



Supporting Information

for

Stability trends in carbocation intermediates stemming from germacrene A and hedycaryol

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Additional figures and Cartesian coordinates for germacrene A and hedycaryol cations

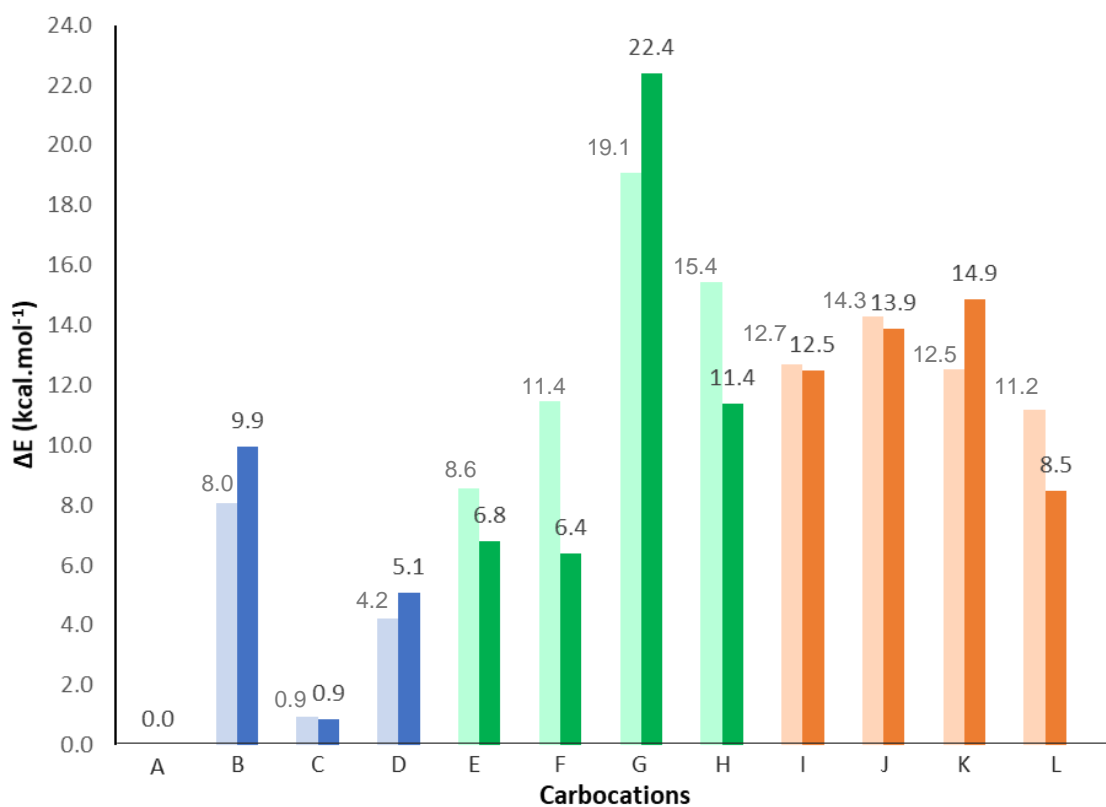


Figure S1: Relative electronic energy bar plots for germacrene A and hedycaryol carbocations with respect to **A** and **A-OH** cations, respectively. Germacrene A carbocations are shown in light color shades and hedycaryol carbocations are represented by dark shades. 6-6 bicyclic molecules are colored in blue; 5-7 bicyclics with the carbocation present on the seven membered ring in green, and 5-7 bicyclics with the carbocation on the five membered ring in orange.

