

Quantum-Chemical Predictions of Redox Potentials of Carbamates in Methanol

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Supporting Information

1.1 Optimized geometries at HF/6-31G(d) level:

tert-butyl indoline-1-carboxylate (1):

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1\1\GINC-HER05-16\FOpt\RHF\6-31G(d)\C13H17N1O2\LHAYA\29-Nov-2010\0\#\#opt freq hf/6-31g(d) geom=connectivity maxdisk=2000MB\261110_1\0,1\N,1.4100298276,0.2792430342,0.4187995437\C,2.8074151281,0.6892935381,0.6152541824\C,3.6307814513,-0.6048674226,0.4596392664\C,2.5905434605,-1.6614690778,0.1791357169\C,1.3162655318,-1.1047472657,0.1646224119\C,0.2053440294,-1.8964269038,-0.0750784563\C,0.4013412477,-3.254115331,-0.2989318177\C,1.6653333243,-3.8157050692,-0.2861525414\C,2.7700610263,-3.0089701636,-0.044381173\C,0.4535771573,1.2387674005,0.5052890035\O,0.7290763353,2.3830525583,0.7331096549\O,-0.766331104,0.7732127918,0.3150186124\H,2.9196495272,1.1360372116,1.5929601238\H,4.3461856894,-0.522767083,-0.3516485329\H,4.1926494111,-0.8263541655,1.3607507323\H,-0.7796373234,-1.4839906483,-0.0895124554\H,-0.4561006065,-3.8761320246,-0.4858832302\H,1.7923130992,-4.868582069,-0.4619825907\H,3.7596653948,-3.4321880234,-0.0314633323\H,3.0715016412,1.4382723155,-0.1178553158\C,-1.9427194809,1.6215852793,0.3619478224\C,-3.076141317,0.6376663655,0.0868750651\H,-4.0296692575,1.154036293,0.0949524061\H,-2.9490911057,0.1690922109,-0.8826665438\H,-3.1009991283,-0.138484127,0.8436308532\C,-1.8780752231,2.6789666881,-0.7374270279\H,-2.8252517485,3.2068581621,-0.7844957106\H,-1.0914295671,3.3950551065,-0.5535350249\H,-1.7070174826,2.2086063858,-1.7002864159\C,-2.0979056105,2.2366843484,1.7506758613\H,-3.0550679086,2.7444826031,1.8138927446\H,-2.0783682855,1.4604182647,2.5087229531\H,-1.3137860334,2.948737517,1.959316785\Version=EM64L-G09RevA.02\State=1-A\HF=-706.4037726\RMSD=6.491e-09\RMSF=1.430e-05\Dipole=-0.1813801,-0.5338234,-0.1106695\Quadrupole=8.4172556,-4.5463012,-3.8709544,-3.5855231,0.4490448,-0.443009\PG=C01 [X(C13H17N1O2)]\@
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tert-butyl 1*H*-indole-1-carboxylate (2):

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1\1\GINC-HER05-14\FOpt\RHF\6-31G(d)\C13H15N1O2\URIETA\22-Jan-2011\0\#\#opt freq hf/6-31g(d) maxdisk=2500MB geom=connectivity\aromatico_1\0,1\C,0.1013656915,-0.3999054575,0.1346727089\C,0.175589108,0.0032762537,1.4695545925\C,1.2185453105,0.7941575627,1.9392444785\C,2.1863419944,1.1694186712,1.0295997213\C,2.1276366812,0.7748418902,-0.3101809084\C,1.0902021757,-0.0086080836,-0.7651939713\C,-1.0968864607,-1.2022735293,-0.0051290694\C,-1.6843759315,-1.2578569749,1.1928616492\H,1.2673597625,1.0984093535,2.9636220176\H,3.0055892962,1.781160466,1.3628246412\H,2.9011624168,1.0877559212,-0.9884506947\H,1.0416778454,-0.3141683015,-1.7953686659\H,-1.4535060886,-1.6687486204,-0.900802415\H,-2.5804832981,-1.7483417113,1.4987526617\C,-1.246038065,-0.3732349358,3.4604564712\O,-0.5727053972,0.2576128496,4.2142452261\O,-2.3604941295,-1.0047081337,3.7602467825\N,-0.9391500529,-0.5328552041,2.1274415526\C,-2.930342923,-1.0118008101,5.0987957643\C,-1.9672812351,-1.6802163226,6.0760962343\C,-3.2969584087,0.4081899393,5.5213532866\C,-4.1855017679,-1.8590785799,4.9178462921\H,-1.6806234772,-2.6606668835,5.7104325857\H,-1.0763464006,-1.0885667191,6.2254267166\H,-2.4612055658,-1.8093524323,7.0336169516\H,-3.9300584813,0.8719546817,4.7721650671\H,-3.850213809,0.372546256,6.4541565687\H,-2.4190902549,1.0204320278,5.6647742046\H,-4.7156420837,-1.946536319,5.8596367224\H,-4.8500255167,-1.4068481503,4.1903938286\H,-3.9280649153,-2.8547753413,4.5749065333\Version=EM64L-G09RevA.02\State=1-A\HF=-705.2352246\RMSD=6.376e-09\RMSF=8.249e-06\Dipole=-0.9199974,-0.543058,0.1669952\Quadrupole=1.0161961,-4.0823799,3.0661838,3.2908278,-4.5799779,-0.4948282\PG=C01 [X(C13H15N1O2)]\@
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tert-butyl (*S,S*)-octahydro-1*H*-indole-1-carboxylate (3):

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1\1\GINC-LOST\FOpt\RHF\6-31G(d)\C13H23N1O2\LUIA\06-Sep-2010\0\#\#opt=c alcfc freq hf/6-31g(d) geom=connectivity\060910_1\0,1\N,0.0762357614,-0.9654796828,-1.0822909513\C,-1.104625167,-0.2432962938,-0.5997540203\C,-0.9234768665,-0.240080162,0.9210460164\C,0.5963919728,-0.2822769436,1.1006867683\C,1.0273375068,-1.2698878616,-0.0007859766\C,1.2080568288,1.1211309902,0.9454447274\C,2.7114338204,1.1011488882,0.6759091943\C,3.0119590015,0.2571047279,-0.5613441413\C,2.5114760795,-1.1734048308,-0.3696596497\H,-2.0138720172,-0.741747577,-0.9026542938\H,-1.3854394127,0.6227104802,1.3886609125\H,-1.3765355726,-1.1302105104,1.3471150674\H,0.8761847095,-0.6811921246,2.0712653131\H,0.8404584918,-2.2843016691,0.3441863012\H,0.7231616994,1.6425207659,0.1238051922\H,0.9877392349,1.6944089068,1.8425827213\H,3.0750059272,2.1170547522,0.5472908718\H,3.2384326035,0.6871503721,1.5344841779\H,2.5381101819,0.7049800482,-1.4319651904\H,4.0798107122,0.2414364114,-0.7614198322\H,3.0629239303,-1.623363479,0.4549792981\H,2.7076134065,-1.7779634363,-1.242082196\H,-1.1327813258,0.7597636265,-1.0094961298\C,0.066680728,-1.6788222824,-2.2319795445\O,0.8661195832,-2.5301477549,-2.5097753671\O,-0.938096049,-1.3069533723,-3.0160992876\C,-1.1793356761,-1.8912664829,-4.3160961753\C,0.0012380744,-1.6248125922,-5.2476255633\C,-1.4851227624,-3.3819526452,-4.1850435579\C,-2.415431066,-1.1360530838,-4.7970937936\H,0.2251659057,-0.5631973023,-5.2734719305\H,0.8837487205,-2.1598808904,-4.9307640938\H,-0.2542875362,-1.9393446305,-6.2546427357\H,-2.2908873745,-3.5380898247,-3.4746806486\H,-1.8052638071,-3.7714214461,-5.1463444
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016\H,-0.6188736924,-3.9366682095,-3.857315286\H,-2.7079813825,-1.4813
788528,-5.7827772516\H,-3.2461073168,-1.292161545,-4.1178353757\H,-2.2
145678994,-0.0720266295,-4.8503593678\Version=EM64L-G09RevA.02\State=
1-A\HF=-709.9034739\RMSD=7.463e-09\RMSF=4.163e-06\Dipole=-0.6876561,0.
5369986,0.3330775\Quadrupole=-0.7083647,-3.6057857,4.3141504,2.1687043
,2.1600573,0.3016507\PG=C01 [X(C13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate (4):

1\1\GINC-HER05-15\FOpt\RHF\6-31G(d)\C10H19N1O2\LHAYA\11-Nov-2010\0\#o
pt freq hf/6-31g(d) geom=connectivity\101110_6\0,1\C,-1.3002220266,0
.5414738154,-0.3718056509\C,-1.7506838916,0.1384067323,1.0336491318\C,
-3.2308527582,0.4464992371,1.247808795\N,-4.0370204493,-0.1614415024,0
.1988238812\C,-3.6765072246,0.2134245194,-1.161150559\C,-2.2042945292,
-0.0975709323,-1.4276298026\C,-5.1703876582,-0.8231231171,0.5389498334
\O,-5.5089029904,-1.0263308291,1.6727743273\O,-5.8489449591,-1.2303171
895,-0.5255228853\C,-7.0790351295,-1.9853362611,-0.4300670882\C,-6.832
6343596,-3.3235195366,0.2632263024\C,-8.1583772678,-1.1622253867,0.269
7225869\C,-7.4472594448,-2.2066777033,-1.8947378951\H,-1.5887735196,-0
.926655661,1.1789247603\H,-1.16446996,0.6590469346,1.7858464555\H,-3.5
732023627,0.0746746158,2.1982763274\H,-3.3853271108,1.5255071303,1.236
0975509\H,-4.3076303359,-0.3120617868,-1.8557550073\H,-3.8530637356,1.
2808473865,-1.2945089848\H,-1.9398532869,0.2554636567,-2.4207633114\H,
-2.0678197065,-1.1760708037,-1.4214204499\H,-6.5833731294,-3.189502557
6,1.3049305097\H,-7.7261822652,-3.9359757696,0.1941829742\H,-6.0224658
605,-3.8549623358,-0.2258359152\H,-8.2663988299,-0.1972160053,-0.21513
82913\H,-9.1094227962,-1.6809853395,0.2011176946\H,-7.9230948763,-1.00
4957609,1.3113910483\H,-6.6651951347,-2.7573130298,-2.4055658987\H,-8.
3701184555,-2.7714474144,-1.9697096688\H,-7.5832300918,-1.2576515401,-
2.4012952121\H,-1.3441983397,1.6253503414,-0.4679579239\H,-0.265843803
5,0.2547715412,-0.5362756244\Version=EM64L-G09RevA.02\State=1-A\HF=-5
93.96297\RMSD=6.643e-09\RMSF=3.931e-06\Dipole=0.2851178,0.1623508,-0.8
955851\Quadrupole=3.4935726,0.8526893,-4.3462619,2.7283172,2.0482,0.79
296\PG=C01 [X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate (5):

