
C,0,-2.1414272782,-1.6778090245,0.1372178995
C,0,-3.6229162122,-3.3489717219,1.8322362785
C,0,-2.9476820105,-2.6886593054,-0.3987392522
C,0,-2.0703656334,-1.5131251152,1.5272141991
C,0,-2.8131127179,-2.3434579776,2.3696224951
C,0,-3.6872001199,-3.5207113345,0.4470378065
H,0,-3.0041360374,-2.8279775355,-1.4748272093
H,0,-1.4426515676,-0.738262949,1.9580988443
H,0,-2.7572652979,-2.2036132455,3.4448958818
H,0,-4.3138466663,-4.2980108925,0.020537947
H,0,-4.1998776801,-3.9928328973,2.4889039141
C,0,-1.2880191605,-0.7924271473,-0.8016514438
H,0,-1.6818365016,-0.9615655192,-1.8174927214

E(RB3LYP) = -1156.92793727 A.U.

Zero-point correction= 0.435091 (Hartree/Particle)
Thermal correction to Energy= 0.458617
Thermal correction to Enthalpy= 0.459561
Thermal correction to Gibbs Free Energy= 0.379956
Sum of electronic and zero-point Energies= -1156.492846
Sum of electronic and thermal Energies= -1156.469321
Sum of electronic and thermal Enthalpies= -1156.468376
Sum of electronic and thermal Free Energies= -1156.547981

11a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.4628886871,-1.4062253033,-0.1914992329
C,0,-1.4293389098,-1.3939949334,-0.1982244783
C,0,0.6910909596,-0.1821983489,-0.1318991623

C,0,0.7887313883,-2.5925336314,-0.2624571471
C,0,-0.6738024629,-2.6672359171,-0.2789344715
C,0,-0.7407625062,-0.1790002206,-0.2040335269
H,0,1.3367402305,-3.526558748,-0.3415273217
C,0,2.9582450838,-1.4247437325,-0.2095914565
C,0,5.762893065,-1.5942886552,-0.29532888
C,0,3.6815936861,-0.754013486,-1.2094305767
C,0,3.656022552,-2.1848643271,0.742041891
C,0,5.0506882891,-2.2658799022,0.7015812658
C,0,5.0738130633,-0.8415848384,-1.2523611466
H,0,3.1576064974,-0.17142301,-1.96060233
H,0,3.1088640019,-2.7013174047,1.5257657848
H,0,5.576919111,-2.8508361747,1.4498250714
H,0,5.6198888469,-0.3234830707,-2.0349089172
H,0,6.8463809379,-1.6566358543,-0.3281857413
C,0,1.4198067547,1.0875193725,0.0997352662
C,0,2.8292767086,3.4604532816,0.6185712619
C,0,1.3660899884,2.160367456,-0.8078242084
C,0,2.2002149317,1.2154866378,1.2660933317
C,0,2.8777919231,2.403304199,1.5333643474
C,0,2.083655231,3.3298023276,-0.5567537398
H,0,0.7962118595,2.0688389362,-1.724183087
H,0,2.2545473424,0.3950994585,1.9738439308
H,0,3.4527067656,2.4981172068,2.4491213512
H,0,2.0532371599,4.140809569,-1.2774924998
H,0,3.3729921479,4.3785261127,0.8188106785
C,0,-1.4919237664,1.11768333,-0.0829668971
C,0,-2.9119425608,3.5274766692,0.1783551944
C,0,-1.8569309214,1.8538461561,-1.218647071
C,0,-1.8462810264,1.5987665313,1.1858477327
C,0,-2.5522411254,2.7975021811,1.3150607998
C,0,-2.5629794013,3.0525263646,-1.0890937966
H,0,-1.5924580931,1.4899578724,-2.2076912864
H,0,-1.570266,1.0362801622,2.0731108985
H,0,-2.8204592393,3.158618802,2.3033047672
H,0,-2.8396378675,3.6117677075,-1.9777414294
H,0,-3.4612915782,4.4585064308,0.2796049107
C,0,-2.8944818327,-1.5224210468,-0.0763313323
C,0,-5.6755050117,-1.8870732513,0.1587900182
C,0,-3.781097571,-0.8619890379,-0.9505996456
C,0,-3.4296597857,-2.3760313748,0.9124345103
C,0,-4.8080700523,-2.5407871363,1.0386043992
C,0,-5.1565249144,-1.0567922983,-0.8402709589
H,0,-3.3938983507,-0.227230378,-1.7369582885
H,0,-2.7717911951,-2.87565167,1.6162584909
H,0,-5.2022485127,-3.1797661676,1.8223442322
H,0,-5.8239618214,-0.55817007,-1.5359953544
H,0,-6.748545064,-2.0238683012,0.2498082732
H,0,-0.9755985687,-3.169290073,-1.2186410418
H,0,-1.0310810737,-3.3911214012,0.4718446182

E(RB3LYP) = -1156.91878311 A.U.

Zero-point correction= 0.433564 (Hartree/Particle)
Thermal correction to Energy= 0.457330
Thermal correction to Enthalpy= 0.458275
Thermal correction to Gibbs Free Energy= 0.378340
Sum of electronic and zero-point Energies= -1156.485219
Sum of electronic and thermal Energies= -1156.461453
Sum of electronic and thermal Enthalpies= -1156.460508
Sum of electronic and thermal Free Energies= -1156.540443

11c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.6388561281,1.151070047,-0.1007788492
C,0,-1.2379162979,1.2078031573,0.3273213541
C,0,0.7892752686,-0.0522844764,-0.4316500712
C,0,1.0382173961,2.2117613247,0.5542559167
C,0,-0.3389435062,2.2007554563,0.7935045626
C,0,-0.7100526409,0.1386569178,-0.3994061558
H,0,1.6143666007,3.0772005427,0.8593904648
H,0,-0.7617580835,3.0352024046,1.346042748
C,0,3.0671847626,1.1396479289,-0.3989907241
C,0,5.8188580667,1.1814468632,-0.9878838414
C,0,3.5670919221,0.5128818593,-1.5638861267
C,0,3.9821981309,1.7889739431,0.4635447999
C,0,5.3422570908,1.8003301616,0.1745723448
C,0,4.9272850199,0.5440511698,-1.8573342838
H,0,2.8898911759,0.0437353325,-2.2686924856
H,0,3.6286847714,2.2470075061,1.3807951985
H,0,6.0332643565,2.2853292446,0.856327644
H,0,5.2916586697,0.0772356772,-2.7665916155
H,0,6.880109454,1.1981875379,-1.2154670056
C,0,1.2298135566,-1.1628231293,0.5883551183
C,0,2.095913266,-3.1280890702,2.3902844623
C,0,2.0593127484,-2.2024108147,0.1509704183
C,0,0.8404998411,-1.1059438493,1.9313621345
C,0,1.2720194912,-2.0870293856,2.8275629301
C,0,2.4875514159,-3.182981318,1.0504565205
H,0,2.3676438959,-2.2594474769,-0.8880375314
H,0,0.202151872,-0.3048043628,2.2892871243
H,0,0.9617358651,-2.0341238892,3.8665895089
H,0,3.1239116072,-3.9888015815,0.6977605825
H,0,2.4283677767,-3.8905481707,3.0878070477
C,0,-1.5398196301,-0.7948560045,-1.180325257
C,0,-3.0809802014,-2.4931155012,-2.8237664659
C,0,-1.2299475345,-2.1674812289,-1.2957207832
C,0,-2.6353663586,-0.2929876644,-1.9198361209
C,0,-3.3857797785,-1.1306090293,-2.740588976
C,0,-2.0030562837,-3.0065782788,-2.0953268127

H,0,-0.4072038072,-2.5901916977,-0.7334645501
H,0,-2.8774021804,0.7619411875,-1.8768929631
H,0,-4.2096982989,-0.7185553002,-3.3146163176
H,0,-1.7621126071,-4.0635979904,-2.1493686464
H,0,-3.675523112,-3.1479360904,-3.4532496695
C,0,-2.6824748002,1.3730373495,0.667447933
C,0,-5.371753787,1.7176486531,1.4144979548
C,0,-3.3886186225,0.3314136658,1.2929155511
C,0,-3.3382035883,2.5928833264,0.4319566172
C,0,-4.6759536866,2.7613259827,0.7977470865
C,0,-4.7224174999,0.5041989522,1.6647776802
H,0,-2.8901811916,-0.6110100959,1.4976563192
H,0,-2.8103586132,3.4072556285,-0.0567378791
H,0,-5.1725347077,3.7060719616,0.598281037
H,0,-5.252877969,-0.3076545467,2.1531189292
H,0,-6.4107375226,1.8493014146,1.7009401147
H,0,1.0613623094,-0.4323003836,-1.4186593722

E(RB3LYP) = -1156.92018789 A.U.

Zero-point correction= 0.435288 (Hartree/Particle)
Thermal correction to Energy= 0.458777
Thermal correction to Enthalpy= 0.459722
Thermal correction to Gibbs Free Energy= 0.380822
Sum of electronic and zero-point Energies= -1156.484900
Sum of electronic and thermal Energies= -1156.461410
Sum of electronic and thermal Enthalpies= -1156.460466
Sum of electronic and thermal Free Energies= -1156.539365

12a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-1.925872706,-2.1140146317,0.1395639485
C,0,-1.3529711997,-1.1984478938,0.2087979228
C,0,0.0326195892,1.2822343071,0.4909708157
C,0,-0.0216368263,-1.2661724624,0.541039835
C,0,-2.0120017824,0.0399897599,-0.0227099849
C,0,-1.2975000269,1.2584325112,0.1453410248
C,0,0.8078658411,-0.0080057994,0.5677456081
H,0,-1.846213627,2.1900185842,0.0948758246
C,0,-3.4342241306,0.0665863443,-0.3741163281
C,0,-6.1614505673,0.1240099056,-1.0709443673
C,0,-3.9680325024,1.1414931772,-1.1221604692
C,0,-4.3031926487,-0.9780047497,0.0173223879
C,0,-5.6529908845,-0.9409489556,-0.3184437881
C,0,-5.3135712467,1.1612238996,-1.4760030866
H,0,-3.3224307034,1.9432862153,-1.462547974
H,0,-3.9350807321,-1.7995072985,0.6211605251
H,0,-6.3100779714,-1.7402407609,0.0084317378
H,0,-5.7016321984,1.9832015588,-2.06866322