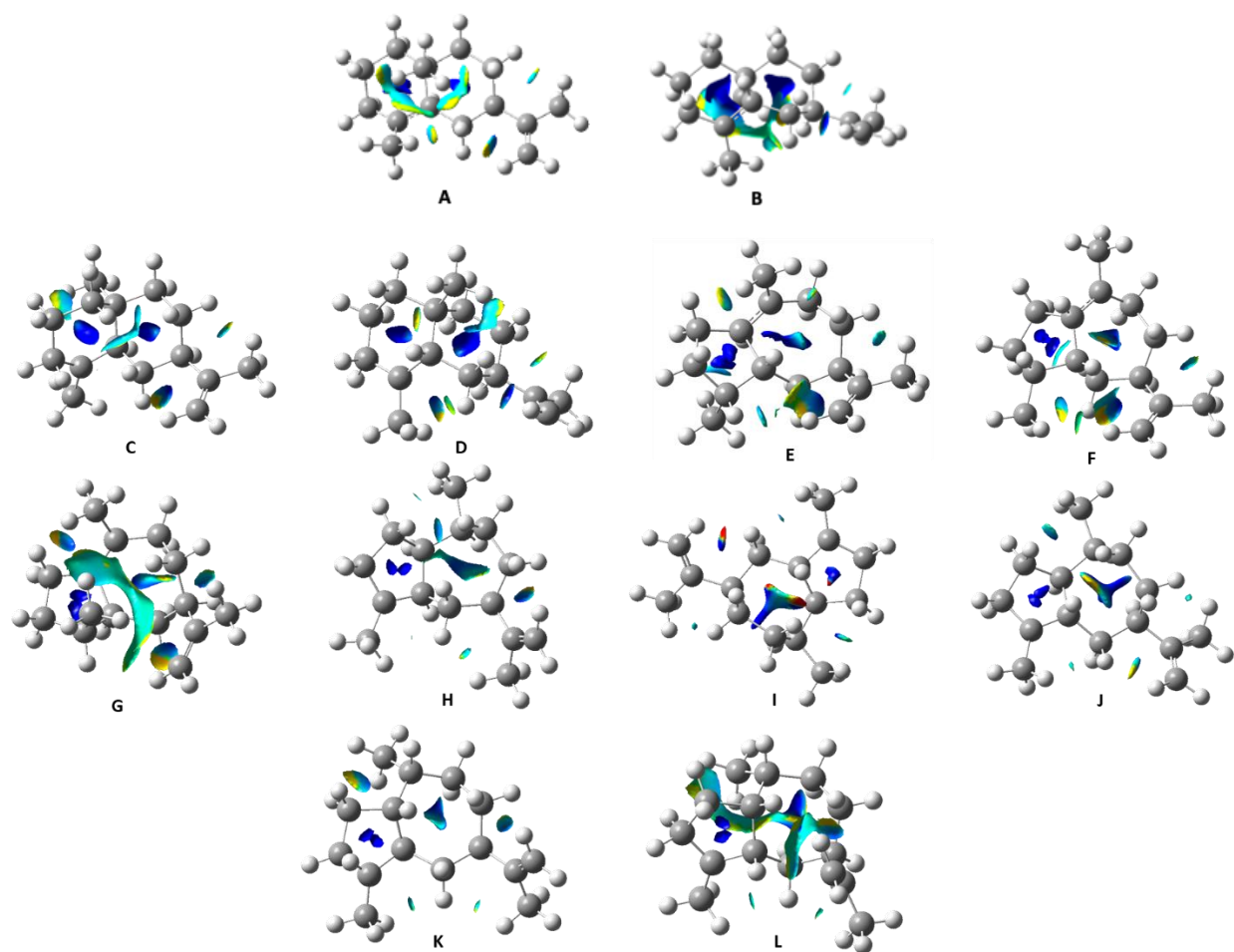


Figure S2: NCI plots for carbocations derived from germacrene A.

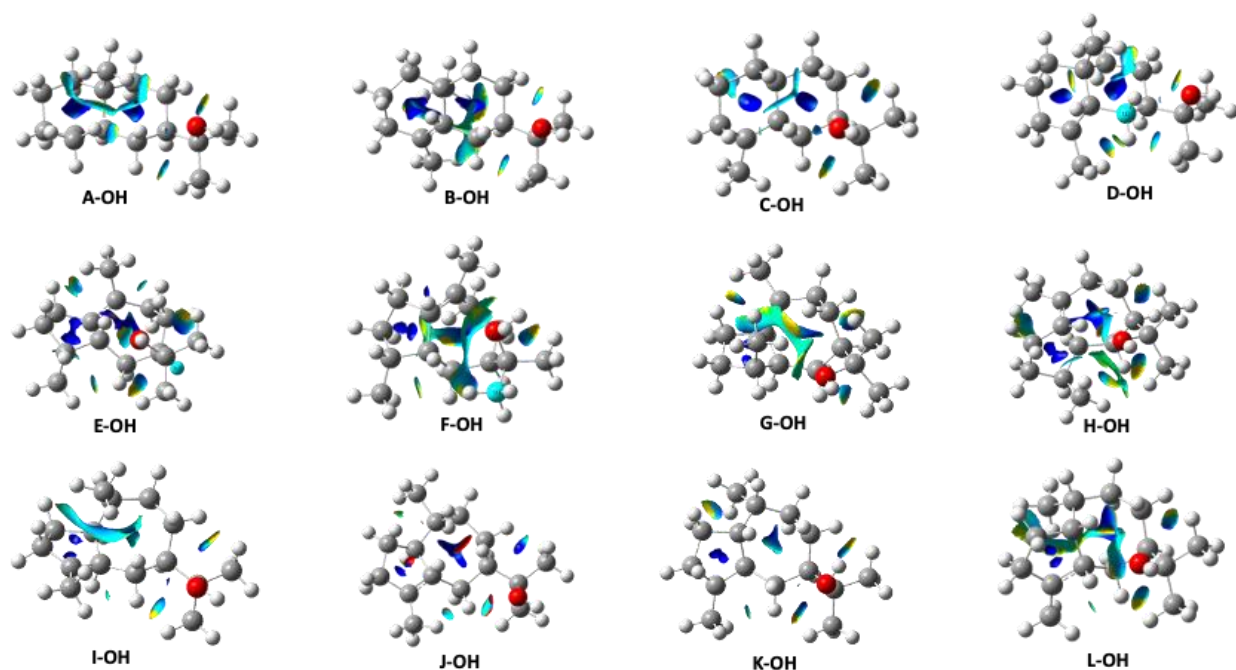


Figure S3: NCI plots for carbocations derived from hedycaryol.