1\1\GINC-LOST\FOpt\RHF\6-31G(d)\C9H17N1O2\LUISA\06-Jul-2010\0\#opt=ca
lfc freq hf/6-31g(d) geom=connectivity\carbamat\0,1\N,0.8447566429
,-0.5347396726,-0.4501271396\C,0.6336070434,-1.4063462204,0.6994202837
\C,0.1352529374,-2.7027383394,0.0559207728\C,-0.5879076554,-2.21896532
64,-1.204749854\C,0.2864224369,-1.061259044,-1.689142088\H,1.547794043
5,-1.5408571223,1.2605899069\H,-0.1088277963,-0.985203382,1.3708084683
\H,0.9809106702,-3.3262855451,-0.2184680405\H,-0.4985002423,-3.2767837
193,0.7215138333\H,-0.7043585029,-2.992647888,-1.9542763932\H,-1.57741
67312,-1.8526970787,-0.9475803519\H,1.0776517866,-1.4061004709,-2.3479
757395\H,-0.2677872614,-0.2957650627,-2.2135529179\C,1.4600214336,0.66
2063625,-0.4255789607\O,1.856967641,0.9734126643,0.8026212629\O,1.6188
092138,1.3467107172,-1.3991513473\C,2.5516766635,2.2020392753,1.113703
3941\C,1.6656148053,3.4073972588,0.8063027005\C,3.8851765794,2.2633905
097,0.3717236209\C,2.7847748045,2.0834302078,2.6173131194\H,0.70756269
35,3.3047643133,1.305928719\H,2.1419349788,4.3105269457,1.1748196716\H
,1.4961690827,3.512537328,-0.2547497198\H,3.740335073,2.3565255121,-0.
6940953661\H,4.4556677058,3.1177664201,0.7222897051\H,4.4653982398,1.3
677356969,0.5697374206\H,3.3812541217,1.2063901204,2.8424344798\H,3.30
6923624,2.9589154682,2.9878484525\H,1.8406549679,1.9974267791,3.143411
9274\Version=EM64L-G09RevA.02\State=1-A\HF=-554.9261569\RMSD=5.637e-0
9\RMSF=4.046e-06\Dipole=-0.2261103,-0.7041551,0.7697953\Quadrupole=0.8
030076,2.7814474,-3.584455,2.6841491,1.6534702,3.9226288\PG=C01 [X(C9H
17N1O2)]\@

tert-butyl diethylcarbamate (6):

1\1\GINC-HER03-41\FOpt\RHF\6-31G(d)\C9H19N1O2\LHAYA\20-Nov-2010\0\#op
t freq hf/6-31g(d) maxdisk=2000MB\191110_25\0,1\N,-1.5048717608,-0.1
352975934,0.6748694638\C,-1.7986758615,1.2550564762,1.0028589286\C,-2.
556369036,-1.1451036992,0.7471619317\H,-2.6297895005,1.2474715503,1.69
74107284\H,-0.9538338946,1.6759761413,1.52689169\H,-3.2938471479,-0.79
04569035,1.456936061\H,-2.1270853455,-2.050510991,1.1504542108\C,-0.28
30512529,-0.5431727943,0.2579898397\O,0.586933056,0.4578703639,0.21469
17987\O,-0.0269020215,-1.6799242096,-0.0333939554\C,1.9676222011,0.281
6847286,-0.1797418666\C,2.0517006372,-0.201354853,-1.626027643\C,2.682
435181,-0.6609834274,0.7859963146\C,2.5323792131,1.6943566479,-0.05788
91866\H,1.488206774,0.4608573833,-2.2756998824\H,3.087215092,-0.189481
5729,-1.9512847699\H,1.6664460524,-1.2042563645,-1.7311861378\H,2.3051
119827,-1.6692977927,0.7067328712\H,3.7449904827,-0.6676485172,0.56427
61079\H,2.5546132109,-0.3178777039,1.8077192433\H,2.4380178717,2.05642
20222,0.9597818503\H,3.5821392402,1.7045014218,-0.3302273312\H,2.00103
46434,2.375795427,-0.7128428608\C,-3.2237448283,-1.4529297246,-0.59068
68438\H,-3.7099359117,-0.5768110094,-1.0065492993\H,-2.4926672093,-1.8
141594244,-1.3032127243\H,-3.9782533691,-2.2235470217,-0.4599581785\C,
-2.142993417,2.1288547867,-0.2011371872\H,-1.3224641936,2.147850906,-0
.9084739537\H,-3.0277248636,1.7684674233,-0.7142468814\H,-2.3350623345

,3.1482364342,0.1217906921\\Version=EM64L-G09RevA.02\\State=1-A\\HF=-556
.0863208\\RMSD=4.624e-09\\RMSF=6.250e-06\\Dipole=-0.1507359,0.8875494,0.2
246947\\Quadrupole=5.0337083,-4.4046702,-0.6290382,0.6991253,-1.83887,-
0.2398361\\PG=C01 [X(C9H19N1O2)]\\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate (7):

1\\1\\GINC-LOST\\FOpt\\RHF\\6-31G(d)\\C11H19N1O4\\LUISA\\06-Jul-2010\\0\\#opt f
req hf/6-31g(d) geom=connectivity\\carb_01\\0,1\\N,-1.2183593712,-0.212
169293,0.0314888175\\C,-1.7040370183,1.1386785543,-0.2069938254\\C,-3.15
07468586,1.0459943204,0.2728178204\\C,-3.558425665,-0.3787532817,-0.115
0217108\\C,-2.2685325613,-1.2056091493,0.0904692614\\H,-1.1185777865,1.8
581488569,0.3450146017\\H,-1.6490873197,1.3900998661,-1.2619874486\\H,-3
.1869996163,1.1680764551,1.3507611026\\H,-3.7893146164,1.7993099094,-0.
172889766\\H,-4.3826315391,-0.766830573,0.4691636265\\H,-3.8472797469,-0
.4027661159,-1.160202308\\H,-2.2643124518,-1.713039388,1.0452865383\\C,0
.0705728908,-0.5992989769,0.1338309769\\O,0.8997754653,0.4198317097,-0.
0118973412\\O,0.3889602697,-1.7373879144,0.3468738488\\C,2.3398294408,0.
2731828615,0.034102518\\C,2.8142603198,-0.6451053124,-1.089695989\\C,2.7
791176689,-0.2216811349,1.4102052708\\C,2.8275039193,1.6997748536,-0.20
06831632\\H,2.4342637276,-0.2964284531,-2.0441637046\\H,3.898866402,-0.6
3210784,-1.1320770416\\H,2.4850434969,-1.6617284716,-0.9358328864\\H,2.4
489562491,-1.2337638708,1.5903529986\\H,3.8621341343,-0.1916567032,1.47
60360979\\H,2.3773133508,0.4219053547,2.1863557066\\H,2.4576090905,2.361
9841334,0.5742251931\\H,3.9115317685,1.7323421919,-0.1919282788\\H,2.479
6079066,2.0679891687,-1.1591127909\\C,-2.1297350943,-2.2472602368,-1.00
67543026\\O,-1.6993276403,-2.0306734442,-2.0917994377\\O,-2.6277989176,-
3.4095720245,-0.6249979609\\C,-2.5877887207,-4.4649437328,-1.5693860685
\\H,-3.0216215725,-5.3198385284,-1.0748255853\\H,-3.1607644654,-4.208700
5845,-2.4490042653\\H,-1.5672217291,-4.6733191866,-1.8545466641\\Versio
n=EM64L-G09RevA.02\\State=1-A\\HF=-781.5685454\\RMSD=5.307e-09\\RMSF=2.259
e-06\\Dipole=-0.5809965,0.6509046,0.3276041\\Quadrupole=5.3659804,1.6909
275,-7.056908,2.8845953,-0.2985267,2.7442371\\PG=C01 [X(C11H19N1O4)]\\@

tert-butyl indoline-1-carboxylate radical cation (1):

1\\1\\GINC-HER05-17\\FOpt\\UHF\\6-31G(d)\\C13H17N1O2(1+,2)\\LHAYA\\29-Nov-2010
\\0\\#opt freq uhf/6-31g(d) maxdisk=2500MB geom=connectivity\\291110_7\\
\\1,2\\N,1.4445102378,0.2226646565,0.4124169951\\C,2.8510819736,0.6698651
731,0.6166313334\\C,3.6838871741,-0.6098801541,0.463440243\\C,2.65387344
41,-1.6676638843,0.1834885292\\C,1.3443156424,-1.0746930541,0.172687049
9\\C,0.1795121572,-1.8729286756,-0.0728982284\\C,0.3693713577,-3.2180267
991,-0.2955143205\\C,1.6585151427,-3.8018612456,-0.2849248911\\C,2.80393
9114,-3.0189345867,-0.0437538312\\C,0.4236232489,1.2461261874,0.5037622
073\\O,0.7849505661,2.3449479863,0.7302927573\\O,-0.7569067189,0.7766736
225,0.3166202346\\H,2.9189677754,1.1203793014,1.5941119295\\H,4.39450054
-0.5261892647,-0.3498173023\\H,4.241344354,-0.8311600651,1.3654679331\\
H,-0.792584681,-1.4347848598,-0.0812457881\\H,-0.4851503968,-3.84052176
76,-0.4822738455\\H,1.7610222939,-4.8553097232,-0.4633800108\\H,3.778412
4456,-3.4703627278,-0.0375364099\\H,3.0712150186,1.4247660807,-0.121425
8363\\C,-1.9898157153,1.6368233958,0.3604986678\\C,-3.0917220897,0.62571
94637,0.0838621615\\H,-4.0507537228,1.1290343397,0.088542638\\H,-2.95947
85769,0.1621804599,-0.8870051534\\H,-3.1123063303,-0.1452067964,0.84555
01269\\C,-1.8981135343,2.6813196749,-0.7425853102\\H,-2.8418568323,3.211
7721965,-0.7953631245\\H,-1.1167904849,3.4034285882,-0.5540032472\\H,-1.
7259407974,2.2104092253,-1.7039805675\\C,-2.1183217133,2.2386509036,1.7
524621057\\H,-3.0729225962,2.7472719174,1.8221289843\\H,-2.0977118163,1.
4628220481,2.5096626935\\H,-1.3385243796,2.9579370834,1.9573748464\\Ver
sion=EM64L-G09RevA.02\\State=2-A\\HF=-706.1822966\\S2=1.185658\\S2=1=0.\\S2
A=0.900101\\RMSD=8.101e-09\\RMSF=7.839e-06\\Dipole=0.9805284,-1.6560178,-
0.207233\\Quadrupole=11.4275314,3.3090108,-14.7365421,-10.9249972,0.415
1701,2.3313689\\PG=C01 [X(C13H17N1O2)]\\@

tert-butyl 1H-indole-1-carboxylate radical cation (2):