H,0,-7.2129938302,0.1457685916,-1.3395285282
C,0,0.6267934733,-2.5557911556,0.8147788002
C,0,1.8330846818,-5.0433727697,1.3546386301
C,0,0.2297417277,-3.7183515651,0.1177822998
C,0,1.644104685,-2.669615553,1.7862250185
C,0,2.2328210565,-3.9028415665,2.0581014103
C,0,0.8323751986,-4.9454748787,0.3811006079
H,0,-0.5239435576,-3.6520255282,-0.6598357062
H,0,1.9504985272,-1.8046156737,2.3644475785
H,0,3.0004521109,-3.9738933698,2.8220774618
H,0,0.5272807238,-5.824518141,-0.1776932385
H,0,2.2981157826,-6.0019294535,1.5628279141
C,0,1.8338836431,-0.0486263158,-0.600247592
C,0,3.6908220516,-0.1203780641,-2.7005944688
C,0,3.2058303025,-0.062744486,-0.32696545
C,0,1.394234118,-0.0701116573,-1.9301372191
C,0,2.3196238973,-0.1061153895,-2.9753046028
C,0,4.1309010657,-0.0986110241,-1.3751867857
H,0,3.5611444211,-0.0462668448,0.6988073548
H,0,0.332313862,-0.0594434337,-2.1579197996
H,0,1.9678255161,-0.1230948431,-4.0023443416
H,0,5.1931819505,-0.1096160344,-1.1508307989
H,0,4.4095502389,-0.1482785278,-3.5138265397
C,0,0.725856888,2.5507356286,0.7514914847
C,0,2.0195443912,5.001523609,1.2579399056
C,0,1.7388566066,2.6446627179,1.7295630309
C,0,0.3778011669,3.7150397353,0.0311203418
C,0,1.0233250524,4.9234252625,0.2779380726
C,0,2.371335818,3.859690649,1.9844110884
H,0,2.0084139769,1.7798207371,2.3258065575
H,0,-0.3723941199,3.663349715,-0.7508381063
H,0,0.7550162376,5.8032394726,-0.298214752
H,0,3.1349326741,3.9158362842,2.7536378947
H,0,2.5179570296,5.9458663039,1.4534332436
H,0,1.4070714755,-0.0043520029,1.4842370317

E(RB3LYP) = -1156.93984795 A.U.

Zero-point correction= 0.435604 (Hartree/Particle)
Thermal correction to Energy= 0.459174
Thermal correction to Enthalpy= 0.460118
Thermal correction to Gibbs Free Energy= 0.380001
Sum of electronic and zero-point Energies= -1156.504244
Sum of electronic and thermal Energies= -1156.480674
Sum of electronic and thermal Enthalpies= -1156.479730
Sum of electronic and thermal Free Energies= -1156.559847

12d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1

C,0,-2.2406923555,-0.0604511645,-0.0475719523
C,0,0.678661952,0.0002921523,0.0044646284
C,0,-1.5449806002,1.127978146,-0.0950698417
C,0,-1.4537751696,-1.3218870428,-0.0097338266
C,0,0.0376788073,-1.2274687754,0.0051794712
C,0,-0.1319819579,1.1946483839,-0.0322883477
H,0,-2.0844016492,2.0652326066,-0.1347691538
C,0,-3.7050240141,-0.1125076261,-0.0159914201
C,0,-6.5221547781,-0.2061844027,0.0446923155
C,0,-4.4008270435,-1.2769559469,-0.4121206212
C,0,-4.459315005,1.0002039851,0.4225846648
C,0,-5.8497970757,0.95053963,0.4541556994
C,0,-5.7921542427,-1.3185160884,-0.3883984665
H,0,-3.8606044054,-2.1471780174,-0.7674717968
H,0,-3.9588706471,1.8947102783,0.7758182221
H,0,-6.409473689,1.811007331,0.8064439956
H,0,-6.3076661615,-2.2170600987,-0.7118096575
H,0,-7.6068790742,-0.2418659368,0.0661372251
C,0,0.4498262849,2.551611981,0.0063664106
C,0,1.4389713134,5.1823547021,0.1083198765
C,0,1.4381600912,2.9098285394,0.9461967701
C,0,-0.0396472188,3.5398065693,-0.8743193421
C,0,0.4677116917,4.8369398431,-0.8370417359
C,0,1.9114315632,4.2186028295,1.0059017539
H,0,1.812483855,2.1749036246,1.6481360607
H,0,-0.7905011745,3.2812464866,-1.6143531775
H,0,0.1018806049,5.5774165295,-1.5411786772
H,0,2.6541147506,4.4851395757,1.7511391975
H,0,1.8240724487,6.1966319973,0.1470822978
C,0,2.1742978432,0.0912781839,0.028579355
C,0,4.9804777676,0.2389208348,0.067624892
C,0,2.8961271142,-0.377332078,1.1367444334
C,0,2.8733851138,0.6352588859,-1.0598679778
C,0,4.2679243717,0.7042910446,-1.0421020173
C,0,4.2905739254,-0.3001519465,1.157708204
H,0,2.3661539932,-0.7983186803,1.9860985523
H,0,2.3272528792,0.9986658298,-1.9255994885
H,0,4.796137971,1.1216927727,-1.894075534
H,0,4.8357318612,-0.662388938,2.0241311964
H,0,6.0647091533,0.2956844513,0.0824039649
C,0,0.7426581665,-2.5301439391,-0.031916401
C,0,1.9865846155,-5.051170195,-0.1610698524
C,0,0.4056041158,-3.5454210608,0.8844067175
C,0,1.7079255381,-2.80352023,-1.0204743034
C,0,2.3138226404,-4.0569357857,-1.0892742549
C,0,1.0350998152,-4.7895901792,0.8286837937
H,0,-0.3201779959,-3.3550505084,1.6686634544
H,0,1.9670566022,-2.0421422976,-1.7470158855
H,0,3.0434102135,-4.2563590875,-1.8680004104
H,0,0.780345084,-5.5522920773,1.5578802749
H,0,2.4696632651,-6.022195767,-0.2096638262

H,0,-1.7883802795,-1.93922732,0.8377161138
H,0,-1.7198338753,-1.9391720042,-0.8819965734

E(RB3LYP) = -1156.93598513 A.U.

Zero-point correction= 0.434323 (Hartree/Particle)
Thermal correction to Energy= 0.458124
Thermal correction to Enthalpy= 0.459068
Thermal correction to Gibbs Free Energy= 0.378923
Sum of electronic and zero-point Energies= -1156.501662
Sum of electronic and thermal Energies= -1156.477861
Sum of electronic and thermal Enthalpies= -1156.476917
Sum of electronic and thermal Free Energies= -1156.557063

12e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.8448303391,-0.0553138341,-1.2433228309
C,0,-0.6158523086,-0.013511216,0.1430004228
C,0,1.8236292028,-0.0202922729,0.1519462028
C,0,0.6425510716,-0.0678281581,-1.9456319434
C,0,-0.5898538958,-0.0338833726,-1.2736537387
C,0,0.6105744531,-0.012720557,0.8556527886
H,0,2.7545041966,-0.0269712957,0.7119785589
H,0,0.6454829587,-0.0764375893,-3.0314323099
C,0,3.1931789156,-0.069864969,-1.9789534544
C,0,5.9943043282,0.1087453337,-1.5705739663
C,0,4.0267594444,-1.2601378132,-1.7050764444
C,0,3.9079993488,1.2257350349,-1.9718950725
C,0,5.2666174017,1.2969421455,-1.7960034114
C,0,5.3844805993,-1.1632071852,-1.5313075057
H,0,3.5276859121,-2.2240278319,-1.6772378213
H,0,3.3186111182,2.1216429871,-2.1424696334
H,0,5.7818828642,2.2503417494,-1.8126042247
H,0,5.9882241699,-2.0453228129,-1.3517474163
H,0,7.0683645415,0.1759809674,-1.4209753851
C,0,0.6851867549,-0.0377824789,2.3494792595
C,0,0.9330114815,-0.1156548124,5.1560009443
C,0,1.3954762776,0.9612236958,3.0357103406
C,0,0.1079138715,-1.0820399049,3.091484201
C,0,0.2327540687,-1.1215363433,4.4816620463
C,0,1.5143542971,0.9263417575,4.4281029143
H,0,1.8442521709,1.778428071,2.477646476
H,0,-0.4350899671,-1.8692459779,2.5781753978
H,0,-0.2160839439,-1.9394756404,5.0378023721
H,0,2.0582224258,1.7139886501,4.9415578508
H,0,1.0251943813,-0.145020126,6.2376683078
C,0,-1.9202897568,0.0040725499,0.8789108008
C,0,-4.3754593943,0.0370184178,2.2598304684
C,0,-2.2750022844,1.0985443549,1.6833656833
C,0,-2.8138275675,-1.0738543729,0.7772189394
C,0,-4.0297082696,-1.0603077148,1.4649753344
C,0,-3.4943495331,1.11782901,2.3647838448

H,0,-1.5956826261,1.9412967014,1.7723434074
H,0,-2.5539027923,-1.9290929181,0.1602847314
H,0,-4.7060652197,-1.9057772318,1.3779789789
H,0,-3.7542950313,1.9761402717,2.9776145861
H,0,-5.3223810604,0.0500810362,2.7914513672
C,0,-1.8254859752,0.0083206967,-2.1151473838
C,0,-4.090200199,0.1169533753,-3.7902598932
C,0,-2.7475400324,1.0631166832,-2.0072421258
C,0,-2.0530670076,-0.9860566752,-3.0812690356
C,0,-3.178485024,-0.9357555484,-3.9088474212
C,0,-3.8681813112,1.1177727522,-2.8384693688
H,0,-2.5841721585,1.8472393933,-1.2749483148
H,0,-1.3532061359,-1.8119334592,-3.1749927513
H,0,-3.3418870449,-1.7198754036,-4.6425024878
H,0,-4.5668357432,1.9440123687,-2.7437056005
H,0,-4.9644577898,0.1582914781,-4.4331709426
H,0,2.9423072576,-0.1981248958,-3.0604460517

E(RB3LYP) = -1156.90720503 A.U.