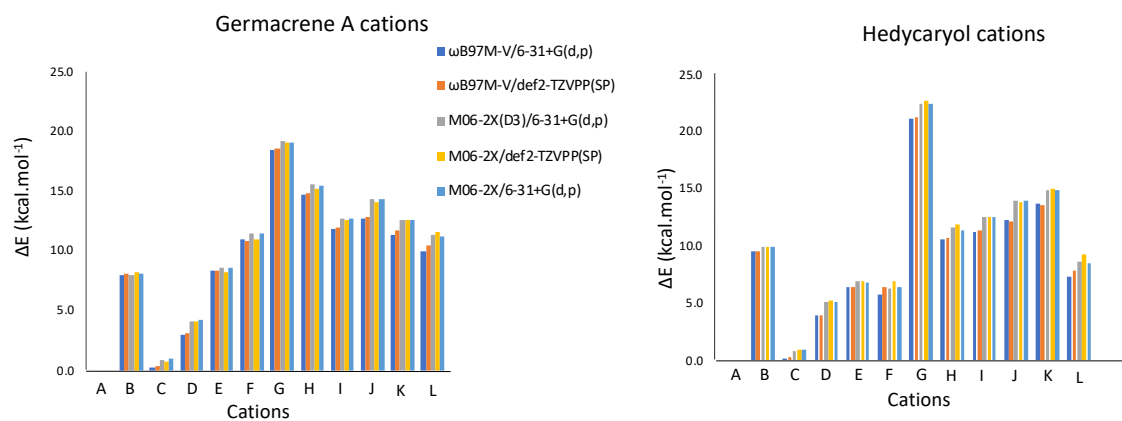


Figure S4: Comparison of energy trends with five different methods tested in this study for both germacrene A and hedycaryol carbocations.

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H -0.1233240000 2.8068580000 -0.4635110000
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H 3.3181040000 1.7902220000 0.2137850000
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H 3.0186790000 -2.0429620000 -0.3801880000
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E

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H 2.095707000 -0.742951000 -1.675384000

Hedycaryl carbocations:

A-OH

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C -0.520721000 0.855524000 -0.213388000
C -1.574242000 -0.210175000 -0.554365000
C -2.974307000 0.246699000 -0.071033000
C -4.026855000 -0.837132000 -0.312465000
C -1.181161000 -1.569192000 0.041933000
C 0.249199000 -1.977031000 -0.305811000
H 2.890331000 2.465851000 1.307650000
H 1.570023000 3.177791000 0.370854000
H 1.167208000 2.002708000 1.612773000
H 4.021601000 1.806096000 -0.689422000
H 3.181592000 0.835139000 -1.948345000
H 4.709356000 -0.608406000 -0.705845000
H 4.010459000 -0.155295000 0.843587000
H 2.616069000 -1.661738000 -1.443624000
H 3.017144000 -2.314386000 0.141390000
H 0.407931000 -0.434051000 2.068482000
H 1.424748000 -1.868415000 2.111287000
H 2.170371000 -0.272325000 2.067397000
H 0.960805000 0.146530000 -1.652641000
H -0.599581000 1.082276000 0.853607000
H -0.737047000 1.782740000 -0.754230000
H -1.627231000 -0.311404000 -1.649199000
H -5.020045000 -0.456003000 -0.054030000
H -4.052326000 -1.135040000 -1.365600000
H -3.836244000 -1.719103000 0.301956000
H -1.324870000 -1.539157000 1.127881000
H -1.847690000 -2.346412000 -0.340379000
H 0.480694000 -2.945313000 0.155563000
H 0.341830000 -2.112638000 -1.391485000
C -3.411435000 1.543922000 -0.757725000
H -2.760648000 2.379179000 -0.490154000
H -3.420707000 1.431284000 -1.846689000
H -4.426395000 1.807067000 -0.444156000
O -2.816866000 0.471831000 1.333118000
H -3.676482000 0.667368000 1.725432000

B-OH

C -1.257673000 2.313550000 0.869400000
C -1.810139000 1.286966000 -0.036390000
C -3.281008000 1.127634000 -0.145619000
C -3.687494000 -0.186375000 -0.814746000
C -2.830821000 -1.365642000 -0.295957000
C -1.438353000 -0.940685000 0.202691000
C -1.444529000 -0.733135000 1.725078000
C -0.331951000 -1.933960000 -0.185632000
C 1.063984000 -1.555871000 0.322581000
C 1.394844000 -0.050768000 0.199035000
C 2.901338000 0.173918000 -0.081749000
C 3.752130000 -0.495636000 1.000210000
C 3.248423000 1.664020000 -0.156113000
C 0.528727000 0.610594000 -0.886473000
C -0.979551000 0.388819000 -0.755742000
H -0.274881000 2.043086000 1.260294000
H -1.942897000 2.586259000 1.673176000
H -1.101755000 3.206206000 0.240470000
H -3.638693000 1.992496000 -0.729672000
H -3.724798000 1.257726000 0.849131000
H -4.749192000 -0.369241000 -0.640445000
H -3.571122000 -0.093994000 -1.898248000
H -3.344787000 -1.872570000 0.526432000
H -2.717803000 -2.099506000 -1.100132000
H -1.527990000 -1.722505000 2.186033000
H -0.530074000 -0.273649000 2.104002000
H -2.300499000 -0.149012000 2.076485000
H -0.628166000 -2.907733000 0.225644000
H -0.326816000 -2.043939000 -1.276084000
H 1.177536000 -1.871639000 1.364349000
H 1.791914000 -2.122864000 -0.264242000
H 1.203145000 0.440550000 1.162961000
H 3.586972000 -1.574519000 0.192664000
H 3.532136000 -0.076535000 1.987539000
H 4.814368000 -0.323546000 0.799005000
H 4.070318000 -0.399507000 -1.564283000
H 4.332483000 1.791622000 -0.235540000
H 2.798664000 2.134590000 -1.033158000
H 0.719146000 1.687436000 -0.924658000
H 0.848611000 0.208799000 -1.852693000
H -1.434334000 0.074889000 -1.698064000
O 3.131046000 -0.442195000 -1.347139000
H 2.922591000 2.193948000 0.745884000