1\\1\\GINC-HER05-16\\FOpt\\UHF\\6-31G(d)\\C13H15N1O2(1+,2)\\URIETA\\25-Jan-201
1\\0\\#opt freq uhf/6-31g(d) maxdisk=2500MB geom=connectivity\\aromatic
o_6\\1,2\\C,-2.6088916137,0.9677341864,-0.0000340799\\C,-1.7149059463,-0
.1463232922,-0.0000209552\\C,-2.1586841915,-1.4465412278,-0.0000174658\\
C,-3.5578842683,-1.637114708,-0.0000274947\\C,-4.4691792593,-0.55870762
23,-0.0000405963\\C,-4.0183989272,0.7487268711,-0.0000441411\\C,-1.84449
14244,2.1188250302,-0.0000344955\\C,-0.4837236312,1.7062403305,-0.00002
12792\\H,-1.4854979419,-2.2776698381,-0.000075684\\H,-3.9361807055,-2.6
41816392,-0.0000250857\\H,-5.5226920461,-0.763260294,-0.0000478455\\H,-4
.6957523285,1.5813612751,-0.0000540873\\H,-2.1693759645,3.1391905527,-0
.0000427937\\H,0.395564022,2.3155367525,-0.0000178372\\C,0.8200910489,-0
.373573595,0.0000006228\\O,0.769973617,-1.5505839189,0.0000233732\\O,1.8
265815015,0.4281072885,0.0000246069\\N,-0.4000850372,0.3878750896,-0.00
00141231\\C,3.2543967979,-0.0389644592,0.0000649979\\C,3.5074502446,-0.8
362000031,1.2713765445\\C,3.5075039467,-0.8362459893,-1.2712067566\\C,4.
0162420332,1.2769873364,0.0000582184\\H,3.2390695572,-0.2569502668,2.14
77664648\\H,2.9617614192,-1.7689599154,1.2799282729\\H,4.5654212378,-1.0
63549839,1.3330362\\H,3.2391690446,-0.2570246786,-2.1476295672\\H,4.5654

760255,-1.0636062369,-1.3328086509\H,2.9618070348,-1.7690012773,-1.279
7511541\H,5.0807298646,1.0765625316,0.0000846548\H,3.78144889,1.861304
3085,-0.8819062237\H,3.781411,1.8613350008,0.8819922448\Version=EM64L
-G09RevA.02\State=2-A\HF=-705.0060876\S2=1.190752\S2-1=0.\S2A=0.907514
\RMSD=5.737e-09\RMSF=2.621e-05\Dipole=-1.375815,1.5423176,-0.0000384\Q
uadrupole=22.8448376,-4.2763219,-18.5685157,-0.2195822,0.0005833,-0.00
012\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate radical carbocation (3):

1\1\GINC-LOST\FOpt\UHF\6-31G(d)\C13H23N1O2(1+,2)\LUISA\07-Sep-2010\0\#
opt=calcfc freq uhf/6-31g(d) geom=connectivity\070910_4\1,2\N,-0.03
93972333,-1.2976533317,-0.8145086292\C,-1.2487816237,-0.7078673403,-0.
2166961499\C,-0.845004495,-0.4749607185,1.242373269\C,0.6767571414,-0.
2756290037,1.1774936389\C,1.1156654924,-1.3115027764,0.1249187626\C,1.
056927638,1.1649223248,0.7917802751\C,2.4972865408,1.2925876932,0.2954
96709\C,2.738008046,0.3735052588,-0.9020375347\C,2.4834302417,-1.08682
57325,-0.5251066804\H,-2.0775422538,-1.3866601712,-0.3662804822\H,-1.3
636422651,0.3767816571,1.6612537504\H,-1.097052595,-1.3453985885,1.836
9474551\H,1.1441003523,-0.5289041112,2.1214202873\H,1.0708412388,-2.31
61573522,0.5398921059\H,0.3907126661,1.5307763396,0.0120977222\H,0.890
3288621,1.8024661667,1.6531029329\H,2.6968869732,2.3231285858,0.025192
0438\H,3.1904760306,1.0394157981,1.0941874256\H,2.0929873651,0.6710259
49,-1.7283403161\H,3.7566395516,0.4698571479,-1.2595186278\H,3.2100990
838,-1.3927842264,0.2211057405\H,2.6155522433,-1.7553148298,-1.3656850
719\H,-1.4542103713,0.201201154,-0.7681610379\C,-0.0606050764,-2.00830
15117,-2.0954371033\O,0.5305874195,-3.022007469,-2.168748397\O,-0.7806
723551,-1.3520213375,-2.9218706112\C,-1.0430557943,-1.8015441781,-4.34
15987814\C,0.2878480934,-1.8741517187,-5.0744869587\C,-1.7797198481,-3
.1314468389,-4.2933321655\C,-1.9228037784,-0.6798353658,-4.8673617321\
H,0.815364099,-0.9293148626,-5.0088426903\H,0.9193600186,-2.6647126168
, -4.6933319382\H,0.0943475166,-2.0754918813,-6.1216291321\H,-2.6816667
052,-3.0510590811,-3.6971403796\H,-2.0708850591,-3.4013477155,-5.30176
26873\H,-1.1600549247,-3.9254718532,-3.9001508887\H,-2.1858758688,-0.8
858999733,-5.8977778602\H,-2.8372492632,-0.6013174329,-4.2919266197\H,
-1.4033871041,0.2700139439,-4.831429643\Version=EM64L-G09RevA.02\Stat
e=2-A\HF=-709.6485672\S2=0.773991\S2-1=0.\S2A=0.750486\RMSD=5.068e-09\
RMSF=4.582e-06\Dipole=-0.7564999,0.360315,0.7631882\Quadrupole=-1.4950
285,-10.3175842,11.8126127,3.6900554,5.5845987,5.0011507\PG=C01 [X(C13
H23N1O2)]\@

tert-butyl piperidine-1-carboxylate radical carbocation (4):

1\1\GINC-HER05-18\FOpt\UHF\6-31G(d)\C10H19N1O2(1+,2)\LHAYA\12-Nov-2010
\0\#opt freq uhf/6-31g(d) geom=connectivity\111110_13\1,2\C,-1.2785
852011,0.3863954932,-0.3321078424\C,-1.823173263,0.180702391,1.0818996
201\C,-3.2658642009,0.6956009783,1.2069565104\N,-4.0852552165,0.066575
9995,0.1593022628\C,-3.6466151966,0.2684568809,-1.2302699578\C,-2.2046
107258,-0.2475103281,-1.3711386312\C,-5.2183033756,-0.7981856445,0.544
8549486\O,-5.343758373,-1.0440087915,1.689320179\O,-5.8831672059,-1.13
67363851,-0.4896371246\C,-7.1196087366,-2.0135556143,-0.4383442614\C,-
6.7193862389,-3.3701506316,0.1201901073\C,-8.1744212037,-1.3012171226,
0.3938407291\C,-7.5057032074,-2.0904003904,-1.9056578018\H,-1.79742330
13,-0.8695980567,1.3543866106\H,-1.2278792663,0.7132031363,1.813608805
2\H,-3.7077786039,0.4747933412,2.1620254748\H,-3.3140844068,1.76186050
78,1.0160398709\H,-4.3367271364,-0.2285252933,-1.8869662258\H,-3.69165
45815,1.3384879592,-1.4001249153\H,-1.8797977049,-0.0188541522,-2.3789
807322\H,-2.202944916,-1.3287780895,-1.2741000378\H,-6.4289324046,-3.3
130592101,1.1599797797\H,-7.5709067614,-4.0365166913,0.0465557865\H,-5
.9088488393,-3.8008817123,-0.456587717\H,-8.3647891651,-0.3070576128,0
.0060739309\H,-9.0979458222,-1.8650752111,0.3329583393\H,-7.893647931,
-1.2322925513,1.4356068854\H,-6.7153950481,-2.5426986213,-2.4926560527
\H,-8.3953966458,-2.6997536434,-2.0079922624\H,-7.7202338908,-1.105844
4856,-2.3031252514\H,-1.1716297264,1.4486338547,-0.53464444083\H,-0.290
3179933,-0.0498867033,-0.4106846085\Version=EM64L-G09RevA.02\State=2-
A\HF=-593.7025157\S2=0.784456\S2-1=0.\S2A=0.750859\RMSD=6.240e-09\RMSF
=8.623e-06\Dipole=1.0032134,0.9439615,-0.6040227\Quadrupole=10.5633736
, -2.0488567,-8.5145168,10.3387228,2.1173563,2.0428015\PG=C01 [X(C10H19
N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate radical carbocation (5):

1\1\GINC-LOST\FOpt\UHF\6-31G(d)\C9H17N1O2(1+,2)\LUISA\07-Jul-2010\0\#
opt freq hf/6-31g(d) geom=connectivity\intermedio\1,2\N,-1.333687882
, -0.1598889939,0.0240122186\C,-1.750914608,1.2487476976,-0.0302379323\
C,-3.2578476032,1.1789515821,0.2278695254\C,-3.658749746,-0.1977972271
, -0.3181584066\C,-2.4714927659,-1.0919575035,0.0425789634\H,-1.1702504
43,1.815995106,0.6817117914\H,-1.5031576225,1.5998738199,-1.0273494216
\H,-3.4539460219,1.2421200109,1.2918640134\H,-3.7784228813,1.992874140
3,-0.2564439941\H,-4.5770871357,-0.5702309682,0.1129382789\H,-3.783830
4232,-0.1636136032,-1.3941934712\H,-2.5244516517,-1.4844213555,1.05357
17125\H,-2.2653317505,-1.9129893339,-0.6272562108\C,0.0515316873,-0.63
72415656,0.0625069848\O,0.8480859651,0.356511975,-0.027244724\O,0.2153