Zero-point correction= 0.433241 (Hartree/Particle)
Thermal correction to Energy= 0.457180
Thermal correction to Enthalpy= 0.458124
Thermal correction to Gibbs Free Energy= 0.376560
Sum of electronic and zero-point Energies= -1156.473964
Sum of electronic and thermal Energies= -1156.450025
Sum of electronic and thermal Enthalpies= -1156.449081
Sum of electronic and thermal Free Energies= -1156.530645

12f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-2.1864377405,-0.0593466743,0.0296634479
C,0,0.6631585971,-0.0213789788,0.0114564188
C,0,-1.4685308279,1.1536089895,0.0928566389
C,0,-1.4364393301,-1.2530334834,-0.0473245998
C,0,-0.0418772564,-1.2542636436,-0.0508172381
C,0,-0.0752097259,1.193270959,0.079810496
H,0,-1.99318038,2.1003661225,0.131486114
H,0,-1.9336709327,-2.2136622104,-0.0880168747
C,0,-3.6414786684,-0.0731594057,0.0375776161
C,0,-6.5426928724,-0.0401620987,0.0446798398
C,0,-4.3865833893,-1.2592985798,0.0565573887
C,0,-4.4024520891,1.2152482814,0.0249191331
C,0,-5.8814764824,1.1482318245,0.0295939579
C,0,-5.7781513753,-1.2394968156,0.0597232442
H,0,-3.8963865997,-2.2232704582,0.0781210298
H,0,-6.4176193689,2.092137697,0.0214585379
H,0,-6.3035013976,-2.1901677902,0.0776029878
H,0,-7.6253306512,-0.088654803,0.0481759389
C,0,0.5756391071,2.5401774725,0.1037380055
C,0,1.6961852574,5.1234735964,0.1210893396
C,0,0.3107648706,3.4287669685,1.1585103596
C,0,1.4048140323,2.9670586811,-0.9468949392

C,0,1.9577015165,4.249056479,-0.9390397764
C,0,0.8710944354,4.7093641039,1.1702651715
H,0,-0.3233925533,3.1107772833,1.9815316234
H,0,1.6119581141,2.2980070015,-1.7761026788
H,0,2.5916755983,4.5649369739,-1.7623260726
H,0,0.6636462682,5.3795167465,1.9993536047
H,0,2.1309076528,6.1185631408,0.1279505849
C,0,2.1550098337,0.0002607762,0.0046817938
C,0,4.9681863804,0.0413976123,-0.0082556203
C,0,2.8667787934,0.5471626718,1.0853828412
C,0,2.8723993955,-0.5257577673,-1.0825706855
C,0,4.2681936257,-0.4962320182,-1.092953637
C,0,4.2628529646,0.5584798312,1.0829569887
H,0,2.3269042876,0.9546809256,1.9345057511
H,0,2.3366259729,-0.9490067254,-1.926557673
H,0,4.8075038248,-0.8967127104,-1.946228947
H,0,4.7980841414,0.9743818545,1.9314128894
H,0,6.0539666212,0.0569427375,-0.0132256433
C,0,0.6442696164,-2.5837484016,-0.0836136033
C,0,1.8345881317,-5.1355635876,-0.1173689813
C,0,1.4970604811,-2.9887285229,0.9564791605
C,0,0.391298661,-3.4781134683,-1.136177235
C,0,0.9859243399,-4.7431183263,-1.1560034155
C,0,2.084907719,-4.2551127653,0.9404635569
H,0,1.6963892719,-2.3145939433,1.7835478336
H,0,-0.2615574335,-3.1773638375,-1.9510171924
H,0,0.7862657686,-5.4180789651,-1.9831252093
H,0,2.7372085379,-4.5541019679,1.755697309
H,0,2.2961138137,-6.1184397119,-0.1304876134
H,0,-4.0932514095,1.8429768337,0.8768567054
H,0,-4.0940122884,1.8195433867,-0.8445698727

E(RB3LYP) = -1156.92806683 A.U.

Zero-point correction= 0.433687 (Hartree/Particle)
Thermal correction to Energy= 0.457677
Thermal correction to Enthalpy= 0.458621
Thermal correction to Gibbs Free Energy= 0.377684
Sum of electronic and zero-point Energies= -1156.494380
Sum of electronic and thermal Energies= -1156.470390
Sum of electronic and thermal Enthalpies= -1156.469445
Sum of electronic and thermal Free Energies= -1156.550383

12g: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-2.1654696877,-0.0128659,0.0078469171
C,0,0.6696551279,0.00552198,0.0036891766
C,0,-1.4588205264,1.1944153025,0.0352521927
C,0,-1.4431276187,-1.210808388,-0.0229541432
C,0,-0.0417086775,-1.2210153268,-0.0104077437
C,0,-0.057702066,1.2227999777,0.01986636
H,0,-1.9971282376,2.1370831671,0.0128926721
H,0,-1.9666125892,-2.1619712143,-0.0004725673

C,0,-3.6502197094,-0.0219096141,0.0149653956
C,0,-6.524214571,-0.1477221003,-0.0662147376
C,0,-4.3769747716,-0.9413330216,-0.7893926512
C,0,-4.390372382,0.8480583814,0.7919727226
C,0,-5.8571826465,0.8401098807,0.7866778666
C,0,-5.7832702092,-1.0146176934,-0.8297138617
H,0,-3.8153482659,-1.6225915246,-1.4225929549
H,0,-3.8969960142,1.5634772533,1.4427919959
H,0,-6.2602355071,-1.7459385475,-1.4719270155
H,0,-7.6091710985,-0.1697879064,-0.0804362888
C,0,0.6012187293,2.5653079973,-0.0195202275
C,0,1.7442217157,5.140420366,-0.1189629517
C,0,0.3333952683,3.5096786539,0.9853818427
C,0,1.4454637855,2.9348808137,-1.0800236763
C,0,2.0097207957,4.2112469109,-1.1303105323
C,0,0.9039059885,4.7850748596,0.9398118153
H,0,-0.3127757917,3.2388120701,1.8159150706
H,0,1.6566516964,2.2232180258,-1.8717868014
H,0,2.6557572857,4.4799376295,-1.9611063622
H,0,0.6925517631,5.4974492473,1.7321037536
H,0,2.1872377779,6.1312163225,-0.1569844805
C,0,2.1668956291,0.0148420273,-0.0000808223
C,0,4.983900481,0.031689947,-0.0073298418
C,0,2.8828888187,0.54652793,1.0842921442
C,0,2.8836773435,-0.5082841319,-1.0881283388
C,0,4.2805393955,-0.4962260126,-1.0945567863
C,0,4.2798391814,0.5511701197,1.0834962159
H,0,2.3439664309,0.9529951869,1.9350996455
H,0,2.3453110422,-0.9214282401,-1.9360510404
H,0,4.8178643562,-0.9000767642,-1.9477982362
H,0,4.8167011,0.9614062465,1.9339755638
H,0,6.0699116518,0.0382212015,-0.010117715
C,0,0.6343880036,-2.555064063,0.0254350582
C,0,1.809273958,-5.1159302579,0.1190705075
C,0,1.485978068,-2.91524811,1.0832855906
C,0,0.3755965488,-3.5015711512,-0.9798431331
C,0,0.9618577548,-4.7698770362,-0.9371286566
C,0,2.0660626174,-4.1846057595,1.1306810922
H,0,1.6903041904,-2.2018897782,1.8753237841
H,0,-0.2760918202,-3.2378587492,-1.8083541231
H,0,0.757107622,-5.4839937247,-1.7295751285
H,0,2.7175502104,-4.4462239336,1.9594741923
H,0,2.2644055748,-6.1013019287,0.1549132213
H,0,-6.233403732,0.7530622188,1.824538531
H,0,-6.2262614799,1.8543008811,0.53198659

E(RB3LYP) = -1156.91788419 A.U.

Zero-point correction= 0.432584 (Hartree/Particle)
Thermal correction to Energy= 0.456727
Thermal correction to Enthalpy= 0.457671
Thermal correction to Gibbs Free Energy= 0.375523
Sum of electronic and zero-point Energies= -1156.485300
Sum of electronic and thermal Energies= -1156.461158
Sum of electronic and thermal Enthalpies= -1156.460213
Sum of electronic and thermal Free Energies= -1156.542361

12h: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.0000000044,0.,2.1163546934
C,0,0.0000000013,0.,-0.7272304827
C,0,1.2085756879,-0.0072306853,1.3866647984
C,0,-1.2085756938,0.0072306853,1.3866647935
C,0,-1.2275080747,-0.0137334474,-0.0071281989
C,0,1.2275080745,0.0137334474,-0.007128194
H,0,2.1577511497,0.0454429277,1.9062726639
H,0,-2.1577511577,-0.0454429277,1.9062726552
C,0,-0.0000000074,0.,3.5692278423
C,0,-0.0000000132,0.,6.4527959673
C,0,-1.1406274315,0.4720105235,4.3004148999
C,0,1.1406274138,-0.4720105235,4.3004149045
C,0,1.148567603,-0.4806373734,5.6616465362
C,0,-1.1485676262,0.4806373734,5.6616465316
H,0,-1.9950529395,0.8618777309,3.7620236463
H,0,1.995052924,-0.8618777309,3.7620236544
H,0,2.0135949533,-0.8585499763,6.198073689
H,0,-2.0135949786,0.8585499763,6.1980736809
C,0,2.5626322264,0.0893400863,-0.6772369714
C,0,5.1233476046,0.2593511189,-1.8359388757
C,0,3.5303793789,-0.8962784845,-0.4237030472
C,0,2.8984174431,1.1661074643,-1.5145594944
C,0,4.1692563642,1.2512971305,-2.0863171302
C,0,4.7998808997,-0.815284111,-1.0031704691
H,0,3.2835784171,-1.7388941246,0.2163420533
H,0,2.1666624448,1.9425907279,-1.713973976
H,0,4.4141220432,2.0937190914,-2.7264926705
H,0,5.5322949423,-1.5920943933,-0.8040460598
H,0,6.1097092767,0.3248783855,-2.2853857285
C,0,0.0000000044,0.,-2.2188649088
C,0,0.0000000101,0.,-5.0319637243
C,0,0.6175489037,-1.0402208772,-2.9333920694
C,0,-0.6175488921,1.0402208772,-2.9333920719
C,0,-0.6078766488,1.0452590613,-4.3293932331
C,0,0.607876666,-1.0452590613,-4.3293932307
H,0,1.0961060525,-1.8527265416,-2.3955969827
H,0,-1.096106043,1.8527265416,-2.3955969872
H,0,-1.0786848118,1.8629757511,-4.8669088431
H,0,1.0786848312,-1.8629757511,-4.8669088387
H,0,0.0000000123,0.,-6.1178495769
C,0,-2.5626322239,-0.0893400863,-0.6772369818
C,0,-5.1233475974,-0.2593511189,-1.8359388965
C,0,-2.8984174372,-1.1661074643,-1.5145595062
C,0,-3.5303793775,0.8962784845,-0.4237030615
C,0,-4.7998808959,0.815284111,-1.0031704886
C,0,-4.169256356,-1.2512971305,-2.086317147
H,0,-2.1666624381,-1.9425907279,-1.7139739848
H,0,-3.2835784183,1.7388941246,0.21634204
H,0,-5.5322949393,1.5920943933,-0.8040460822
H,0,-4.4141220324,-2.0937190914,-2.7264926884

H,0,-6.1097092677,-0.3248783855,-2.2853857532
H,0,-0.3316827914,-0.790613736,7.1505706236
H,0,0.3316827622,0.790613736,7.1505706249

E(RB3LYP) = -1156.93085444 A.U.