C-OH

C 2.125806000 2.554292000 -1.051761000
C 1.904273000 1.336648000 -0.261241000
C 2.522704000 1.229188000 1.070581000
C 2.814136000 -0.194460000 1.572407000
C 1.711771000 -1.177618000 1.175693000
C 1.400148000 -1.140426000 -0.330802000
C 2.632042000 -1.556807000 -1.146585000
C 1.020106000 0.296644000 -0.750391000
C -0.367106000 0.780047000 -0.128100000
C -1.489372000 -0.198519000 -0.519020000
C -2.820173000 0.280252000 0.126630000
C -2.263590000 1.636549000 -0.429848000
O -2.527871000 0.398434000 1.520626000
C -3.933944000 -0.745998000 -0.092851000
C -1.120255000 -1.629765000 -0.114006000
C 0.228625000 -2.064610000 -0.686948000
H 2.303878000 3.438472000 -0.434877000
H 3.070476000 2.352575000 -1.589925000
H 1.355466000 2.724431000 -1.805536000
H 1.747375000 1.699505000 1.711419000
H 3.381113000 1.905166000 1.145020000
H 3.779245000 -0.514305000 1.693110000
H 2.927737000 -0.163064000 2.658126000
H 0.807274000 -0.967564000 1.757095000
H 2.020529000 -2.193562000 1.442624000
H 2.406022000 -1.563215000 -2.217707000
H 2.952499000 -2.565006000 -0.866679000
H 3.483357000 -0.882104000 -0.993573000
H 0.901089000 0.375883000 -1.839717000
H -0.304999000 0.819960000 0.962211000
H -0.587955000 1.785755000 -0.494803000
H -1.623423000 -0.159768000 -1.610045000
H -4.227156000 1.917640000 0.005883000
H -2.554244000 2.429426000 -0.182570000
H -3.391763000 1.595089000 -1.516166000
H -3.345503000 0.553388000 2.009224000
H -3.731555000 -1.671286000 0.449412000
H -4.057329000 -0.975711000 -1.156042000
H -4.884745000 -0.341860000 0.269521000
H -1.134588000 -1.704340000 0.979505000
H -1.880380000 -2.321419000 -0.485096000
H 0.469680000 -3.080800000 -0.351886000
H 0.149841000 -2.112491000 -1.782292000

D-OH

C -0.997145000 0.305799000 -0.787308000
C -1.629117000 1.466220000 -0.146779000
C -1.008279000 2.799788000 -0.230665000
C -2.955618000 1.384409000 0.481169000
C -3.453557000 0.010303000 0.924322000
C -2.995892000 -1.070826000 -0.048194000
C -1.477480000 -1.083234000 -0.287513000
C -1.177720000 -2.152007000 -1.347010000
C -0.709991000 -1.374067000 1.016397000
C 0.811685000 -1.302975000 0.874445000
C 1.280424000 0.055512000 0.335277000
C 2.812265000 0.112176000 0.106912000
C 3.579236000 -0.378287000 1.236827000
C 3.271410000 1.531269000 -0.244852000
C 0.530742000 0.391996000 -0.967626000
H -1.456420000 0.473077000 -1.782340000
H -1.694783000 3.603966000 0.033645000
H -0.178368000 2.792865000 0.496729000
H -0.541730000 2.979021000 -1.202777000
H -3.589011000 1.772806000 -0.347611000
H -3.045995000 2.164961000 1.246644000
H -3.090874000 -0.192844000 1.935572000
H -4.543794000 0.034560000 0.087239000
H -3.506583000 -0.936497000 -1.012541000
H -3.299903000 -2.054169000 0.325336000
H -1.529721000 -3.124301000 -0.989402000
H -1.702444000 -1.932672000 -2.283453000
H -0.114198000 -2.250872000 -1.569980000
H -1.013156000 -0.645665000 1.784425000
H -1.009202000 -2.36801000 1.388785000
H 1.251418000 -1.482748000 1.858822000
H 1.183137000 -2.094259000 0.139440000
H 1.046679000 0.820669000 1.096143000
H 3.290125000 1.079090000 2.234022000
H 3.407705000 -1.442297000 1.599300000
H 4.653701000 -0.229608000 1.188831000
H 3.014170000 2.237831000 0.551984000
H 4.359213000 1.553194000 -0.361683000
H 0.831986000 -0.323025000 -1.735588000
H 0.819650000 1.374084000 -1.345282000
H 2.383190000 1.875089000 -1.186795000
O 3.042804000 -0.762226000 -0.997172000
H 3.991997000 -0.870126000 -1.133725000