296116, -1.7987419219, 0.1650215785\C, 2.3580095841, 0.2198399098, -0.02165
5294\C, 2.7647908044, -0.6141953633, -1.2265038134\C, 2.7757286666, -0.3903
07055, 1.307242546\C, 2.8016475824, 1.6669231839, -0.1516828455\H, 2.374597
9757, -0.1849790871, -2.1422632121\H, 3.8464141072, -0.6158114901, -1.29408
44717\H, 2.4344098165, -1.640270945, -1.142002772\H, 2.4448455435, -1.41482
93123, 1.4070494154\H, 3.8579188284, -0.3813034564, 1.3645731219\H, 2.39354
07619, 0.1933688508, 2.1369214989\H, 2.4468109885, 2.2589039048, 0.68325734
33\H, 3.8840475525, 1.7076532997, -0.1613557699\H, 2.4364820593, 2.10410970
13, -1.0730106532\Version=EM64L-G09RevA.02\State=2-A\HF=-554.664374\S2
=0.785391\S2-1=0.\S2A=0.750877\RMSD=9.035e-09\RMSF=3.941e-06\Dipole=-1
.6917494, 0.7223119, -0.0598354\Quadrupole=17.4863868, -9.1942481, -8.2921
387, 0.7606307, -0.1033171, 0.2310149\PG=C01 [X(C9H17N1O2)]\@

tert-butyl diethylcarbamate radical carbocation (6):

1\1\GINC-LOST\FOpt\UHF\6-31G(d)\C9H19N1O2(1+, 2)\LUISA\24-Nov-2010\0\#\
opt freq hf/6-31g(d) geom=connectivity\191110_38\1, 2\N, 1.478652246,
0.0591027812, -0.5547132672\C, 1.5694430454, 1.4540826744, -1.0213035462\C
, 2.6963057712, -0.7410705445, -0.3208282732\H, 2.3520802073, 1.4706650339,
-1.7669884664\H, 0.6286109956, 1.7090624759, -1.4779011106\H, 3.5248606987
, -0.16009954, -0.6944000334\H, 2.5838138332, -1.6360465896, -0.9161506082\
C, 0.1755739101, -0.6039476426, -0.3452965999\O, -0.717864509, 0.2726119404
, -0.0979913662\O, 0.1476212402, -1.7764499916, -0.4332490682\C, -2.1764127
717, -0.0660498235, 0.1519183891\C, -2.2551106247, -0.9447446936, 1.3904704
288\C, -2.7314185419, -0.7290547849, -1.098995127\C, -2.7784689066, 1.3086
535563, 0.3869685078\H, -1.7701202591, -0.4667072349, -2.2339234965\H, -3.29
89466697, -1.0878991479, 1.6441962522\H, -1.8147774174, -1.9186183775, 1.22
7430573\H, -2.2875916506, -1.6986786644, -1.2771324336\H, -3.7983802542, -0
.8679949339, -0.9692423324\H, -2.581383146, -0.0997070605, -1.9688086072\H
, -2.6543185789, 1.9420785951, -0.4830320873\H, -3.8388732528, 1.2036389411
, 0.5815365508\H, -2.3221772448, 1.7921436778, 1.242190674\C, 2.8739895324,
-1.0897104437, 1.1590769107\H, 2.948203157, -0.202300402, 1.774983142\H, 2.
0676786482, -1.7139232028, 1.5189093668\H, 3.7976805392, -1.6458400242, 1.2
580930518\C, 1.8907968648, 2.3947419229, 0.1446605402\H, 1.1200967222, 2.35
27576536, 0.9028189296\H, 2.8502793252, 2.1690818937, 0.592405831\H, 1.9321
650907, 3.4041229559, -0.2447103319\Version=EM64L-G09RevA.02\State=2-A\
HF=-555.8243486\S2=0.778559\S2-1=0.\S2A=0.750651\RMSD=7.790e-09\RMSF=3
.880e-06\Dipole=1.4993215, 0.9333097, -0.3290373\Quadrupole=14.0403508, -
6.9894196, -7.0509312, 1.2922473, -2.234295, -2.4842927\PG=C01 [X(C9H19N1O
2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate radical carbocation (7):

1\1\GINC-LOST\FOpt\UHF\6-31G(d)\C11H19N1O4(1+, 2)\LUISA\07-Jul-2010\0\#\
#opt freq hf/6-31g(d) geom=connectivity\carb_02\1, 2\N, -1.2758759601,
-0.2435943925, 0.2456215052\C, -1.8018008216, 1.1253562798, 0.1968010439\C
, -3.2877158496, 0.9277427234, 0.4984288255\C, -3.6048812419, -0.4442409754
, -0.1104112724\C, -2.3264040599, -1.2690877925, 0.1387114443\H, -1.2528952
922, 1.7469945718, 0.88809153\H, -1.6133513121, 1.4785834662, -0.8126044114
\H, -3.4505816515, 0.9219797915, 1.5698117344\H, -3.8870846827, 1.71999341,
0.0726376323\H, -4.4656070574, -0.9201411701, 0.3351842952\H, -3.784645627
7, -0.3531897171, -1.1753611128\H, -2.3456884135, -1.8009068923, 1.08206958
26\C, 0.1352508374, -0.6108761701, 0.4554460028\O, 0.8767247725, 0.30872197
36, -0.0178066031\O, 0.339409273, -1.6182413959, 1.0254328847\C, 2.39028486
02, 0.2330211204, -0.03583669\C, 2.7934669196, -0.9999053962, -0.8269692172\
C, 2.8806876519, 0.2168258257, 1.4033656888\C, 2.7572064031, 1.5206469231, -
0.753294118\H, 2.3311118818, -0.9947108317, -1.8095138214\H, 3.8690268152, -
0.9851892777, -0.9628536024\H, 2.5315043521, -1.915822153, -0.3183962251\
H, 2.5932483677, -0.6888980855, 1.9194095818\H, 3.9631285382, 0.2715402202,
1.3994239576\H, 2.505538352, 1.0751994302, 1.9489976893\H, 2.3982169427, 2.
3853087141, -0.2081637803\H, 3.8355366903, 1.5904911698, -0.8295598539\H, 2
.3422170636, 1.5383998226, -1.7535171286\C, -1.9605326896, -2.213600296, -0
.9963589155\O, -1.0777189282, -1.9703625504, -1.7525454423\O, -2.759014872
2, -3.2351947899, -1.0178185197\C, -2.5728741226, -4.2141444298, -2.0542267
788\H, -3.3323914471, -4.9564266217, -1.8813597698\H, -2.698948163, -3.7496
351926, -3.0193958766\H, -1.5873396384, -4.6439574319, -1.9713068443\Vers
ion=EM64L-G09RevA.02\State=2-A\HF=-781.3045649\S2=0.775358\S2-1=0.\S2A
=0.750531\RMSD=8.930e-09\RMSF=8.875e-06\Dipole=-1.4335093, 1.0960831, 0.
3306988\Quadrupole=12.6315068, 0.156591, -12.7880978, 5.1361008, 1.1063636
, 7.2926442\PG=C01 [X(C11H19N1O4)]\@

tert-butyl piperidine-1-carboxylate cation (4):

1\1\GINC-HERO3-03\FOpt\RHF\6-31G(d)\C10H18N1O2(1+)\LHAYA\11-Nov-2010\0
\#opt freq hf/6-31g(d) geom=connectivity\111110_25\1, 1\C, -1.4071609
765, 0.8903779619, -0.3622834834\C, -1.5719803353, 0.1745123172, 0.97443238
06\C, -3.0405671387, 0.0595761164, 1.3517670872\N, -3.8515212652, -0.467931
7242, 0.2084257171\C, -2.1392195846, 0.1043590141, -1.448497529\C, -5.17993
19354, -0.9895296921, 0.5653729686\O, -5.5066026894, -0.9331333275, 1.69257
61114\O, -5.7885454168, -1.4356782528, -0.4720577029\C, -7.1757602819, -2.0
310336591, -0.4267440062\C, -7.1426010424, -3.2656816646, 0.4611547962\C, -
8.1440772753, -0.9629226404, 0.0583287824\C, -7.4099688547, -2.3882776026,
-1.8854340603\H, -1.1261433791, -0.8147637695, 0.9282084052\H, -1.06781470

03,0.7122728911,1.7677455797\H,-3.1966425488,-0.6188397968,2.172646677
5\H,-3.4701109038,1.0147854145,1.6191738099\H,-2.321856244,0.690628551
6,-2.3440052443\H,-1.5622253834,-0.7594600895,-1.7793018393\H,-6.96487
81389,-3.0157065766,1.4974403472\H,-8.102968126,-3.7636896125,0.394984
0243\H,-6.3824860534,-3.9616281475,0.1245565871\H,-8.074916231,-0.0725
743426,-0.5564670337\H,-9.1534094622,-1.3485789552,-0.0265766522\H,-7.
9717830678,-0.6980140335,1.0918229417\H,-6.673775742,-3.1030268877,-2.
2338468551\H,-8.3912630676,-2.8343453374,-1.9916996873\H,-7.3698074622
, -1.5059731055,-2.5133501866\H,-1.8117971675,1.8953603114,-0.299890228
\H,-0.3623014431,0.9837459423,-0.6268351122\C,-3.4505472793,-0.4440193
203,-1.0045152415\H,-4.1161341233,-0.8615659328,-1.7353912642\Version
=EM64L-G09RevA.02\State=1-A\HF=-593.1578991\RMSD=7.804e-09\RMSF=6.692e
-06\Dipole=1.7079951,0.5628273,-1.1798966\Quadrupole=13.2541718,-5.380
9681,-7.8732037,10.3995934,0.9315195,0.4263795\PG=C01 [X(C10H18N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate cation (5):