Zero-point correction= 0.433732 (Hartree/Particle)
Thermal correction to Energy= 0.457583
Thermal correction to Enthalpy= 0.458528
Thermal correction to Gibbs Free Energy= 0.379135
Sum of electronic and zero-point Energies= -1156.497123
Sum of electronic and thermal Energies= -1156.473271
Sum of electronic and thermal Enthalpies= -1156.472327
Sum of electronic and thermal Free Energies= -1156.551719

12i: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.8553531093,0.9710322898,0.0539470113
C,0,-0.7096195073,-0.2753215038,0.0852931627
C,0,1.7344704749,-0.4239769028,0.1148726489
C,0,0.6746835884,1.725541361,0.0068006936
C,0,-0.5971302039,1.1356584527,0.0238943771
C,0,0.4778585839,-1.035275114,0.1281210154
H,0,2.6284523028,-1.0405490143,0.1200896406
H,0,0.7382455195,2.8088699754,-0.0035424495
C,0,3.1901111314,1.6259267663,0.0405736304
C,0,5.7229181965,2.8688777251,0.0119679247
C,0,3.4263459635,2.7622568624,-0.7544803842
C,0,4.2477488302,1.1250396152,0.8211631918
C,0,5.5012879978,1.7403097535,0.8072344177
C,0,4.6799372775,3.3770572361,-0.7686932992
H,0,2.6320383184,3.155545741,-1.3818360399
H,0,4.0837430311,0.2639171057,1.4623141684
H,0,6.301563046,1.3428567428,1.424640803
H,0,4.8429848425,4.2489383115,-1.3954504879
H,0,6.6974618925,3.3477162371,0.0012167558
C,0,0.4367907764,-2.5711892268,0.1164124602
C,0,1.9232861948,-4.9723909375,-0.1486098831
C,0,1.0665249126,-3.2343347634,1.2713312543
C,0,0.6920807697,-3.1957167371,-1.1953797033
C,0,1.3891092774,-4.3739361437,-1.3078763047
C,0,1.7601354452,-4.4122727922,1.1348770716
H,0,0.9297500729,-2.7806314331,2.2483061482
H,0,0.27141822,-2.7138049143,-2.0726090541
H,0,1.5453150747,-4.8361175266,-2.2758452139
H,0,2.1927638463,-4.904897024,1.9980758631
H,0,2.4806370805,-5.8995009014,-0.247889134
C,0,-2.0407759344,-0.9584905003,0.0492386199
C,0,-4.5205154526,-2.2919415132,-0.0484858676
C,0,-2.5473341851,-1.6184573915,1.1841338943
C,0,-2.7978378293,-0.9762130679,-1.1347720507
C,0,-4.026366145,-1.6374261335,-1.1828190342
C,0,-3.7789812388,-2.2801871163,1.1350605191

H,0,-1.9884204643,-1.589736271,2.1156554319
H,0,-2.4208238378,-0.4701031884,-2.018475623
H,0,-4.5984565373,-1.6417495147,-2.1057983712
H,0,-4.1580251557,-2.7769347342,2.023115071
H,0,-5.4774347299,-2.8033544066,-0.0879086636
C,0,-1.7881347874,2.0377240498,-0.0106608776
C,0,-3.9751911922,3.8157498012,-0.0718755186
C,0,-2.7733848169,1.9979275261,0.9903222897
C,0,-1.9134582939,2.9886475355,-1.0379414776
C,0,-2.9997486711,3.867104091,-1.0717140294
C,0,-3.8555497476,2.88030886,0.9609538035
H,0,-2.6867181063,1.2839103648,1.802820779
H,0,-1.1631524525,3.0305652682,-1.8225014605
H,0,-3.0831711442,4.5886246807,-1.879263298
H,0,-4.602668214,2.8391767066,1.7482706088
H,0,-4.8189370701,4.499037419,-0.0951702362
H,0,-0.6513546694,-2.8246548861,0.2743582656

E(RB3LYP) = -1156.91242845 A.U.

Zero-point correction= 0.433321 (Hartree/Particle)
Thermal correction to Energy= 0.457094
Thermal correction to Enthalpy= 0.458038
Thermal correction to Gibbs Free Energy= 0.377574
Sum of electronic and zero-point Energies= -1156.479108
Sum of electronic and thermal Energies= -1156.455334
Sum of electronic and thermal Enthalpies= -1156.454390
Sum of electronic and thermal Free Energies= -1156.534854

12j: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,2.1942431971,0.0035451659,0.0313970692
C,0,-0.6660824096,0.0331882734,-0.0156537002
C,0,1.4658951099,-1.1874450109,0.0859056551
C,0,1.4708898894,1.2028099892,-0.0294185425
C,0,0.0680506859,1.2406236136,-0.0360751957
C,0,0.0570443078,-1.1947848188,0.0386230441
H,0,2.0063285012,-2.1268992883,0.0727556679
H,0,2.0088676913,2.1453705764,-0.0225854185
C,0,3.6805107135,-0.001474198,0.0423192002
C,0,6.4996172154,-0.0098967636,0.061381875
C,0,4.4076608388,0.8912920457,-0.7652516722
C,0,4.3915800107,-0.8973925579,0.8607533823
C,0,5.7878919805,-0.9010991646,0.8703866198
C,0,5.8039574662,0.8861275571,-0.7562244801
H,0,3.8801796938,1.5784238879,-1.4202094816
H,0,3.8514950901,-1.5774443053,1.5130801161
H,0,6.3188333466,-1.5938136458,1.5166727273
H,0,6.3474139386,1.5777080449,-1.3931943963
H,0,7.5854198625,-0.0127028732,0.0691350135
C,0,-0.6015955489,-2.506562396,-0.029838118
C,0,-1.6941364212,-5.1695883099,-0.2317325463
C,0,-0.1570183161,-3.5898296376,0.8913787147

C,0,-1.6072284146,-2.7998514106,-0.9491102696
C,0,-2.1210387334,-4.0939801323,-1.0537959735
C,0,-0.7291407829,-4.9370634078,0.7033396542
H,0,-1.9605969988,-2.0378519213,-1.6316123699
H,0,-2.8704527018,-4.2881084112,-1.8159285124
H,0,-0.3666086869,-5.7306995086,1.3490873602
H,0,-2.1252184098,-6.1548270713,-0.3665631881
C,0,-2.160247277,0.0477806846,0.0024528251
C,0,-4.9757858074,0.058659991,0.0280732635
C,0,-2.869490934,-0.4918856525,1.0887602182
C,0,-2.8834211765,0.6027689545,-1.0671970478
C,0,-4.2791624539,0.6011277181,-1.0575715438
C,0,-4.2665002366,-0.4833320429,1.1035254241
H,0,-2.3274894127,-0.9022101055,1.9359750225
H,0,-2.3506532076,1.0270303586,-1.9126595634
H,0,-4.8224311269,1.0253128472,-1.8967097989
H,0,-4.7979370819,-0.8963346521,1.9557523726
H,0,-6.0615435498,0.0639339591,0.0370576055
C,0,-0.5822721402,2.5880023094,-0.0209079323
C,0,-1.7013382774,5.1720659542,0.0320048553
C,0,-1.4203238283,2.9832277695,1.034741
C,0,-0.306596237,3.5092791075,-1.044394819
C,0,-0.866200357,4.7899287869,-1.0215322
C,0,-1.9730603002,4.2653046525,1.0617358579
H,0,-1.6341285924,2.2894346013,1.8416535081
H,0,0.3387625169,3.218303347,-1.8686209038
H,0,-0.6484296101,5.4861495371,-1.8261608301
H,0,-2.6136004769,4.5561995947,1.8891976101
H,0,-2.1342692327,6.1677566065,0.052787453
H,0,-0.4333031042,-3.2630083541,1.9142954489
H,0,0.9382431684,-3.643262434,0.9769263397

E(RB3LYP) = -1156.92602487 A.U.

Zero-point correction= 0.433438 (Hartree/Particle)
Thermal correction to Energy= 0.457380
Thermal correction to Enthalpy= 0.458324
Thermal correction to Gibbs Free Energy= 0.377632
Sum of electronic and zero-point Energies= -1156.492587
Sum of electronic and thermal Energies= -1156.468645
Sum of electronic and thermal Enthalpies= -1156.467701
Sum of electronic and thermal Free Energies= -1156.548393

12k: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.0517332214,0.0826918324,-2.2759477989
C,0,0.0460896198,0.0880002885,0.5784109142
C,0,-0.5783120607,-0.9390853055,-1.5539318076
C,0,0.6747144886,1.1035202675,-1.5458118548
C,0,0.6920631058,1.1207011519,-0.1435552779
C,0,-0.5938161096,-0.9421139809,-0.1533685643
H,0,-1.1122391403,-1.7180662854,-2.0887908527
H,0,1.2050504419,1.8881893089,-2.0759806304