E-OH

C 3.1597150000 -1.7874300000 -0.1993710000
C 2.6089890000 -0.4253820000 -0.2299660000
C 1.6112830000 0.1512110000 -0.8073940000
C 0.3456630000 -0.7318250000 -0.9365050000
C -0.7939140000 -0.4176580000 -0.0255590000
C -1.7264700000 -1.5902210000 0.4331840000
C -2.1141520000 -2.4869030000 -0.7413510000
C -2.9378110000 -0.9019740000 1.0651550000
C -3.2943010000 0.2231350000 0.0751240000
C -1.9877140000 0.5889010000 -0.6349010000
C -1.1898710000 1.6855110000 -0.2433000000
C -1.4299770000 2.4130980000 1.0291360000
C -0.0436340000 2.1354380000 -1.0820280000
C 1.2938120000 1.6242360000 -0.4843060000
C 3.7858070000 0.5248870000 0.4701740000
H 3.8648000000 -2.1524650000 0.5541180000
H 2.3785040000 -2.5422860000 -0.3052170000
H 3.7022280000 -1.7071020000 -1.1459910000
H 2.1208810000 0.1121390000 -1.7781200000
H 0.6287470000 -1.7690570000 -0.7414350000
H -0.0238950000 -0.7209510000 -1.9674090000
H -0.3832830000 -0.0129630000 0.9835340000
H -1.1683050000 -2.1780690000 1.1721130000
H -1.2463530000 -2.9773780000 -1.1881140000
H -2.6320120000 -1.9343490000 -1.5329400000
H -2.7914390000 -3.2709160000 -0.3929010000
H -2.6617840000 -0.4841990000 2.0399110000
H -3.7707810000 -1.5891380000 1.2300970000
H -4.0038350000 -0.1273410000 -0.6773790000
H -3.7547210000 1.0862690000 0.5620540000
H -1.9540200000 0.3715850000 -1.7024770000
H -2.0854570000 3.2564910000 1.7622930000
H -1.9518460000 1.8168130000 0.7727030000
H -0.5127500000 2.8345110000 1.4442960000
H -0.1570230000 1.8112710000 -2.1197030000
H -0.0373380000 3.2312620000 -1.0591350000
H 2.0897560000 2.2648770000 -0.8692400000
H 1.2753050000 1.7647320000 0.6020820000
H 3.4643630000 1.4664980000 0.9195940000
H 4.5056100000 0.0600850000 1.1551261000
H 4.3118760000 0.7403910000 -0.4653570000
O 1.8336600000 -0.5631470000 1.4289480000
H 2.3989490000 -0.8847860000 2.1423730000

F-OH

C -2.1793050000 2.0888160000 0.8563620000
C -2.2294940000 0.6950410000 0.2272160000
C -1.2829590000 0.5747620000 -0.9891060000
C 0.1349330000 1.1514150000 -0.7769700000
C 0.9399570000 0.7231840000 0.4659780000
C 2.4288720000 1.1560150000 0.4000360000
C 2.7075540000 2.0515276000 -0.2306870000
C 3.1059620000 -0.2474990000 -0.2960360000
C 2.5266420000 -1.2615650000 0.3946900000
C 1.0347190000 -0.7852270000 0.8203970000
C 0.3082420000 -1.7954130000 0.0982890000
C -0.1643710000 -3.0004300000 0.7977110000
C 0.0578150000 -1.6633300000 -1.3476950000
C -1.2599480000 -0.8597430000 -1.5695650000
C -3.6799870000 0.3960660000 -0.1644120000
H -2.9021520000 2.1552450000 1.6757810000
H -1.1948180000 2.3323440000 1.2576160000
H -2.4502930000 2.8504250000 0.1187310000
H -1.7373260000 1.2097970000 -1.7588640000
H 0.0477250000 2.2408300000 -0.7148120000
H 0.7118290000 0.9727790000 -1.6930140000
H 0.4595870000 1.1836180000 1.3325410000
H 2.7978660000 1.1784870000 1.4353930000
H 2.1503230000 3.3094610000 0.2754180000
H 2.4420340000 2.5342520000 -1.2917850000
H 3.7704500000 2.7569070000 -0.1519700000
H 4.1968110000 -0.0113350000 -0.2125540000
H 2.8665130000 -0.0225300000 -1.3675670000
H 2.5681710000 -2.1590250000 -0.2331310000
H 3.0410810000 -1.5041280000 1.3268080000
H 0.9217010000 -0.9315660000 1.8951000000
H 0.3333860000 -3.1599350000 1.7553360000
H -1.2202650000 -2.7607360000 1.0147160000
H -0.1465860000 -3.8950090000 0.1735270000
H 0.8827140000 -1.1283670000 -1.8240730000
H -0.0515990000 -2.6439490000 -1.8154370000
H -1.3817540000 -0.8262540000 -2.6552060000
H -2.0854710000 -1.4568780000 -1.1776550000
H -3.8042150000 -0.6035250000 -0.5854400000
H -4.3239100000 0.4658750000 0.7185010000
H -0.4262400000 1.1268280000 -0.8927560000
O -1.7739260000 -0.2989390000 1.1668580000
H -2.3495610000 -0.2825440000 1.9426790000