1\1\GINC-LOST\FOpt\RHF\6-31G(d)\C9H16N1O2(1+)\LUIA\07-Jul-2010\0\#\#opt
freq hf/6-31g(d) geom=connectivity\producto\1,1\N,-1.3460764714,-0.
.1403325724,-0.0819176425\C,-1.7294266173,1.2996772483,-0.1005065689\C
, -3.2504446078,1.2407764292,0.1177086315\C,-3.6415222005,-0.2148097287
, -0.2123325446\C,-2.3411114449,-0.9330562278,-0.1453878148\H,-1.192560
7736,1.8164475272,0.6771550293\H,-1.4401240851,1.7075673313,-1.0579800
08\H,-3.4873625622,1.4629288509,1.149416796\H,-3.7697564956,1.95489128
53,-0.504099769\H,-4.36602865,-0.6499422975,0.4649562547\H,-4.03539335
15,-0.3388250377,-1.2189382748\H,-2.1805834661,-1.995355372,-0.1670049
663\C,0.02523765,-0.6480419409,-0.0549370952\O,0.8314504362,0.34185523
28,-0.0461740895\O,0.1950442139,-1.8133966805,-0.046663455\C,2.3331659
53,0.1919048407,-0.0194328962\C,2.7654981308,-0.5412103172,-1.28029166
46\C,2.7216444771,-0.529724257,1.2621690607\C,2.7925669434,1.640569365
4,-0.0181755842\H,2.3982575914,-0.034106222,-2.1653590166\H,3.84841615
58,-0.5442169512,-1.3233599578\H,2.4265559151,-1.5676537107,-1.2893130
172\H,2.3826618999,-1.5561600709,1.2687453928\H,3.8024353081,-0.531821
1093,1.3426838693\H,2.3238999344,-0.0149428794,2.1294297598\H,2.423030
1061,2.1643016769,0.8552181777\H,3.8751885602,1.6721770332,-0.00082619
7\H,2.4511434505,2.1568445542,-0.9072514096\Version=EM64L-G09RevA.02\
State=1-A\HF=-554.1182989\RMSD=4.290e-09\RMSF=2.084e-05\Dipole=-2.4857
387,0.4942988,-0.1208955\Quadrupole=20.5460082,-10.2180941,-10.3279141
,2.0652385,0.946513,0.2385011\PG=C01 [X(C9H16N1O2)]\@

tert-butyl diethylcarbamate cation (6):

1\1\GINC-HERO3-25\FOpt\RHF\6-31G(d)\C9H18N1O2(1+)\LHAYA\25-Nov-2010\0\
\#opt freq hf/6-31g(d) maxdisk=2000MB geom=connectivity\221110_1\1,1
\N,1.6060883709,0.0953200199,-0.2544578358\C,1.8863100643,1.3414937184
, -0.193055689\C,2.692153525,-0.8922252284,-0.5870999886\H,2.9060949273
, 1.5714309828,-0.4492349513\H,3.3686079031,-0.3802496913,-1.2555323271
\H,2.2220992104,-1.6967420749,-1.1254226286\C,0.293910565,-0.50454723,
0.0351152271\O,-0.6464419441,0.3586246472,-0.0725603836\O,0.2645413125
, -1.6518135023,0.2892425707\C,-2.1049504587,0.0086221293,0.1169437765\
C,-2.3077442022,-0.4780039239,1.5439989539\C,-2.4945575318,-1.02053342
57,-0.9337806963\C,-2.7852013911,1.3459703531,-0.1275910911\H,-1.94633
38789,0.2545972592,2.2572180873\H,-3.3697126863,-0.6108940299,1.714832
3908\H,-1.8177769502,-1.4240380948,1.724493805\H,-2.0115287158,-1.9729
953074,-0.7693534832\H,-3.5662704527,-1.173994601,-0.8836843294\H,-2.2
55425701,-0.6634803563,-1.9291148064\H,-2.5734269702,1.713641011,-1.12
45546521\H,-3.8571719662,1.2233507752,-0.0331457344\H,-2.4667210125,2.
0861720577,0.5969768665\C,3.4027374425,-1.3935341453,0.6610011466\H,3.
8787485069,-0.5809213308,1.199484081\H,2.7184752397,-1.9068201349,1.32
19118072\H,4.1746466821,-2.0925671405,0.3619089613\C,1.0265643854,2.50
01008492,0.1850919187\H,0.3978826809,2.2825055506,1.0338952793\H,1.664
6040708,3.3457137756,0.3978108755\H,0.3838439748,2.7493008081,-0.65280
61505\Version=EM64L-G09RevA.02\State=1-A\HF=-555.2696499\RMSD=3.451e-
09\RMSF=4.004e-06\Dipole=1.701801,1.6353007,-0.4402907\Quadrupole=13.6
572654,-4.2066774,-9.450588,2.6991423,-2.5814561,0.6395371\PG=C01 [X(C
9H18N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate carbocation (7):

1\1\GINC-LOST\FOpt\RHF\6-31G(d)\C11H18N1O4(1+)\LUIA\08-Jul-2010\0\#\#opt
freq hf/6-31g(d) geom=connectivity\carb_03_1\1,1\N,-0.3279868418,
0.9020646896,0.26344479\C,-0.2847246004,1.9617690146,-0.4411790171\C,-
1.6055940935,2.6430023533,-0.5198851396\C,-2.4178906519,1.924503522,0.
5745908144\C,-1.6886646464,0.5765030644,0.7488230835\H,0.6292089989,2.
2670456007,-0.9131597983\H,-1.51262623,3.7128362392,-0.3824258044\H,-1
.9965924217,2.4756018315,-1.5210486591\H,-2.3757490548,2.482096563,1.5
00677615\H,-3.4567156784,1.7922581143,0.3106299551\H,-1.6430550914,0.2
294754996,1.7669058653\C,0.7671144944,-0.0369487214,0.4707254849\O,1.8
310672283,0.3967408623,-0.0953732269\O,0.540540662,-1.0036116758,1.100
5261117\C,3.1393429301,-0.3572754413,-0.0888757962\C,2.9275654202,-1.6
941201023,-0.7830570604\C,3.609997457,-0.4908380977,1.3513651184\C,4.0
366504934,0.5659969297,-0.8963910547\H,2.5091503323,-1.5520185878,-1.7

728096286\H, 3.8894582397, -2.1815359103, -0.8926167675\H, 2.2820369633, -2.3484652664, -0.2144839594\H, 2.9631755796, -1.1343495355, 1.9309068699\H, 4.6034111276, -0.9242554182, 1.3512200512\H, 3.6699895834, 0.4807415967, 1.8286793642\H, 4.1242573739, 1.5360730748, -0.4215214024\H, 5.0267619124, 0.1322088425, -0.9656800713\H, 3.6537136107, 0.6984005664, -1.9013382322\C, -2.2558908891, -0.5058826118, -0.1632431353\O, -1.8271965428, -0.6991913523, -1.2537985921\O, -3.2659252539, -1.1008420039, 0.3975281877\C, -3.93711139741, -2.1283899304, -0.3463696914\H, -4.7236151462, -2.478997343, 0.2991470064\H, -4.3415806948, -1.7155851004, -1.2573253956\H, -3.2433965957, -2.9223222664, -0.5734918854\Version=EM64L-G09RevA.02\State=1-A\HF=-780.7595118\RMSD=4.654e-09\RMSF=2.160e-05\Dipole=-0.5598811, 2.2270019, -0.1140816\Quadrupole=15.7179235, 0.6691922, -16.3871157, -2.2222232, -1.042039, -0.4626277\PG=C01 [X(C11H18N1O4)]\@\

1.2 Optimized geometries at HF/6-31G(d,p) level:

tert-butyl indoline-1-carboxylate (1):

1\1\GINC-HER05-13\FOpt\RHF\6-31G(d,p)\C13H17N1O2\LHAYA\29-Nov-2010\0\#\opt freq hf/6-31g(d,p) geom=connectivity maxdisk=2000MB\261110_3\0, 1\N, 1.4089620099, 0.2785399844, 0.4185438999\C, 2.8062733891, 0.6894037111, 0.6151427397\C, 3.6300132361, -0.6040074394, 0.4597717899\C, 2.5907152737, -1.6611288735, 0.1792324221\C, 1.3160293128, -1.1054132971, 0.1644547414\C, 0.2055398054, -1.8973790311, -0.0752982075\C, 0.4026047063, -3.2547245983, -0.2989782079\C, 1.6666749482, -3.815372955, -0.2859730985\C, 2.7709853452, -3.0083877779, -0.0441576322\C, 0.4520967323, 1.2374564686, 0.5049240791\O, 0.7276572495, 2.38202117, 0.7328191655\O, -0.7677665083, 0.772178985, 0.3146997386\H, 2.9186111175, 1.1368935325, 1.5932504094\H, 4.3453796987, -0.5220617326, -0.3520008171\H, 4.1916671652, -0.8257711065, 1.3613414597\H, -0.7794837885, -1.4844339177, -0.0896879075\H, -0.4545574236, -3.8777078763, -0.4861063873\H, 1.7941008766, -4.8684877473, -0.4617938814\H, 3.7610993503, -3.4312196726, -0.0310875915\H, 3.0705536295, 1.4391354218, -0.1181338118\C, -1.9444092249, 1.6217340599, 0.3618227027\C, -3.0780954927, 0.6384228904, 0.0868609577\H, -4.0312217099, 1.1558180197, 0.0951656547\H, -2.9510523178, 0.1700662439, -0.8829611255\H, -3.1029996142, -0.137616731, 0.8439541294\C, -1.8772840669, 2.6789356075, -0.7373275271\H, -2.8228884819, 3.2100396478, -0.7827849359\H, -1.0871083795, 3.3912542602, -0.5529163705\H, -1.7090903424, 2.2077364003, -1.7004184701\C, -2.0970088165, 2.2366251507, 1.7507191475\H, -3.0523613532, 2.7481024808, 1.8138517155\H, -2.0804105955, 1.4595398974, 2.5081697905\H, -1.3090836305, 2.9450775244, 1.9581949992\Version=EM64L-G09RevA.02\State=1-A\HF=-706.43161\RMSD=5.624e-09\RMSF=1.282e-05\Dipole=-0.1781945, -0.5238401, -0.1086236\Quadrupole=8.4560487, -4.5936283, -3.8624204, -3.5657465, 0.4554373, -0.4515918\PG=C01 [X(C13H17N1O2)]\@\

tert-butyl 1H-indole-1-carboxylate (2):