C,0,0.059655157,0.0806476253,-3.7625549409
C,0,0.0773321058,0.0751583492,-6.5841265535
C,0,-0.0890847659,1.2775562235,-4.4864378747
C,0,0.2181633842,-1.1188840877,-4.4802989281
C,0,0.2272951162,-1.1216805198,-5.8767244323
C,0,-0.0808428762,1.274629807,-5.8828841642
H,0,-0.2335451798,2.2136516575,-3.9552697413
H,0,0.3603026275,-2.0526046924,-3.9440332419
H,0,0.3607259671,-2.0577506831,-6.411225251
H,0,-0.20505038,2.2089977591,-6.4224401385
H,0,0.0848660113,0.073334294,-7.6699973476
C,0,-1.3435890107,-2.0424390117,0.5215212922
C,0,-2.9099322371,-4.0734530594,1.8232923647
C,0,-1.1402171104,-3.3663938535,0.1957336583
C,0,-2.3470681687,-1.7629198015,1.4893831466
C,0,-3.1113396343,-2.754179268,2.1388935445
C,0,-1.9092119836,-4.4511619728,0.8196754386
H,0,-0.3881758669,-3.6433296164,-0.5370498169
H,0,-2.5508787258,-0.7247472345,1.7308773526
H,0,-3.8576469121,-2.4584667814,2.8672625194
H,0,-3.4879576494,-4.8605000269,2.2972848996
C,0,0.0381137222,0.0781160379,2.075472664
C,0,0.0224697389,0.0613213724,4.8940214926
C,0,0.6515628845,-0.9647349194,2.7915089375
C,0,-0.5835565782,1.1129246563,2.796571767
C,0,-0.5946358736,1.1027648461,4.1926415635
C,0,0.6476245585,-0.9712052534,4.1890579931
H,0,1.1501341486,-1.7650995246,2.2518351687
H,0,-1.0607092998,1.9273313438,2.2597423196
H,0,-1.0826693889,1.9091547759,4.7320384948
H,0,1.1360856222,-1.7800072878,4.7245421134
H,0,0.0177523579,0.0564313342,5.9798608889
C,0,1.4393767126,2.2303320097,0.5253871607
C,0,2.8892771243,4.3479109733,1.6911690173
C,0,2.5212221536,1.971747133,1.3837216325
C,0,1.1018474801,3.5668212372,0.2542844597
C,0,1.8169446062,4.6174649432,0.8360295292
C,0,3.2407875202,3.0210073706,1.9596101363
H,0,2.8074199327,0.9460753595,1.5942164775
H,0,0.2666007186,3.7844096249,-0.4056003462
H,0,1.5349005858,5.6440377246,0.6206631578
H,0,4.0782656773,2.8012089212,2.615447419
H,0,3.447593439,5.1631198078,2.1418521805
H,0,-1.2130998763,-5.1966699218,1.2513232148
H,0,-2.3923919615,-5.0637653285,0.0326963745

E(RB3LYP) = -1156.92040764 A.U.

Zero-point correction= 0.432847 (Hartree/Particle)
Thermal correction to Energy= 0.456866
Thermal correction to Enthalpy= 0.457810
Thermal correction to Gibbs Free Energy= 0.377052
Sum of electronic and zero-point Energies= -1156.487561
Sum of electronic and thermal Energies= -1156.463542
Sum of electronic and thermal Enthalpies= -1156.462597
Sum of electronic and thermal Free Energies= -1156.543355

12l: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.0915151278,0.0364307833,-2.2567583927
C,0,0.0547839571,0.0979083676,0.6048625089
C,0,-0.4940806708,-1.0012234347,-1.5292894739
C,0,0.6688120428,1.0901367436,-1.5313590891
C,0,0.6824570066,1.1295943685,-0.128547403
C,0,-0.5571079675,-0.9670758512,-0.1203871079
H,0,-0.989348613,-1.8052359701,-2.0619949649
H,0,1.1788066908,1.8827983588,-2.0695414159
C,0,0.1119650073,0.0222927255,-3.742680113
C,0,0.1494738961,-0.0025299568,-6.561279796
C,0,-0.0952081667,1.2050197452,-4.4748072278
C,0,0.3395970142,-1.1728535131,-4.4482503332
C,0,0.3588069717,-1.1847327427,-5.8443407942
C,0,-0.0776249786,1.1920626037,-5.8709787275
H,0,-0.2930357733,2.1359959358,-3.9518303206
H,0,0.5281301756,-2.0936036372,-3.9040112592
H,0,0.5462118905,-2.1157971258,-6.3710032095
H,0,-0.2479764435,2.1143249544,-6.4184493797
H,0,0.1646331291,-0.0119049628,-7.6469499538
C,0,-1.356293286,-2.0176260116,0.5190129981
C,0,-3.0032305813,-4.0891217041,1.6393985183
C,0,-1.2573171424,-3.3632943123,0.0375431392
C,0,-2.295579849,-1.7125820547,1.5549647663
C,0,-3.0951286985,-2.6846904159,2.0780026653
C,0,-2.0195303581,-4.3570558034,0.5750858958
H,0,-0.5312587419,-3.5928491245,-0.7334165989
H,0,-2.3954754844,-0.6892280736,1.8916234716
H,0,-3.833611853,-2.4343561657,2.8335126263
H,0,-1.9063422641,-5.3802971319,0.2300962712
C,0,0.0994908962,0.0723298147,2.0958041979
C,0,0.1699381769,-0.0110569136,4.908448179
C,0,0.6915316979,-1.0121368698,2.7664799567
C,0,-0.4472270511,1.1210664183,2.8560642404
C,0,-0.4199681144,1.0744832558,4.2501406641
C,0,0.7303545832,-1.0513318553,4.1625280386
H,0,1.1425952853,-1.8174715197,2.1935766313
H,0,-0.9076805433,1.9659286503,2.3536333773
H,0,-0.8578166452,1.8863623266,4.8230764383
H,0,1.2008458907,-1.8916401796,4.6642152758
H,0,0.1966109627,-0.0412463962,5.9934835701
C,0,1.4177198178,2.2602487096,0.5192906642
C,0,2.8476032215,4.41611503,1.6315864149
C,0,2.52790116,2.0300535771,1.3484745255
C,0,1.0403496562,3.5855773006,0.2486562371
C,0,1.7463100385,4.6559856787,0.8051200957
C,0,3.2380155634,3.0995914806,1.8977647099
H,0,2.8428382611,1.0125623852,1.5576175421
H,0,0.1831031884,3.7795580123,-0.3900881801
H,0,1.4349345788,5.6743150093,0.5916885127
H,0,4.0980937354,2.9036882173,2.5313443175
H,0,3.3990117971,5.2467540613,2.0619523706

H,0,-2.8017901843,-4.7419657113,2.5089646754
H,0,-3.9998083502,-4.4482770271,1.3219499647

E(RB3LYP) = -1156.92914033 A.U.

Zero-point correction= 0.433695 (Hartree/Particle)
Thermal correction to Energy= 0.457458
Thermal correction to Enthalpy= 0.458403
Thermal correction to Gibbs Free Energy= 0.378808
Sum of electronic and zero-point Energies= -1156.495445
Sum of electronic and thermal Energies= -1156.471682
Sum of electronic and thermal Enthalpies= -1156.470738
Sum of electronic and thermal Free Energies= -1156.550332

12m: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,0.0322029105,0.0428705561,-2.2910064553
C,0,0.0726392053,0.1798900626,0.5336590694
C,0,-0.7357412756,-0.8369216015,-1.5132421914
C,0,0.8131184165,0.9979124857,-1.6247980163
C,0,0.8354566149,1.0900283189,-0.2273431303
C,0,-0.7197230463,-0.7902713969,-0.1143896729
H,0,-1.368054961,-1.5729410796,-1.9991046705
H,0,1.4220505231,1.6896550834,-2.1977422775
C,0,0.0141999315,-0.0318383842,-3.7760316061
C,0,-0.0150636438,-0.1745782179,-6.5935600716
C,0,0.0469321811,1.137621306,-4.5572986087
C,0,-0.0340520219,-1.2743176427,-4.4341476212
C,0,-0.0478242772,-1.3447561692,-5.8286972095
C,0,0.0318164458,1.0668978881,-5.9517935457
H,0,0.0615054545,2.1093335638,-4.0727681362
H,0,-0.0379415428,-2.1920412798,-3.8535649888
H,0,-0.0762194925,-2.3145281451,-6.3169033119
H,0,0.0492437752,1.9823472909,-6.5359287305
H,0,-0.0260770434,-0.2296105045,-7.6780138372
C,0,-1.5540209141,-1.769729221,0.6483448014
C,0,-3.1436420605,-3.6394220426,2.0238382133
C,0,-0.9749297088,-2.9143307105,1.2225225978
C,0,-2.9458650114,-1.5864249915,0.7549413794
C,0,-3.7337361719,-2.514249164,1.4390560559
C,0,-1.7640010718,-3.8393183296,1.9105615806
H,0,0.0911946734,-3.0900328696,1.1118583668
H,0,-3.4060537661,-0.7148490105,0.298069912
H,0,-4.8059396252,-2.3595259885,1.5134652888
H,0,-1.3035464216,-4.7208581511,2.3466068064
H,0,-3.7565561526,-4.3628586932,2.553086504
C,0,0.1238171656,0.2081490062,2.0656015805
C,0,-0.3721460116,-1.011330146,4.5827153175
C,0,1.0928735389,-0.7100782236,2.6998904409
C,0,-1.1687158341,0.3377977199,2.7609013657
C,0,-1.3801345333,-0.2237119028,4.0006204912
C,0,0.8573341931,-1.2590944073,3.935791224
H,0,2.0323006814,-0.8835197671,2.1840793288

H,0,-1.9242614103,0.9680244009,2.3029243528
H,0,-2.3191119829,-0.0739046831,4.5209562796
H,0,1.5980287337,-1.8933126912,4.4094785329
H,0,-0.5466825592,-1.4481874309,5.5617197689
C,0,1.6682310969,2.1573569839,0.4078110729
C,0,3.2363533291,4.1851192675,1.5735897862
C,0,3.070453226,2.107014741,0.3354115233
C,0,1.062618722,3.2452028381,1.0635996311
C,0,1.8424967571,4.2504807223,1.6444535979
C,0,3.8477727501,3.1128679529,0.9146355561
H,0,3.5501451561,1.275193248,-0.1722237917
H,0,-0.0212738134,3.3190416719,1.0930677988
H,0,1.359028975,5.0868061518,2.1403784575
H,0,4.9305281707,3.0584597004,0.852097675
H,0,3.8425521569,4.9661471935,2.0223177374
H,0,0.5964201288,1.2023249219,2.3105055988

E(RB3LYP) = -1156.91390463 A.U.