G-OH

C -3.6966700000 -0.3770130000 1.0351280000

C -2.6764180000 -0.0581600000 -0.0619620000
C -1.4582020000 0.6848740000 0.5476840000
C -0.5767950000 -0.2483260000 1.4117090000
C 0.7810230000 -0.8046720000 0.9467070000
C 0.9757790000 -1.8297410000 -0.1993400000
C 2.4719130000 -2.1423850000 -0.0089800000
C 3.1284080000 -0.7545240000 0.1655210000
C 1.9847080000 0.1507280000 0.7241690000
C 1.8233540000 1.4683150000 0.1281440000
C 2.9812370000 2.1313060000 -0.4932940000
C 0.5583660000 2.2294890000 0.1850590000
C -0.6543300000 1.5024370000 -0.4648450000
C -3.3578010000 0.7515300000 -1.1669660000
H -4.5096790000 -0.9828010000 0.6216780000
H -3.2488720000 -0.9375770000 0.8592270000
H -4.1388580000 0.5398010000 1.4356410000
H -1.8984660000 1.4209430000 1.2356450000
H -1.1675730000 -1.1289010000 1.6764670000
H -0.3735730000 0.2578340000 2.3649580000
H 2.9037850000 -2.6802100000 -0.8560530000
H 2.6256470000 -2.7518600000 0.8862160000
H 3.9933930000 -0.7793380000 0.8309010000
H 3.4731970000 -0.3834210000 -0.8026610000
H 3.9431230000 1.7011410000 -0.2178040000
H 2.8409340000 1.9664820000 -1.5788310000
H 2.9578100000 3.2135610000 -0.3485080000
H 0.3331990000 2.3916620000 1.2519370000
H 0.7091170000 3.2145180000 -0.2603850000
H -1.2781750000 2.2947220000 -0.8848860000
H -0.3237490000 0.8883820000 -1.3050640000
H -2.7028320000 0.8675620000 -2.0344020000
H -4.2638750000 0.2351750000 -1.4994630000
C 0.7362590000 -1.3484750000 -1.6306140000
H 1.0495690000 -2.1301600000 -2.3289550000
H -0.3141810000 -1.1302270000 -1.8515489000
H 1.3396260000 -0.4603670000 -1.8736630000
H 0.3468300000 -2.7043640000 -0.0072630000
H 1.0974900000 -1.3755870000 1.8299890000
H 2.2946460000 0.5680240000 1.7207520000
H -3.6584330000 1.7419270000 -0.8094800000
O -2.1583810000 -1.2732250000 -0.6060540000
H -2.8880390000 -1.8034200000 -0.9507800000

H-OH

C -3.0166170000 -1.3789390000 0.5809210000
C -2.4463470000 -0.1790100000 -0.1772100000
C -1.5058930000 0.6831140000 1.7041240000
C -0.3819720000 -0.0847430000 1.4586410000
C 1.0276950000 -0.2684650000 0.8589060000
C 1.6037940000 -1.7083840000 0.6903030000
C 2.8429030000 -1.5114010000 -0.1879170000
C 2.3587840000 -0.5996120000 -1.3276870000
C 1.2427870000 0.2590480000 -0.7312710000
C 1.5033880000 1.5099490000 -0.1299380000
C 2.8864490000 2.0117450000 0.1015520000
C 0.3849410000 2.4147880000 0.2756410000
C -1.0204150000 1.9361650000 -0.0728190000
C -3.6060290000 0.6775320000 -0.6971990000
H -3.7778570000 -1.8746760000 -0.0293720000
H -2.2467580000 -2.1186890000 0.8051840000
H -3.4940140000 -1.0667400000 1.5149760000
H -2.1584400000 1.0388240000 1.1510093000
H -0.7545850000 -1.0761590000 1.7240180000
H -0.2443800000 0.4278000000 2.4151370000
H 3.2445600000 -2.4590860000 -0.5531450000
H 3.6384010000 -1.0260380000 0.3890320000
H 3.1601200000 0.0064950000 -1.7583330000
H 1.9335390000 -1.1895770000 -2.1423470000
H 3.6310570000 1.2185210000 0.1607510000
H 3.1299230000 2.6247290000 -0.7786060000
H 2.9466400000 2.6605900000 0.9775040000
H 0.5007770000 2.6387020000 1.3459850000
H 0.5996470000 3.3706360000 -0.2259910000
H -1.7079270000 2.7650490000 0.1128720000
H -1.0625520000 1.7447040000 -1.1498630000
H -3.2573080000 1.5057550000 -1.3173660000
H -4.2771230000 0.0632480000 -1.3061800000
C 0.6096590000 -2.6921400000 0.0776480000
H 1.1296890000 -3.6196650000 -0.1772310000
H -0.1847700000 -2.9527230000 0.7805080000
H 0.1356250000 -2.2942480000 -0.8239390000
H 1.8874760000 -2.0544280000 1.6914400000
H 1.7466340000 0.2249720000 1.5279480000
H 0.2577700000 1.3268700000 -1.1780480000
H -4.1950120000 1.0816070000 0.1318240000
O -1.6565020000 -0.6385310000 -1.2833270000
H -2.2279400000 -1.0821920000 -1.9229460000