1\1\GINC-HER03-42\FOpt\RHF\6-31G(d,p)\C13H15N1O2\URIETA\24-Jan-2011\0\#\opt freq hf/6-31g(d,p) maxdisk=2500MB geom=connectivity\aromatico_3\0, 1\C, -2.5813516394, 0.951038939, -0.0003418903\C, -1.6997958874, -0.1317692227, 0.0000592261\C, -2.1530622716, -1.4463297289, 0.000676998\C, -3.5188962891, -1.643177497, 0.0008802818\C, -4.4156249899, -0.5711076068, 0.0004825035\C, -3.9562176458, 0.7271581432, -0.0001284293\C, -1.7792085426, 2.157459571, -0.0009404814\C, -0.4964193517, 1.7861003293, -0.0008790853\H, -1.468974017, -2.2691276196, 0.0009785949\H, -3.9006067928, -2.6488878396, 0.0013546524\H, -5.4734529469, -0.7659428054, 0.0006567559\H, -4.6436704011, 1.5547811499, -0.0004349884\H, -2.1393014796, 3.1661231181, -0.0013527811\H, 0.3917430142, 2.376842483, -0.0012087233\C, 0.7663427793, -0.3401006472, -0.0000866076\O, 0.7896044525, -1.5315709094, 0.000546405\O, 1.8143708602, 0.4547009488, -0.0003451245\N, -0.4003613593, 0.3914862123, -0.0002911314\C, 3.1830477024, -0.0408301561, 0.0000411508\C, 3.4482261491, -0.8456188475, 1.2692369863\C, 3.4481003614, -0.8476372145, -1.2678919178\C, 3.9994739972, 1.2471729046, -0.0010128964\H, 3.1892099448, -0.2610104893, 2.145915225\H, 2.8824891277, -1.7655091741, 1.2818021733\H, 4.5047786723, -1.0870064364, 1.3253656123\H, 3.189044369, -0.2644114674, -2.1454782263\H, 4.5046332674, -1.0891816433, -1.3237170037\H, 2.8823023609, -1.7675160041, -1.2789459671\H, 5.0591024176, 1.0166292865, -0.0008526053\H, 3.7766183323, 1.8396497553, -0.8812803396\H, 3.776658806, 1.8410614681, 0.8783126334\Version=EM64L-G09RevA.02\State=1-A\HF=-705.2607798\RMSD=6.731e-09\RMSF=9.623e-06\Dipole=0.8168305, 0.718539, -0.0002778\Quadrupole=7.2396806, -1.2234982, -6.0161824, 0.3383907, -0.0000374, -0.0023849\PG=C01 [X(C13H15N1O2)]\@\

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate (3):

1\1\GINC-LOST\FOpt\RHF\6-31G(d,p)\C13H23N1O2\LUIISA\15-Sep-2010\0\#\opt=calcfreq freq hf/6-31g(d,p) geom=connectivity\140910_4\0, 1\N, 0.0763525977, -0.9636669438, -1.0836865911\C, -1.1035249516, -0.2396339052, -0.6012434904\C, -0.9235272915, -0.2391784821, 0.9192629276\C, 0.5961610428, -0.2827098407, 1.1001061848\C, 1.0273044172, -1.2693055748, -0.0020868794\C, 1.2095126735, 1.1201841618, 0.9477141867\C, 2.7125237655, 1.0993167521, 0.677840997\C, 3.0125545334, 0.2568883886, -0.5602571741\C, 2.5111335779, -1.1732739539, -0.3713854335\H, -2.0141569676, -0.7355216408, -0.9060402537\H, -1.38543834, 0.6232033409, 1.3881526556\H, -1.3771691161, -1.1303555311, 1.343

4500102\H,0.8749314217,-0.6837351977,2.0706223347\H,0.8404789724,-2.28
47254016,0.342400604\H,0.7248981491,1.6436370876,0.1267089925\H,0.9897
980913,1.6920132357,1.8462398619\H,3.0768787112,2.1153881946,0.5505659
373\H,3.2394814585,0.6835592793,1.536163017\H,2.5383536543,0.706372362
3,-1.430409692\H,4.0805843537,0.2408523172,-0.7605698434\H,3.062390443
5,-1.6257929134,0.4524338944\H,2.7049078694,-1.7764536419,-1.245717177
6\H,-1.1295134004,0.76350428993,-1.0091132307\H,0.065902897,-1.67694801
91,-2.2331104568\O,0.8660445774,-2.5279156829,-2.5115547618\O,-0.93980
13086,-1.3065755452,-3.0164802946\C,-1.1808630645,-1.891836341,-4.3169
891864\C,0.0001450176,-1.623953105,-5.247274867\C,-1.4833520033,-3.382
8259657,-4.1837843298\C,-2.4179998019,-1.1385064551,-4.797626912\H,0.2
204234281,-0.5615012109,-5.2752592765\H,0.8831948987,-2.1558913918,-4.
926058662\H,-0.2532514526,-1.942066773,-6.2538415874\H,-2.2905370282,-
3.5391864852,-3.4748933891\H,-1.8002933992,-3.7745260072,-5.1453839329
\H,-0.6155398377,-3.933333183,-3.8525357347\H,-2.7098487914,-1.484771
603,-5.7833572627\H,-3.2482431555,-1.2960430448,-4.1179483078\H,-2.218
2966417,-0.074124044,-4.8509528763\Version=EM64L-G09RevA.02\State=1-A
\HF=-709.939159\QRMSD=5.618e-09\RMSF=4.239e-06\Dipole=-0.6897654,0.5365
581,0.3298727\Quadrupole=-0.7009422,-3.5902573,4.2911995,2.1611733,2.1
675986,0.2918744\PG=C01 [X(C13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate (4):

1\1\GINC-HER03-46\FOpt\RHF\6-31G(d,p)\C10H19N1O2\LHAYA\11-Nov-2010\0\#
#opt freq hf/6-31g(d,p) geom=connectivity\111110_2\0,1\C,-1.30068837
11,0.5377550844,-0.3707289535\C,-1.7530904527,0.1368334173,1.034461831
9\C,-3.2322111131,0.4484043833,1.2479281766\N,-4.0392151344,-0.1571952
551,0.1980271507\C,-3.6770125715,0.2162049089,-1.1620045944\C,-2.20574
66981,-0.0983646256,-1.4271422685\C,-5.1711845936,-0.8209946259,0.5373
458756\O,-5.5094210105,-1.0253619838,1.6714444901\O,-5.8495935131,-1.2
284666131,-0.5269601988\C,-7.0792573422,-1.985749733,-0.4310256048\C,-
6.8288866553,-3.3227902057,0.2626178224\C,-8.157692639,-1.1634824486,0
.2707266457\C,-7.4478870702,-2.2069852567,-1.8953999491\H,-1.594013943
5,-0.9290208054,1.180343321\H,-1.1659376823,0.6565199909,1.7869633307\
H,-3.5765776733,0.0764811939,2.1982915489\H,-3.383719139,1.5285289947,
1.2367313194\H,-4.3092116602,-0.3083285852,-1.8571741702\H,-3.85057713
09,1.2847230293,-1.2961425144\H,-1.9397200765,0.2543302052,-2.42025776
08\H,-2.0721783761,-1.1776827839,-1.4209517108\H,-6.5756526659,-3.1855
927055,1.3031401955\H,-7.7223830866,-3.9359625787,0.1973142661\H,-6.01
99004049,-3.8537039167,-0.2292472276\H,-8.2688084437,-0.1995100057,-0.
2157735516\H,-9.107917881,-1.6844952461,0.2058667771\H,-7.917562229,-1
.004599976,1.3112349798\H,-6.6650618255,-2.7564407905,-2.4066182568\H,
-8.3701373666,-2.7731674772,-1.9695215082\H,-7.5855472361,-1.257662219
1,-2.4012349048\H,-1.3411323748,1.6222046342,-0.4672426263\H,-0.266859
9291,0.2476955956,-0.5344299208\Version=EM64L-G09RevA.02\State=1-A\HF
=-593.992702\QRMSD=2.888e-09\RMSF=8.827e-06\Dipole=0.2839614,0.160893,-
0.8954198\Quadrupole=3.4892686,0.850171,-4.3394397,2.7249189,2.0554131
,0.7992392\PG=C01 [X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate (5):

1\1\GINC-HER05-22\FOpt\RHF\6-31G(d,p)\C9H17N1O2\LHAYA\02-Dec-2010\0\#
opt freq hf/6-31g(d,p) maxdisk=2000MB geom=connectivity\011210_1\0,1
\N,-1.2934672261,-0.1595855044,0.0352962735\C,-1.7050263166,1.23748475
84,-0.0346282883\C,-3.2087631899,1.1623696494,0.2390037239\C,-3.602598
4983,-0.2109354456,-0.31281596\C,-2.4115671257,-1.0942651754,0.0602229
509\H,-1.1751779318,1.8381282859,0.6923260033\H,-1.5005991346,1.651072
9024,-1.0185349746\H,-3.3903473411,1.1972050352,1.3094809272\H,-3.7526
619994,1.9814192466,-0.217120928\H,-4.5371396712,-0.5823424909,0.09111
52317\H,-3.7025950632,-0.1619040022,-1.3934984604\H,-2.5280603755,-1.5
248369896,1.0510148643\H,-2.2456798609,-1.9069502055,-0.6335900413\C,-
0.0233140618,-0.6039232252,0.0465951602\O,0.8393012517,0.4029473798,-0
.0225213725\O,0.2725903121,-1.7662614095,0.1091396004\C,2.2722206732,0
.2083487476,-0.0215149419\C,2.6993853702,-0.5967269774,-1.2468455893\C
,2.7187637491,-0.4477464906,1.283179195\C,2.8040788639,1.6359437118,-0
.1097900168\H,2.3209369322,-0.1305455237,-2.1511341462\H,3.7831682885,
-0.6169662088,-1.3067579718\H,2.3340558677,-1.6116556002,-1.1974113713
\H,2.3543300416,-1.4613965162,1.3587017417\H,3.8033486526,-0.461096755
5,1.3286710041\H,2.3533445985,0.1212827401,2.1322960589\H,2.4687297337
,2.220471986,0.7398110351\H,3.8888072501,1.6333757022,-0.119484172\H,2
.452446211,2.1177193752,-1.015369536\Version=EM64L-G09RevA.02\State=1
-A\HF=-554.9527601\QRMSD=4.703e-09\RMSF=2.300e-05\Dipole=-0.4135653,0.9
812073,-0.0672384\Quadrupole=6.3618517,-5.3895132,-0.9723385,0.6265207
,0.0301663,0.3763989\PG=C01 [X(C9H17N1O2)]\@

tert-butyl diethylcarbamate (6):

1\1\GINC-HER05-26\FOpt\RHF\6-31G(d,p)\C9H19N1O2\LHAYA\20-Nov-2010\0\#
opt freq hf/6-31g(d,p) maxdisk=2000MB\191110_27\0,1\N,-1.5030468702,
-0.1323598348,0.678633595\C,-1.7963261224,1.2586915105,1.0045403577\C,
-2.55232383965,-1.1432147775,0.7572794503\H,-2.6253394215,1.2527642974,
1.7024880412\H,-0.9489773368,1.68163507,1.5242503636\H,-3.290176449,-0
.7869147818,1.4676276314\H,-2.1210657496,-2.0472892172,1.1624047693\C,