Zero-point correction= 0.433549 (Hartree/Particle)
Thermal correction to Energy= 0.457223
Thermal correction to Enthalpy= 0.458167
Thermal correction to Gibbs Free Energy= 0.378501
Sum of electronic and zero-point Energies= -1156.480355
Sum of electronic and thermal Energies= -1156.456682
Sum of electronic and thermal Enthalpies= -1156.455738
Sum of electronic and thermal Free Energies= -1156.535404

12n: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.0029728189,0.0208216857,-2.293992565
C,0,0.0131798606,0.0218954943,0.5512642592
C,0,-0.6081947797,-1.0147414035,-1.5644969801
C,0,0.5919199096,1.0678277504,-1.5719740432
C,0,0.6140279788,1.0904484703,-0.1759579718
C,0,-0.6200439374,-1.0344793916,-0.1682384447
H,0,-1.1413463831,-1.7979217754,-2.092298857
H,0,1.1044185784,1.861881008,-2.1040787126
C,0,0.0026874444,0.010549393,-3.7772654513
C,0,0.0193302868,-0.0149135118,-6.5969045112
C,0,-0.0921551289,1.2090931722,-4.509166176
C,0,0.106237949,-1.2009224883,-4.4866446296
C,0,0.1171237471,-1.2128913752,-5.8820835356
C,0,-0.0866528486,1.1956712489,-5.9046945564
H,0,-0.1953128114,2.1551740433,-3.9869000023
H,0,0.2041130929,-2.1370832785,-3.9456662157
H,0,0.2084703506,-2.1572381313,-6.410382358
H,0,-0.1712750013,2.1303455258,-6.4509736536
H,0,0.025789961,-0.0245146565,-7.6826694234
C,0,-1.4151090404,-2.1084963034,0.4993472135
C,0,-2.9579110703,-4.1435082436,1.6885486095
C,0,-1.1543716098,-3.4610676486,0.2201983576
C,0,-2.4696642763,-1.7906621,1.3731263115

C,0,-3.2338641494,-2.8008560496,1.9631835262
C,0,-1.916614197,-4.4701632738,0.8141237961
H,0,-0.3417446633,-3.7236160102,-0.4510097791
H,0,-2.7100727086,-0.7508155208,1.5736102962
H,0,-4.0497881605,-2.5368289883,2.629335941
H,0,-1.6942467998,-5.5102138552,0.5950266182
H,0,-3.5516819538,-4.9280113267,2.1476672104
C,0,0.0376437297,0.0158318747,2.0209735904
C,0,-0.0468465247,-0.1091047862,4.8994512578
C,0,0.5762233249,-1.1658188469,2.7520319701
C,0,-0.3848597262,1.111301553,2.7720215954
C,0,-0.4395804632,1.0404155716,4.1658962659
C,0,0.4292478399,-1.1927336807,4.2197243237
H,0,-0.7420760439,2.0043059291,2.2735834435
H,0,-0.82658915,1.8972773776,4.7100831274
H,0,0.7462762317,-2.0903666278,4.7413385472
H,0,-0.1383655594,-0.11611068,5.9794245487
C,0,1.3603766213,2.205850193,0.4816676856
C,0,2.7953473643,4.336020566,1.6357215808
C,0,2.4991106352,1.9599129275,1.2675662292
C,0,0.9622070051,3.5363337046,0.2675318281
C,0,1.6701499475,4.5926198774,0.8459654648
C,0,3.2112457671,3.016681832,1.8392482291
H,0,2.8474797755,0.9413980075,1.4119636737
H,0,0.0867989496,3.7417515323,-0.341887335
H,0,1.3422612202,5.6142831718,0.6788818356
H,0,4.0942000629,2.8090295886,2.4363326264
H,0,3.3478084783,5.1573407011,2.0819686158
H,0,1.6719912091,-1.1286455633,2.5696543587
H,0,0.3056725641,-2.1223366024,2.2908223838

E(RB3LYP) = -1156.92669880 A.U.

Zero-point correction= 0.433550 (Hartree/Particle)
Thermal correction to Energy= 0.457377
Thermal correction to Enthalpy= 0.458321
Thermal correction to Gibbs Free Energy= 0.378218
Sum of electronic and zero-point Energies= -1156.493149
Sum of electronic and thermal Energies= -1156.469322
Sum of electronic and thermal Enthalpies= -1156.468378
Sum of electronic and thermal Free Energies= -1156.548481

12o: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.014926497,0.021115984,-2.3356771774
C,0,0.0040969562,0.0107430458,0.5025323257
C,0,-0.6364464722,-1.0056025087,-1.6112354957
C,0,0.6138077526,1.0442717597,-1.6124012461
C,0,0.6430641033,1.0533537149,-0.2125247636
C,0,-0.6484147049,-1.0245190122,-0.2109657961
H,0,-1.1698256241,-1.7875538409,-2.1417111136
H,0,1.1389739631,1.8308752295,-2.1441992064
C,0,-0.0228546973,0.025522245,-3.8221686776

C,0,-0.0362471312,0.033928015,-6.6434230416
C,0,-0.1648674189,1.2278729879,-4.5386775526
C,0,0.1121343664,-1.1725513557,-4.5471190856
C,0,0.1066560488,-1.1681847151,-5.9434599916
C,0,-0.1725831294,1.2318376699,-5.9349937698
H,0,-0.2929753038,2.1631180684,-4.0018898279
H,0,0.2453704775,-2.1109359509,-4.0170898079
H,0,0.2213907436,-2.103283291,-6.4838651625
H,0,-0.2923672469,2.1701491381,-6.4686935353
H,0,-0.0412863725,0.0371712218,-7.7293163051
C,0,-1.4016905548,-2.12704234,0.463425486
C,0,-2.8684718179,-4.2294926124,1.6365989004
C,0,-1.0633330572,-3.4676752052,0.2105588535
C,0,-2.4930667867,-1.8577903847,1.3087634671
C,0,-3.2213317754,-2.899770095,1.8877013854
C,0,-1.7873273669,-4.5099143048,0.7953583655
H,0,-0.2240251083,-3.693230657,-0.4411839067
H,0,-2.7874264385,-0.829427767,1.4973578602
H,0,-4.0683685817,-2.6720867399,2.5281910453
H,0,-1.5069107383,-5.5392001275,0.5919604503
H,0,-3.4342908968,-5.039137514,2.0875671343
C,0,0.0183703191,0.0036989227,1.9953592759
C,0,-0.0312271649,0.1134489744,4.8697064934
C,0,0.4496162488,-1.0871221049,2.7222788176
C,0,-0.4255562848,1.133385593,2.731075674
C,0,-0.4463341596,1.197178583,4.1410423308
C,0,0.4477519604,-1.0965655532,4.1906830633
H,0,0.8193955856,-1.9735671156,2.2174538989
H,0,-0.7895257087,1.9937037348,2.1778804352
H,0,-0.8052456043,2.0971336987,4.6270966954
H,0,-0.0503439859,0.1231493641,5.9548259315
C,0,1.3951489527,2.1559470374,0.4624716712
C,0,2.8530950455,4.2614545141,1.6410698543
C,0,2.4866062342,1.8891699911,1.3084442859
C,0,1.0519569384,3.4965126342,0.2119894629
C,0,1.7715385837,4.5398295415,0.7993601481
C,0,3.2105372324,2.9329168447,1.8900232964
H,0,2.7844178239,0.8617100588,1.4956310248
H,0,0.2120484901,3.7202821039,-0.4395420223
H,0,1.4872980866,5.5685089655,0.5983847949
H,0,4.0575151011,2.7072064306,2.5312221091
H,0,3.4150003308,5.0722935072,2.0947349711
H,0,1.4651212151,-1.3450100506,4.552657509
H,0,-0.1136434711,-1.9778265232,4.5567304479

E(RB3LYP) = -1156.92140365 A.U.

Zero-point correction= 0.432922 (Hartree/Particle)
Thermal correction to Energy= 0.456933
Thermal correction to Enthalpy= 0.457877
Thermal correction to Gibbs Free Energy= 0.377269
Sum of electronic and zero-point Energies= -1156.488481
Sum of electronic and thermal Energies= -1156.464471
Sum of electronic and thermal Enthalpies= -1156.463527
Sum of electronic and thermal Free Energies= -1156.544135

12p: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,-0.0000000044,0.,-2.3301846304
C,0,0.0000000012,0.,0.5171680941
C,0,-1.2019765134,-0.0322411535,-1.6038935042
C,0,1.2019765075,0.0322411535,-1.6038935089
C,0,1.2295625629,0.0293046498,-0.2089637384
C,0,-1.2295625633,-0.0293046498,-0.2089637335
H,0,-2.1473806926,0.0079142483,-2.1335185623
H,0,2.1473806846,-0.0079142483,-2.1335185708
C,0,-0.0000000073,0.,-3.8124349313
C,0,-0.0000000129,0.,-6.6319489409
C,0,0.9900439376,0.6946622692,-4.5332871277
C,0,-0.9900439551,-0.6946622692,-4.5332871238
C,0,-0.9875473332,-0.6971393487,-5.9285847584
C,0,0.9875473101,0.6971393487,-5.9285847623
H,0,1.7515812798,1.2572158215,-4.0023718987
H,0,-1.7515812952,-1.2572158215,-4.0023718918
H,0,-1.7534092548,-1.2482571777,-6.4659943593
H,0,1.7534092297,1.2482571777,-6.4659943662
H,0,-0.0000000151,0.,-7.7177476919
C,0,-2.5641899641,0.0759578009,0.4507242488
C,0,-5.1168923907,0.3033994164,1.6148997028
C,0,-3.5581907188,-0.8827774742,0.1885895075
C,0,-2.874157722,1.1599846908,1.2903431348
C,0,-4.1412991682,1.2728569555,1.8663395642
C,0,-4.821704295,-0.7740748307,0.7731013211
H,0,-3.3335609719,-1.7252045314,-0.4592185392
H,0,-2.1301108367,1.92936363,1.475863829
H,0,-4.3676065963,2.1215102943,2.5049266282
H,0,-5.5740779991,-1.5305359236,0.5709714495
H,0,-6.1011948396,0.3902928361,2.0649049726
C,0,0.0000000041,0.,1.9829270576
C,0,0.0000000098,0.,4.8595738403
C,0,-0.8124839007,-0.930495041,2.7084419031
C,0,0.8124839118,0.930495041,2.7084418999
C,0,0.7973781995,0.9578633025,4.0705145868
C,0,-0.797378183,-0.9578633025,4.0705145899
H,0,-1.4049157647,-1.6495365311,2.1569097192
H,0,1.4049157736,1.6495365311,2.1569097136
H,0,1.3758963561,1.7035610632,4.6072415049
H,0,-1.3758963375,-1.7035610632,4.6072415103
C,0,2.5641899663,-0.0759578009,0.4507242387
C,0,5.1168923974,-0.3033994164,1.6148996826
C,0,2.8741577275,-1.1599846908,1.2903431234
C,0,3.5581907199,0.8827774742,0.1885894935
C,0,4.8217042984,0.7740748307,0.7731013021
C,0,4.141299176,-1.2728569555,1.8663395478
H,0,2.1301108429,-1.92936363,1.4758638206
H,0,3.3335609705,1.7252045314,-0.4592185524
H,0,5.5740780018,1.5305359236,0.5709714274
H,0,4.3676066066,-2.1215102943,2.504926611
H,0,6.1011948481,-0.3902928361,2.0649049484
H,0,0.659305537,-0.5474987909,5.5583841334

H,0,-0.6593055146,0.5474987909,5.558384136

E(RB3LYP) = -1156.93009974 A.U.