I-OH

C 1.9429860000 2.5813060000 0.9594350000
C 2.1198620000 1.4184090000 0.0891600000

C 3.4238620000 0.8450350000 -0.2683460000
C 3.1220860000 -0.3250050000 -1.2182030000
C 1.6393010000 -0.6902700000 -0.9647690000
C 1.0305900000 0.6702860000 -0.5138670000
C -0.3532640000 0.8087350000 0.1289550000
C -1.3952160000 -0.2389460000 -0.3089390000
C -2.8151910000 0.3650190000 -0.1065820000
C -3.1062810000 1.4264150000 -1.1742710000
C -3.9254350000 -0.6866140000 -0.1542190000
C -1.1715170000 -1.5564820000 0.4524440000
C 0.0056440000 -2.4117850000 -0.0296590000
C 1.4268640000 -1.8324280000 0.0446220000
C 1.8632880000 -1.4911570000 1.4724240000
H 2.8545770000 3.1602200000 1.1036230000
H 1.6215900000 2.1735810000 1.9343830000
H 1.1072860000 3.2071530000 0.6307250000
H 3.8498570000 0.5138470000 0.6963620000
H 4.1227030000 1.6114810000 -0.6263200000
H 3.7897630000 -1.1727970000 -1.0518190000
H 3.2617280000 0.0029070000 -2.2526110000
H 1.1700460000 -0.9949510000 -1.9048600000
H -0.2601350000 0.7428570000 1.2186780000
H -0.7275400000 1.8171850000 -0.0659540000
H -1.2954810000 -0.4353890000 -1.3878600000
H -4.0548830000 1.9249640000 -0.9527910000
H -2.3350550000 2.1995810000 -1.3295460000
H -3.1962080000 0.9653020000 -2.1626410000
H -3.8488500000 -1.3076750000 -1.0525810000
H -3.8999740000 -1.3308420000 0.7264710000
H -1.0867370000 -1.3364140000 1.5247940000
H -2.0541960000 -2.1900760000 0.3453290000
H 0.0003730000 -3.3419510000 0.5498120000
H -0.1839270000 -2.7056130000 -1.0709880000
H 2.0854980000 -2.6393060000 -0.3055540000
H 1.3702520000 -0.5911940000 1.8625230000
H 1.6026450000 -2.3057640000 2.1536550000
H 2.9467080000 -1.3522400000 1.4507050000
H 1.0349490000 1.2803890000 -1.4624760000
H -4.9010430000 -0.1902020000 -0.1805440000
O -2.7702980000 0.9683610000 1.1891780000
H -3.6570380000 1.2529540000 1.4419490000

J-OH

C -1.3560760000 3.2261470000 -0.2948260000
C -1.8122470000 1.8451520000 -0.1076820000
C -3.2220590000 1.4118380000 -0.1334700000
C -3.1783600000 -0.1270680000 -0.1472120000
C -1.8718640000 -0.4355780000 0.6009280000
C -0.9594710000 0.7064920000 0.1163660000
C 0.4698340000 0.8284980000 0.6088100000
C 1.3621780000 -0.3874610000 0.2295180000
C 2.8293760000 0.0965060000 0.0886300000
C 3.3037130000 0.7700660000 1.3812790000
C 3.7865430000 -1.0471280000 -0.2562120000
C 0.8558710000 -1.0951860000 -1.0399480000
C -0.4430570000 -1.9491430000 -0.8992280000
C -1.2473100000 -1.8264230000 0.4043570000
C -2.3194940000 -2.9152550000 0.4938980000
H -2.1096460000 3.8711220000 -0.7453550000
H -0.4127860000 3.2612670000 -0.4895230000
H -1.1153540000 3.6067830000 0.7117820000
H -3.8285910000 1.9193200000 -0.8887680000
H -3.5995060000 1.7641470000 0.8484270000
H -3.1226880000 -0.4824960000 -1.1840010000
H -4.0608640000 -0.5704670000 0.1322960000
H -2.0467920000 -0.2786420000 1.6765620000
H 0.9255730000 1.7234880000 0.1719630000
H 0.4403960000 0.9677040000 1.6957270000
H 1.3614190000 1.1034690000 1.0596700000
H 4.3406060000 1.1019240000 1.2699380000
H 2.7025690000 1.6486660000 1.6265650000
H 3.2688120000 0.0706820000 2.2228750000
H 4.8216940000 -0.6974970000 -0.1841500000
H 3.6746120000 -1.8806620000 0.4443990000
H 0.7531580000 -0.3416090000 -1.8316880000
H 1.6398030000 -1.7613060000 -1.4008290000
H -1.1087780000 -1.7514870000 -1.1751250000
H -0.1715960000 -3.0047950000 -0.9962140000
H -0.5579020000 -1.9822600000 1.2423230000
H -2.9976410000 -2.8765840000 -0.3656110000
H -1.8599420000 -3.9063350000 0.5067330000
H -2.9175590000 -2.8133670000 1.4050870000
H -0.9229400000 0.5579000000 -1.0161320000
H 3.6281740000 -1.4133820000 -1.2716770000
O 2.7990150000 1.0524750000 -0.9758530000
H 3.6981940000 1.3427580000 -1.1720410000