-0.2823464035,-0.540573702,0.2596310196\O,0.5871261375,0.4604536248,0.2098590353\O,-0.0265173726,-1.6785700833,-0.028630397\C,1.9677155129,0.2823093419,-0.1869580119\C,2.0468006701,-0.2074538238,-1.631080385\C,2.6825041045,-0.6574995568,0.7813199756\C,2.5329913193,1.6951294485,-0.0719766107\H,1.4843617563,0.4543195093,-2.2823204379\H,3.081906191,-0.2009305055,-1.9582233954\H,1.6566779338,-1.2093837176,-1.7291586009\H,2.3002890315,-1.6645723683,0.7074191377\H,3.7443847543,-0.6684005126,0.5559360544\H,2.5587904166,-0.3083532369,1.8016398858\H,2.4408552811,2.0610131007,0.9446787576\H,3.5822954455,1.7032629882,-0.346753833\H,2.0002409893,2.3739178943,-0.728754283\C,-3.2225223347,-1.4576072985,-0.5774882515\H,-3.7105653153,-0.5838682048,-0.9966313638\H,-2.4914943143,-1.821364993,-1.2890580119\H,-3.9757600029,-2.2287075564,-0.4415089535\C,-2.144795874,2.1295485651,-0.1997010149\H,-1.3261037758,2.1468212968,-0.9094616672\H,-3.0314002057,1.7681842598,-0.7092160964\H,-2.3356899089,3.1496013738,0.1222162696\Version=EM64L-G09RevA.02\State=1-A\HF=-556.1163576\RMSD=8.372e-09\RMSF=3.422e-06\Dipole=-0.1497621,0.8882915,0.2190138\Quadrupole=5.0022566,-4.3840793,-0.6181773,0.7072634,-1.8258525,-0.2338197\PG=C01 [X(C9H19N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate (7):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C11H19N1O4\LUISA\06-Jul-2010\0\#opt freq b3lyp/6-31g(d)\carb2_01\0,1\N,-1.2537175232,-0.184505671,0.0128451518\C,-1.72825667587,1.1887483991,-0.1749021521\C,-3.19225424,1.0947821446,0.2737960867\C,-3.601510592,-0.3220457426,-0.1638870004\C,-2.3273907498,-1.172010667,0.0750386325\H,-1.1331843788,1.8835376598,0.421806214\H,-1.6479939735,1.4894060334,-1.2288023894\H,-3.2551590342,1.1907421645,1.3641780058\H,-3.8199533523,1.8728964589,-0.1709724978\H,-4.462967395,-0.7180696353,0.380265189\H,-3.8404411979,-0.3249621976,-1.233224048\H,-2.3424922911,-1.6672507072,1.0515674537\C,0.0438505002,-0.5954043794,0.0949781519\O,0.8880085898,0.4573995088,-0.0242118127\O,0.3599062122,-1.766306202,0.2640594458\C,2.3458794867,0.2643868374,0.0222367577\C,2.7932289081,-0.6332603968,-1.136456329\C,2.7589546386,-0.2971316341,1.3870678012\C,2.8748182405,1.6894739262,-0.1610557242\H,2.445064001,-0.2232175215,-2.0907612674\H,3.8879863839,-0.6795320402,-1.1642014937\H,2.3994406404,-1.6442471475,-1.0235372861\H,2.3644071706,-1.3039637704,1.5310146365\H,3.8523092767,-0.3314922429,1.4556592657\H,2.3887024362,0.3480686896,2.1917494975\H,2.5196118484,2.3413121529,0.6439870064\H,3.9698266043,1.6887134688,-0.1484046114\H,2.5393101976,2.106173328,-0.1162961916\C,-2.1718148534,-2.2413262115,-1.0075965466\O,-1.8392406054,-2.0209976196,-2.1502731211\O,-2.5322198245,-3.4513753139,-0.5391464414\C,-2.448547083,-4.5251167031,-1.4903735443\H,-2.7879075964,-5.4146437665,-0.9588082743\H,-3.0867078569,-4.3247238045,-2.3553599647\H,-1.4167624188,-4.6493733774,-1.8287947601\Version=EM64L-G09RevA.02\State=1-A\HF=-786.3031962\RMSD=7.677e-09\RMSF=1.070e-05\Dipole=-0.5185614,0.5611698,0.3352002\Quadrupole=4.7665122,1.9364898,-6.703002,2.2501631,-0.7632419,2.438455\PG=C01 [X(C11H19N1O4)]\@

tert-butyl indoline-1-carboxylate radical carbocation (1):

1\1\GINC-HERO5-13\FOpt\UHF\6-31G(d,p)\C13H17N1O2(1+,2)\LHAYA\29-Nov-2010\0\#opt freq uhf/6-31g(d,p) maxdisk=2500MB geom=connectivity\291110_9\1,2\N,1.4436858323,0.2218016617,0.4122474202\C,2.8499587508,0.6696395852,0.6165932885\C,3.6830955752,-0.6093368343,0.4635516394\C,2.654037775,-1.6674643419,0.1835508098\C,1.344160625,-1.0756137156,0.1725084333\C,0.179847617,-1.8742164304,-0.0731719575\C,0.3709690108,-3.2188622492,-0.2956474318\C,1.6602681937,-3.8017348512,-0.2848557434\C,2.8050878212,-3.0186345058,-0.0436385762\C,0.4224098904,1.2448845839,0.5035040389\O,0.7839687199,2.3438544748,0.7300765172\O,-0.7580728273,0.7758580416,0.3164510558\H,2.9177264854,1.1209499321,1.5944360567\H,4.3937576868,-0.5256632945,-0.3500756035\H,4.2404756279,-0.8308291548,1.3659454803\H,-0.7925873342,-1.4360446514,-0.0815597843\H,-0.4834059719,-3.8422426233,-0.4826081038\H,1.7632606343,-4.8555999873,-0.4633835847\H,3.7801804911,-3.4695211809,-0.0372605536\H,3.070050132,1.4254589355,-0.1214927928\C,-1.9915863026,1.6374021027,0.3604470358\C,-3.0934958916,0.6266734516,0.0839760169\H,-4.0521525846,1.1309977708,0.0887147399\H,-2.9614169879,0.1633390285,-0.8871854147\H,-3.114442089,-0.1438882526,0.8462451416\C,-1.8974833094,2.6814147039,-0.7424857451\H,-2.8399313051,3.2145599128,-0.7938111316\H,-1.113442695,3.4006754493,-0.5535494212\H,-1.7279195454,2.2097178317,-1.7040974024\C,-2.1176082671,2.2389603023,1.7524264495\H,-3.0707174942,2.7506654423,1.8218432241\H,-2.099626411,1.4625007824,-2.5092233977\H,-1.3349097529,2.9555667798,1.956376071\Version=EM64L-G09RevA.02\State=2-A\HF=-706.2104558\S2=1.185583\S2-1=0.\S2A=0.90003\RMSD=3.967e-09\RMSF=8.579e-06\Dipole=0.9768206,-1.639303,-0.204639\Quadrupole=11.5109926,3.2623706,-14.7733632,-10.9358794,0.4245699,2.3292534\PG=C01 [X(C13H17N1O2)]\@

tert-butyl 1H-indole-1-carboxylate radical carbocation (2):

1\1\GINC-HERO5-19\FOpt\UHF\6-31G(d,p)\C13H15N1O2(1+,2)\URIETA\26-Jan-2011\0\#opt freq uhf/6-31g(d,p) maxdisk=2500MB geom=connectivity\aromatico_14\1,2\C,-2.6109153721,0.971295027,-0.0000101305\C,-1.7163791496,-0.1420511775,-0.0000279575\C,-2.1586435284,-1.4426730504,-0.0000997

244\C, -3.5574706654, -1.6340155414, -0.0001559055\C, -4.4694021976, -0.556
4980688, -0.0001400268\C, -4.0201688051, 0.7512379866, -0.0000676845\C, -1.
8475599943, 2.1230256756, 0.0000659158\C, -0.4865554479, 1.711565203, 0.000
0940704\H, -1.4834014354, -2.2726406466, -0.0001125942\H, -3.9353758826, -2
.639376719, -0.0002125723\H, -5.5230892788, -0.7620717755, -0.0001849332\H
, -4.6987378686, 1.5833000151, -0.0000545734\H, -2.1737295106, 3.1432376318
, 0.0000991491\H, 0.3934104078, 2.3212455483, 0.0001503676\C, 0.8183692132,
-0.3670275148, 0.000050008\O, 0.7696451202, -1.5443321875, -0.0000299037\O
, 1.8241146505, 0.4354152165, 0.0000854362\N, -0.4022981829, 0.3931732333, 0
.0000407195\C, 3.2531565332, -0.0313053801, 0.0000727351\C, 3.5045114584, -
0.8286466717, 1.2713244443\C, 3.5044115797, -0.8288431061, -1.2710747523\C
, 4.0139427084, 1.2849841415, -0.0000574058\H, 3.2377048522, -0.248280345, 2
.1475887519\H, 2.9563569005, -1.76011577, 1.2791531186\H, 4.5622014308, -1.
0580420283, 1.332243344\H, 3.237544782, -0.2486095159, -2.1474085551\H, 4.
5620947516, -1.0582581379, -1.3320174346\H, 2.9562470939, -1.7603086609, -1
.278718709\H, 5.0785611195, 1.0845085063, -0.0000818901\H, 3.7788512659, 1.
8688690198, -0.8823863415\H, 3.7789174516, 1.8690050926, 0.8821990439\Ver
sion=EM64L-G09RevA.02\State=2-A\HF=-705.0316943\S2=1.190173\S2-1=0.\S2
A=0.906929\RMSD=9.813e-09\RMSF=5.526e-06\Dipole=-1.3619746, 1.5420022, 0
.0000655\Quadrupole=22.8753905, -4.2893468, -18.5860438, -0.2057911, 0.001
1396, 0.000667\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate radical carbocation (3):