Zero-point correction= 0.433628 (Hartree/Particle)
Thermal correction to Energy= 0.457373
Thermal correction to Enthalpy= 0.458317
Thermal correction to Gibbs Free Energy= 0.379380
Sum of electronic and zero-point Energies= -1156.496472
Sum of electronic and thermal Energies= -1156.472727
Sum of electronic and thermal Enthalpies= -1156.471783
Sum of electronic and thermal Free Energies= -1156.550719

13a: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
C,0,1.2638090272,-0.6747944227,0.0280428729
C,0,-1.2923854076,0.717572995,0.0059246931
C,0,1.2921803492,0.7181159456,-0.012316793
C,0,0.000443676,-1.308967134,-0.0033949871
C,0,-1.2633619211,-0.6753734888,-0.0341589823
C,0,-0.0002577455,1.4591504328,-0.004316663
H,0,0.0007169105,-2.3984889788,-0.0035734867
C,0,2.4777641454,-1.5387454737,0.1401425498
C,0,4.7176350283,-3.2173449816,0.3862285147
C,0,2.7301756273,-2.532832657,-0.8187547876
C,0,3.3545850134,-1.3983325643,1.228375296
C,0,4.4656316354,-2.235370395,1.3506672453
C,0,3.8473950373,-3.3641835554,-0.6982651908
H,0,2.0622086869,-2.648002467,-1.6719271452
H,0,3.1628160292,-0.6406615204,1.9861263549
H,0,5.1340009638,-2.1209603158,2.202421726
H,0,4.0367734742,-4.1246192531,-1.4540278325
H,0,5.5866936995,-3.8661203941,0.4815596555
C,0,2.5171198582,1.5265671127,-0.1052427996
C,0,4.8106589067,3.1372884379,-0.3716888864
C,0,3.556315611,1.1592056316,-0.9878889999
C,0,2.6489962963,2.7213857461,0.6353332069
C,0,3.7923623787,3.5093374752,0.5124394461
C,0,4.683573025,1.9654978063,-1.1266603537
H,0,3.4627402083,0.2632821912,-1.5924761557
H,0,1.8798388047,3.0191737079,1.3451532148
H,0,3.888849667,4.4135878226,1.1106360777
H,0,5.4656351611,1.6783138773,-1.8272819351
H,0,5.6998013827,3.7575827184,-0.4724572228
C,0,-2.4769974651,-1.5401378476,-0.1433477309
C,0,-4.7197771803,-3.2160418443,-0.3815906257
C,0,-3.3579177952,-1.398221782,-1.2281031873
C,0,-2.7263602797,-2.5350576611,0.8155420563
C,0,-3.8452957333,-3.3646329097,0.6992450117
C,0,-4.4703223858,-2.233966592,-1.346558552

H,0,-3.1683708834,-0.6403648785,-1.9861826252
H,0,-2.0554424797,-2.651544306,1.6661733423
H,0,-4.0325953676,-4.1252732437,1.455319021
H,0,-5.1418931231,-2.118318879,-2.1956265582
H,0,-5.5900977802,-3.8635843322,-0.4737200433
C,0,-2.5173387296,1.5257058128,0.1019262386
C,0,-4.8092994971,3.1373105693,0.3769513628
C,0,-2.6516138214,2.7204623608,-0.6382822662
C,0,-3.5531850615,1.1591373214,0.9888482988
C,0,-4.6795275687,1.9659017003,1.1321305126
C,0,-3.7943291243,3.5087090877,-0.5112835023
H,0,-1.8850375014,3.0179303133,-1.3510731277
H,0,-3.457142929,0.2637490256,1.5937024422
H,0,-5.4587529653,1.6793623357,1.8361712823
H,0,-3.8928441137,4.4128185161,-1.1093623873
H,0,-5.6977907569,3.7579910706,0.4810337943
H,0,0.0051395119,2.1534060085,-0.8632906374
H,0,-0.0057174984,2.1561118549,0.8524522481

E(RB3LYP) = -1156.94163812 A.U.

Zero-point correction= 0.430502 (Hartree/Particle)
Thermal correction to Energy= 0.454570
Thermal correction to Enthalpy= 0.455514
Thermal correction to Gibbs Free Energy= 0.373643
Sum of electronic and zero-point Energies= -1156.511136
Sum of electronic and thermal Energies= -1156.487068
Sum of electronic and thermal Enthalpies= -1156.486124
Sum of electronic and thermal Free Energies= -1156.567995

13c: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-0.0130286987,0.1740987496,-2.3074001851
C,0,-0.0304095473,0.117688681,-1.2226749633
C,0,-0.1003012882,-0.0277199278,1.5260763442
C,0,-0.0896431291,1.2988212072,-0.4777833862
C,0,-0.0164018372,-1.1494892206,-0.6214414355
C,0,-0.0321383933,-1.222370954,0.7932994175
C,0,-0.1415184196,1.2386159697,0.9268167354
H,0,-0.1110333345,-0.0836719691,2.6101020888
C,0,-0.0356560697,2.6367253158,-1.2278227599
C,0,0.4444521078,3.9215183841,-3.7101701183
C,0,-1.1072319447,2.8610147369,-2.2143875118
C,0,1.3160271143,3.0568894417,-1.6465061786
C,0,1.5312453492,3.7041792818,-2.8383222602
C,0,-0.8678108327,3.5078027125,-3.4021468548
H,0,-2.107953743,2.5293276932,-1.9544440934
H,0,2.1337897038,2.8709278275,-0.9569213972
H,0,2.5249786285,4.0318114493,-3.1216448328
H,0,-1.6709587379,3.6908970117,-4.1067055174
H,0,0.6248038823,4.4263047697,-4.6550134036
C,0,-0.2149024318,2.456430563,1.785785443

C,0,-0.3481328923,4.7451815429,3.4230079474
C,0,-1.3326002398,3.3110666083,1.7367718825
C,0,0.82849227,2.7609473471,2.6771658448
C,0,0.762021652,3.8957231675,3.4882724173
C,0,-1.3962248774,4.4484196439,2.548430022
H,0,-2.1707626716,3.0668359899,1.0894505334
H,0,1.695793262,2.1090103759,2.7275192918
H,0,1.5780684556,4.1178492354,4.1694094428
H,0,-2.2696353323,5.0920184271,2.5037232825
H,0,-0.3977861979,5.6266553631,4.0549470111
C,0,0.0536212529,-2.505163254,1.5520466799
C,0,0.2555496777,-4.8742750051,3.0662198166
C,0,-0.8749147736,-2.7904300604,2.5676118205
C,0,1.089013778,-3.4248112233,1.3111645619
C,0,1.1905025907,-4.5966606151,2.0632808335
C,0,-0.7779451291,-3.966820509,3.3157245226
H,0,-1.6862543219,-2.0948127646,2.7629231651
H,0,1.8228334874,-3.2169181181,0.5388445323
H,0,2.0015058381,-5.291953464,1.866856308
H,0,-1.5107565586,-4.1734420046,4.0903306183
H,0,0.3333148171,-5.7880781912,3.6478405526
C,0,-0.02161831,-2.3468174152,-1.5133414384
C,0,-0.0780052565,-4.5468185983,-3.2748589208
C,0,-1.0115301721,-3.3373273777,-1.3926926088
C,0,0.9359542521,-2.4752791011,-2.5337634262
C,0,0.9111189157,-3.567800632,-3.4049960357
C,0,-1.0407503,-4.4254250188,-2.2671089661
H,0,-1.7658778866,-3.2505796815,-0.6169135857
H,0,1.7147512532,-1.724489809,-2.6358250176
H,0,1.665904068,-3.6541460596,-4.1812846968
H,0,-1.8170455435,-5.1777605227,-2.1618643375
H,0,-0.0995515459,-5.3958927792,-3.9515696756
H,0,-0.2753611895,3.4121927201,-0.4460175692

E(RB3LYP) = -1156.91170830 A.U.

Zero-point correction= 0.433273 (Hartree/Particle)
Thermal correction to Energy= 0.457089
Thermal correction to Enthalpy= 0.458033
Thermal correction to Gibbs Free Energy= 0.377126
Sum of electronic and zero-point Energies= -1156.478435
Sum of electronic and thermal Energies= -1156.454619
Sum of electronic and thermal Enthalpies= -1156.453675
Sum of electronic and thermal Free Energies= -1156.534582

13d: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,0.065321344,-0.1019729526,-2.4003487211
C,0,0.0466306265,-0.0741441808,-1.3171410086
C,0,0.0409716765,0.0426810877,1.4285645684
C,0,-1.1955755049,-0.0124590528,-0.6479208366
C,0,1.2768275791,-0.0463339019,-0.6578273996
C,0,1.2762374128,0.0412087805,0.7586742739
C,0,-1.194015993,0.0111939265,0.7779075359