K-OH

C -3.2549740000 1.5411850000 -0.5203080000
C -2.8423180000 0.2059310000 0.1036490000
C -3.9369310000 -0.8263740000 -0.1722960000

O	-2.7300900000	0.4513220000	1.5070750000
C	-1.4512840000	-0.2681160000	-0.4318160000
C	-0.4460200000	0.8711630000	-0.1901470000
C	1.0637230000	0.5250870000	-0.3738770000
C	1.6613060000	-0.5012090000	0.6172450000
C	3.0811810000	0.0235860000	0.8970140000
C	2.9164550000	1.5475020000	0.7891490000
C	1.8736400000	1.7391600000	-0.2189090000
C	1.6158520000	3.0056610000	-0.9030340000
C	1.5588990000	-1.9681660000	0.1574100000
C	2.6779110000	-2.3963230000	-0.7951050000
C	0.1997540000	-2.2566140000	-0.4998650000
C	-1.0346640000	-1.6240210000	0.1621560000
H	-3.2007680000	1.5008450000	-1.6132780000
H	-4.2821210000	1.7749590000	-0.2329650000
H	-2.6278540000	2.3588400000	-0.1578140000
H	-4.9064680000	-0.4115780000	0.1144770000
H	-3.7901120000	-1.7512330000	0.3926030000
H	-3.9761880000	-1.0823230000	-1.2355060000
H	-3.0205340000	-0.3234690000	2.0017010000
H	-1.5549810000	-0.4078480000	-1.5184310000
H	-0.6939260000	1.6999540000	-0.8581560000
H	-0.5747310000	1.2218610000	0.8431000000
H	1.2218380000	0.2141950000	-1.4286370000
H	1.0791720000	-0.3935080000	1.5433910000
H	3.4694730000	-0.2855620000	1.8686520000
H	3.7875840000	-0.3068710000	0.1307240000
H	3.8055490000	2.1689420000	0.6583360000
H	2.4052150000	1.9233970000	1.7049620000
H	0.9411360000	3.5642040000	-0.2277770000
H	2.5167480000	3.6105140000	-1.0188270000
H	1.0793940000	2.8791250000	-1.8452060000
H	1.6327170000	-2.5825190000	1.0638000000
H	3.6546920000	-2.4374990000	-0.3071040000
H	2.4682320000	-3.3952850000	-1.1867680000
H	2.7533700000	-1.7228380000	-1.6591860000
H	0.0786530000	-3.3438240000	-0.5309660000
H	0.2396360000	-1.9429480000	-1.5542700000
H	-1.8678630000	-2.3152180000	0.0212090000
H	-0.8923200000	-1.5356010000	1.2477310000

L-OH

C	-1.9988120000	-2.4951490000	-1.1748210000
C	-1.8491880000	-1.4556370000	-0.1498400000
C	-2.9031120000	-1.0891370000	0.8098010000
C	-2.2975050000	0.0038840000	1.7073980000
C	-1.0843970000	0.5549140000	0.9227550000
C	-0.6694840000	-0.6497530000	0.0409380000
C	0.2995340000	-0.4505380000	-1.1232140000
C	1.5564500000	0.3670800000	-0.7742870000
C	2.5325030000	-0.3910880000	0.1582090000
C	2.9436890000	-1.7484720000	-0.4176760000
C	3.7823240000	0.4460270000	0.4319600000
C	1.2368730000	1.7921900000	-0.2483270000
C	-0.1238160000	2.3553330000	-0.6776110000
C	-1.3638260000	1.8284450000	0.1033110000
C	-2.5661660000	1.6952810000	-0.8344590000
H	-2.1169470000	-1.9667510000	-2.1355710000
H	-2.8623890000	-3.1397440000	-1.0145760000
H	-1.0794250000	-3.0806020000	-1.2799410000
H	-3.3276010000	-1.9676820000	1.3110830000
H	-3.7227020000	-0.7084910000	0.1726190000
H	-1.9621770000	-0.4450600000	2.6466620000
H	-3.0238220000	0.7800670000	1.9580100000
H	-0.2668610000	0.7604330000	1.6137660000
H	-0.1760440000	-1.3530310000	0.7783070000
H	0.5936990000	-1.4188060000	-1.5386410000
H	-0.2433440000	0.0667500000	-1.9222550000
H	2.0884090000	0.4798180000	-1.7282630000
H	2.0977020000	-2.4400920000	-0.4600580000
H	3.3640570000	-1.6426570000	-1.4226290000
H	3.7079830000	-2.2083060000	0.2162690000
H	4.4762970000	-0.1124450000	1.0690740000
H	4.3055510000	0.6760050000	-0.5011950000
H	1.3141340000	1.8067140000	0.8436760000
H	2.0163800000	2.4688440000	-0.6101400000
H	-0.0991910000	3.4434590000	-0.5678770000
H	-0.2645890000	2.1807870000	-1.7518790000
H	-1.6208110000	2.5855610000	0.8558610000
H	-3.5029290000	1.5227700000	-0.2951050000
H	-2.6948110000	2.6102100000	-1.4188960000
H	-2.4256960000	0.8789130000	-1.5596490000
H	3.5364230000	1.3827270000	0.9354460000
O	1.8115190000	-0.6039640000	1.3868010000
H	2.4261470000	-0.9079610000	2.0666620000