H,0,0.0448538047,0.0694402254,2.5133912648
C,0,-2.4118905375,0.092866754,-1.450445078
C,0,-4.7112671745,0.4052420605,-3.1718448589
C,0,-2.5459589119,-0.7015447388,-2.7067421826
C,0,-3.4648622143,0.9427845761,-1.1004758019
C,0,-4.5646092208,1.1017128772,-1.9415611921
C,0,-3.7291537577,-0.4562369237,-3.5573956935
H,0,-3.4075365296,1.5347973716,-0.1961923203
H,0,-5.3360671688,1.8088948546,-1.6502902575
H,0,-3.7934181356,-1.0029426002,-4.492955272
H,0,-5.5856719505,0.5791600298,-3.7882891313
C,0,-2.4247967278,-0.0787364569,1.6123016818
C,0,-4.701722637,-0.2813679615,3.2568049649
C,0,-3.3503187042,-1.1221210379,1.4300597616
C,0,-2.6508859525,0.8524034737,2.6414152336
C,0,-3.7837083191,0.7553694399,3.452180945
C,0,-4.477891335,-1.2227684835,2.2470283253
H,0,-3.1760536754,-1.871096947,0.6630723248
H,0,-1.9473979783,1.665838338,2.7933901108
H,0,-3.9489677128,1.4903738909,4.2342064888
H,0,-5.1770147616,-2.0404322973,2.0990387208
H,0,-5.5804202283,-0.3588713422,3.8898614702
C,0,2.514621242,0.1526963623,1.5772401142
C,0,4.8003648756,0.4161032713,3.2019886553
C,0,2.695778381,-0.6726693696,2.7013894896
C,0,3.4958857352,1.1164712229,1.2832628893
C,0,4.6245096005,1.2504958787,2.092912591
C,0,3.8330354787,-0.5473112879,3.5023789767
H,0,1.9537753466,-1.4296718418,2.9382468111
H,0,3.3677570333,1.7717491867,0.4279858928
H,0,5.3667780396,2.0073554746,1.8572740685
H,0,3.9620718347,-1.2024614466,4.3587774626
H,0,5.6828495172,0.5174247269,3.8265670204
C,0,2.5178968503,-0.1384647571,-1.4834479446
C,0,4.8030579122,-0.3604373299,-3.1152007245
C,0,3.4681128669,-1.1474350149,-1.2511729869
C,0,2.7282878804,0.7536947044,-2.548045805
C,0,3.8639762149,0.6464227035,-3.3555239794
C,0,4.5990491199,-1.2586267353,-2.0621606148
H,0,3.3171373106,-1.8518101943,-0.4390131173
H,0,2.0093267743,1.5467357241,-2.7346589956
H,0,4.0148575045,1.3514002098,-4.1678055269
H,0,5.3201736972,-2.0481430394,-1.8719967604
H,0,5.6856417538,-0.4455767775,-3.742105594
H,0,-2.5856387578,-1.7654397869,-2.3998894654
H,0,-1.630945264,-0.6854408031,-3.3154705034

E(RB3LYP) = -1156.92826717 A.U.

Zero-point correction= 0.433800 (Hartree/Particle)
Thermal correction to Energy= 0.457593
Thermal correction to Enthalpy= 0.458537
Thermal correction to Gibbs Free Energy= 0.378683
Sum of electronic and zero-point Energies= -1156.494467
Sum of electronic and thermal Energies= -1156.470675
Sum of electronic and thermal Enthalpies= -1156.469730

Sum of electronic and thermal Free Energies= -1156.549584

13e: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,0.104778459,-0.0118189686,-2.4010513408
C,0,0.0993149801,-0.0084844119,-1.3151040399
C,0,0.0918373932,0.0187408586,1.4325436789
C,0,-1.1307419463,-0.0003313255,-0.6443971898
C,0,1.3324011808,-0.0064858197,-0.6479535177
C,0,1.3274066222,0.0267384698,0.7674710603
C,0,-1.141627418,-0.0029305074,0.7694735798
H,0,0.0909932973,0.0308555556,2.5179994175
C,0,-2.3788459461,0.0363951449,-1.4563207337
C,0,-4.8057974726,0.2550531539,-2.985113693
C,0,-2.5753959943,-0.7969550099,-2.5375918461
C,0,-3.4084907561,0.9750715767,-1.1695354159
C,0,-4.6039161381,1.081497739,-1.9093676144
C,0,-3.7897054268,-0.7335397021,-3.3615299515
H,0,-1.8289777192,-1.5394952389,-2.8033714329
H,0,-3.258158328,1.6636361482,-0.3438514556
H,0,-5.3402344694,1.8248202908,-1.6260849935
H,0,-5.7104891801,0.3182731364,-3.5815087081
C,0,-2.3927388967,-0.0485726457,1.5812868491
C,0,-4.7142503249,-0.1561434813,3.178374632
C,0,-3.3553489234,-1.0561932588,1.3850261494
C,0,-2.6120969649,0.9000348515,2.5964954007
C,0,-3.7629408415,0.8481466818,3.3858458859
C,0,-4.5044845322,-1.1099352286,2.1781337934
H,0,-3.1927447336,-1.8152299714,0.6256506433
H,0,-1.8822126648,1.6877428552,2.7596900224
H,0,-3.916801986,1.5931485508,4.1608504427
H,0,-5.2303855938,-1.9018215219,2.0186142428
H,0,-5.6080769356,-0.1973087048,3.7934666471
C,0,2.5669272759,0.1004447335,1.5957887243
C,0,4.8481711079,0.2846030491,3.2417047932
C,0,2.7683405132,-0.807332961,2.6496551964
C,0,3.5259676517,1.1058326837,1.3831779219
C,0,4.6540147067,1.1987741152,2.2006830459
C,0,3.9012797831,-0.7195323236,3.4629867666
H,0,2.0414827324,-1.5956618648,2.8244822087
H,0,3.382715505,1.8237153802,0.5816614239
H,0,5.3803295417,1.9871425179,2.0254480489
H,0,4.0432388477,-1.436438432,4.2665065393
H,0,5.728034571,0.3556877908,3.8742916354
C,0,2.5762682129,-0.0699562003,-1.4711204956
C,0,4.8693670652,-0.2358796941,-3.1031039508
C,0,3.5336692341,-1.0779687179,-1.2635777528
C,0,2.7856202428,0.8498780469,-2.5127561667
C,0,3.9240316324,0.7707062458,-3.319686056
C,0,4.6678394759,-1.161487276,-2.0736221598
H,0,3.3849863571,-1.8042341406,-0.4705338563
H,0,2.0616631982,1.6422898758,-2.6819543058
H,0,4.0724746341,1.4974205105,-4.1132099977
H,0,5.3933820044,-1.9512266645,-1.9013569934

H,0,5.7541449554,-0.299410595,-3.7295990373
H,0,-4.2532509349,-1.7386609509,-3.4090328306
H,0,-3.5129667639,-0.5936145356,-4.4249729642

E(RB3LYP) = -1156.92103615 A.U.

Zero-point correction= 0.432875 (Hartree/Particle)
Thermal correction to Energy= 0.456830
Thermal correction to Enthalpy= 0.457774
Thermal correction to Gibbs Free Energy= 0.377318
Sum of electronic and zero-point Energies= -1156.488161
Sum of electronic and thermal Energies= -1156.464206
Sum of electronic and thermal Enthalpies= -1156.463262
Sum of electronic and thermal Free Energies= -1156.543719

13f: *1,2-dichloroethane*

Charge = 1 Multiplicity = 1
H,0,-0.0934348052,0.1831838622,-2.3862300471
C,0,-0.0848797681,0.1319868461,-1.3033673064
C,0,-0.0807591939,-0.0258351442,1.4432111653
C,0,1.1565395372,0.0541012365,-0.6307044665
C,0,-1.3145142838,0.0857814262,-0.6475847859
C,0,-1.3142882725,-0.0257395588,0.7693908214
C,0,1.1548262532,0.0186402961,0.7954488661
H,0,-0.088017313,-0.0597004719,2.5277251898
C,0,2.3575842298,-0.0734842526,-1.4469812645
C,0,4.6577076174,-0.4134526677,-3.1483873666
C,0,2.4532357492,0.6289480297,-2.6946977267
C,0,3.4227042428,-0.9539333012,-1.0635170755
C,0,4.5037486501,-1.1363406338,-1.871080986
C,0,3.5443068818,0.4893880438,-3.4972941295
H,0,1.6652023948,1.3179013956,-2.9741298408
H,0,3.3372466363,-1.513227883,-0.1411259977
H,0,5.2809001212,-1.8398930537,-1.5884206045
H,0,3.6190282366,1.059159296,-4.4185536626
C,0,2.3856724419,0.1263761319,1.6232472865
C,0,4.6742355802,0.3719032208,3.2441178518
C,0,3.3205098162,1.1524778557,1.3932803442
C,0,2.6079376741,-0.764848387,2.6886925641
C,0,3.7468500475,-0.6469085991,3.4870415134
C,0,4.4541082831,1.2741851001,2.198748518
H,0,3.1464197326,1.872441389,0.5990069972
H,0,1.8984987689,-1.5653728622,2.8765459127
H,0,3.910518713,-1.35159072,4.2967701435
H,0,5.1604261302,2.0780408333,2.0142169647
H,0,5.5575315966,0.4655392398,3.868511858
C,0,-2.5532346439,-0.155292199,1.5825550584
C,0,-4.8429083783,-0.4576739534,3.1942915537
C,0,-2.7368733789,0.6425180102,2.7263926814
C,0,-3.534149114,-1.1115726576,1.2624114028
C,0,-4.6642321811,-1.2653789677,2.0660178078
C,0,-3.8764923659,0.4983206761,3.5204923928
H,0,-1.9962881219,1.394262466,2.9831291721
H,0,-3.4040260112,-1.7461441211,0.392073684

H,0,-5.4057131701,-2.0165139938,1.8106150356
H,0,-4.0082446806,1.1330311469,4.3916778003
H,0,-5.7271693247,-0.5737443345,3.8137338862
C,0,-2.5550180013,0.1912162096,-1.4723478246
C,0,-4.8383485521,0.4398628785,-3.1021245762
C,0,-3.5077391631,1.1933193862,-1.2212801094
C,0,-2.7615916876,-0.680222142,-2.5545541198
C,0,-3.8965739786,-0.5598083878,-3.3611414459
C,0,-4.637784795,1.3177885624,-2.0314757471
H,0,-3.3593109924,1.8822340345,-0.3955126075
H,0,-2.0399404972,-1.4671523543,-2.7558880453
H,0,-4.0445368687,-1.2486740692,-4.1876386739
H,0,-5.3608586933,2.1019033856,-1.8269823732
H,0,-5.7203249208,0.5353089717,-3.7283935927
H,0,5.6101079689,0.147915269,-3.1505203726
H,0,4.8214054537,-1.1352303739,-3.9694114633

E(RB3LYP) = -1156.93169051 A.U.

Zero-point correction= 0.433734 (Hartree/Particle)
Thermal correction to Energy= 0.457506
Thermal correction to Enthalpy= 0.458450
Thermal correction to Gibbs Free Energy= 0.378557
Sum of electronic and zero-point Energies= -1156.497956
Sum of electronic and thermal Energies= -1156.474184
Sum of electronic and thermal Enthalpies= -1156.473240
Sum of electronic and thermal Free Energies= -1156.553134