1\1\GINC-LOST\UHF\6-31G(d,p)\C13H23N1O2(1+, 2)\LUIA\15-Sep-2010\0
\#opt=calcfc freq uhf/6-31g(d,p) geom=connectivity\140910_8\1,2\N, -
0.0393548916, -1.2955836032, -0.8156344353\C, -1.2485695961, -0.7045484399
, -0.2198213054\C, -0.8465760916, -0.4709787288, 1.2392178897\C, 0.67551755
64, -0.2740769938, 1.1766129468\C, 1.1142524245, -1.3110948923, 0.125279540
2\C, 1.0593756738, 1.1653689992, 0.7911752862\C, 2.5005192996, 1.2899368546
, 0.2972647106\C, 2.7421953779, 0.3694863575, -0.8986425038\C, 2.4833837366
, -1.0898076346, -0.5221231505\H, -2.0786477344, -1.3824703643, -0.36994991
7\H, -1.3648006299, 0.3819763616, 1.6568052071\H, -1.1004410741, -1.3409813
496, 1.8342548778\H, 1.1412267952, -0.5282183726, 2.121650278\H, 1.06673308
08, -2.3162287271, 0.5408710405\H, 0.3950834267, 1.5325064618, 0.0099310305
\H, 0.8925746341, 1.803699232, 1.6522208842\H, 2.7025245486, 2.3201348918, 0
.0263934244\H, 3.192014923, 1.0361828316, 1.097847936\H, 2.0995295316, 0.66
80901087, -1.7269581989\H, 3.7620525168, 0.463475143, -1.2539757332\H, 3.20
77173926, -1.3977083295, 0.2260937063\H, 2.6150224411, -1.7591065251, -1.36
23977014\H, -1.4525503166, 0.2047756947, -0.7727181161\C, -0.0595180624, -2
.0049559103, -2.0970460561\O, 0.5361765901, -3.0161214078, -2.1725749561\O
, -0.7835765139, -1.3514121528, -2.9219885949\C, -1.0453510078, -1.80180875
11, -4.342771983\C, 0.2858010123, -1.8674696705, -5.0752791485\C, -1.774439
0648, -3.1355007966, -4.2928177447\C, -1.9310790407, -0.6842840394, -4.8665
831578\H, 0.8073661857, -0.9190957179, -5.01108533\H, 0.9213091259, -2.6541
396246, -4.6923499462\H, 0.0928642622, -2.0715668991, -6.122118946\H, -2.67
7211311, -3.0590374648, -3.6971316839\H, -2.0635263086, -3.4078253887, -5.3
01328989\H, -1.1495855064, -3.9250072427, -3.8984009308\H, -2.1938584213, -
0.8915352748, -5.8969994914\H, -2.8455031772, -0.6110822313, -4.2901491959
\H, -1.416051787, 0.2681135971, -4.8306715422\Version=EM64L-G09RevA.02\St
ate=2-A\HF=-709.6848676\S2=0.774045\S2-1=0.\S2A=0.750488\RMSD=3.935e-
09\RMSF=4.757e-06\Dipole=-0.7607868, 0.3646761, 0.7565396\Quadrupole=-1.
4854536, -10.3163176, 11.8017712, 3.7068332, 5.6122882, 5.025033\PG=C01 [X(
C13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate radical carbocation (4):

1\1\GINC-HER05-18\FOpt\UHF\6-31G(d,p)\C10H19N1O2(1+, 2)\LHAYA\11-Nov-20
10\0\#opt freq uhf/6-31g(d,p) geom=connectivity\111110_15\1,2\C, -1.
2796543863, 0.3907316197, -0.337144348\C, -1.8175399334, 0.1731222209, 1.07
72335\C, -3.2602444798, 0.6835545022, 1.2135228372\N, -4.0835857987, 0.0630
131915, 0.1640642915\C, -3.6510073267, 0.274555083, -1.2258177887\C, -2.208
9508863, -0.2368500954, -1.3765189342\C, -5.2209763764, -0.7968932573, 0.54
74998991\O, -5.3547326394, -1.0352809503, 1.6928339221\O, -5.8803673447, -1
.1407363414, -0.4885949036\C, -7.1199898834, -2.0154788342, -0.4386052189\
C, -6.7243279738, -3.3679063291, 0.1323053803\C, -8.1766228004, -1.29435287
52, 0.3830694595\C, -7.4970287556, -2.1013478245, -1.9074629093\H, -1.78847
53408, -0.879777314, 1.3410801914\H, -1.2200221543, 0.7008832615, 1.8109406
429\H, -3.6975707244, 0.4525090964, 2.1688878623\H, -3.3112754662, 1.752090
1053, 1.0323860276\H, -4.3428468632, -0.2202431667, -1.8831198419\H, -3.698
7970393, 1.3463247402, -1.3882504319\H, -1.8892388351, -0.0002306427, -2.38
44307459\H, -2.2048471336, -1.3192378179, -1.2872326445\H, -6.4382270102, -
3.3020283779, 1.172909431\H, -7.5772339087, -4.0328868316, 0.0603563443\H,
-5.912383526, -3.8046366622, -0.4381737114\H, -8.363740474, -0.3032310048,
-0.0142861308\H, -9.1006447894, -1.8577022077, 0.3227976329\H, -7.89919014
, -1.2177149634, 1.4253180544\H, -6.7040045305, -2.559580521, -2.4863877568
\H, -8.3874709421, -2.7097742915, -2.0104346492\H, -7.7074662242, -1.118896
6312, -2.3126522278\H, -1.1756751457, 1.4551655988, -0.5320547156\H, -0.290
6474574, -0.0430388796, -0.423456508\Version=EM64L-G09RevA.02\State=2-A
\HF=-593.7328908\S2=0.784461\S2-1=0.\S2A=0.750859\RMSD=7.307e-09\RMSF=
8.400e-06\Dipole=1.0044228, 0.9328811, -0.6046948\Quadrupole=10.6239582,

-2.093523,-8.5304352,10.371641,2.1773504,2.0045851\PG=C01 [X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate radical carbocation (5):

1\1\GINC-HER05-22\FOpt\UHF\6-31G(d,p)\C9H17N1O2(1+,2)\LHAYA\02-Dec-2010\0\#opt freq uhf/6-31g(d,p) maxdisk=2000MB geom=connectivity\1121210_5\1,2\N,-1.3329428093,-0.1607615836,0.021874562\C,-1.7488401218,1.2480940467,-0.0226818789\C,-3.2545144075,1.1779432261,0.2399987387\C,-3.658032143,-0.1949324614,-0.3130454668\C,-2.4709931767,-1.0917806923,0.0397201201\H,-1.1643431981,1.8113070405,0.6900995103\H,-1.5043847722,1.6048259771,-1.0193830513\H,-3.4467657229,1.2342770134,1.3055027491\H,-3.7762359793,1.9956500043,-0.2371970804\H,-4.5760278482,-0.5693612697,0.1176508285\H,-3.7850799817,-0.1542226214,-1.3890434622\H,-2.5216563425,-1.4883816926,1.049993671\H,-2.267200583,-1.9110671875,-0.6337466056\C,0.0520656982,-0.6391654649,0.0494923532\O,0.8489930749,0.355404126,-0.0242660195\O,0.2157244305,-1.8025209705,0.1308599917\C,2.3600444757,0.216820734,-0.0242804807\C,2.7614451389,-0.5964415743,-1.2446364539\C,2.7779052682,-0.4182120571,1.2924958766\C,2.8045997082,1.6653432744,-0.1291473061\H,2.3712223775,-0.1488643347,-2.1516975736\C,3.8430954672,-0.6003257983,-1.3136708338\H,2.4272583065,-1.6226849582,-1.1772262742\H,2.4434503981,-1.4433536486,1.3736923686\H,3.860378237,-0.4135818665,1.3472985907\H,2.3992791462,0.1522293454,2.1330995253\H,2.4523432401,2.2423495486,0.7174669001\H,3.8871950122,1.7044897154,-0.1404344795\H,2.437976107,2.1192251294,-1.0419478195\Version=EM64L-G09RevA.02\State=2-A\HF=-554.6917018\S2=0.7852\S2-1=0.\S2A=0.750871\RMSD=7.813e-09\RMSF=9.133e-06\Dipole=-1.6877354,0.7280587,-0.0442758\Quadrupole=17.5433572,-9.2072355,-8.3361217,0.753121,-0.1423811,0.1694886\PG=C01 [X(C9H17N1O2)]\@

tert-butyl diethylcarbamate radical carbocation (6):

1\1\GINC-LOST\FOpt\UHF\6-31G(d,p)\C9H19N1O2(1+,2)\LUIA\24-Nov-2010\0\#opt freq uhf/6-31g(d,p) geom=connectivity\191110_39\1,2\N,1.4790243343,0.0618539461,-0.5503205063\C,1.5704244688,1.4580948209,-1.0124349417\C,2.6954707661,-0.7405863624,-0.3199502318\H,2.3524357536,1.4763804725,-1.7596554245\H,0.6280550478,1.7155094652,-1.465893872\H,3.5250532457,-0.1600333453,-0.6934869075\H,2.5792116822,-1.6350130694,-0.9166449984\C,0.1757412613,-0.6009850099,-0.343771855\O,0.7190139875,0.2748690588,-0.0992185768\O,0.1482191276,-1.7738179687,-0.4308663616\C,-2.1788381756,-0.0657446511,0.1475791045\C,-2.2576183449,-0.9440253799,1.3860635997\C,-2.7280769606,-0.730705457,-1.1044880228\C,-2.7828672293,1.3081908434,0.3801390724\H,-1.7769521338,-0.4633967873,2.2306806131\H,-3.3019293168,-1.0906416906,1.6363767961\H,-1.8130648113,-1.9162257762,1.223677419\H,-2.2798634266,-1.6988428213,-1.2804861586\H,-3.7949500133,-0.8731766628,-0.976802848\H,-2.5781836016,-0.1005366633,-1.9738853845\H,-2.6575847054,1.9410114351,-0.4903098722\H,-3.8437127671,1.2012944907,0.5721501194\H,-2.3293025226,1.7925964036,1.2364586167\C,2.8745773228,-1.0933546178,1.1582411026\H,2.9518875226,-0.2075817649,1.7764150113\H,2.0670710901,-1.7169533989,1.5170240316\H,3.7972660061,-1.6519244391,1.2537660387\C,1.8944879352,2.3946895325,0.1552455369\H,1.1253099519,2.3497406635\O,0.9150706809\H,2.8554686071,2.1679660549,0.5996439543\H,1.9342618734,3.4052496787,-0.2314807358\Version=EM64L-G09RevA.02\State=2-A\HF=-555.8551083\S2=0.778546\S2-1=0.\S2A=0.75065\RMSD=3.641e-09\RMSF=9.772e-06\Dipole=1.4951691,0.9376781,-0.3165668\Quadrupole=14.0640086,-6.9599747,-7.1040339,1.3048309,-2.1536965,-2.4614976\PG=C01 [X(C9H19N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate radical carbocation (7):

1\1\GINC-HER03-22\FOpt\UHF\6-31G(d,p)\C11H19N1O4(1+,2)\LHAYA\15-Dec-2010\0\#opt freq uhf/6-31g(d,p) maxdisk=3000MB geom=connectivity\151210_9\1,2\N,-0.4050164867,0.9765131098,0.1948040805\C,-0.309344395,2.2940186448,-0.4428401128\C,-1.6662348997,2.9221116615,-0.125206563\C,-2.6269063415,1.7264289167,-0.1055773922\C,-1.7896631741,0.583129303,0.5009982701\H,0.5586824374,2.8151037689,-0.0664880095\H,-0.1650892631,2.0997764542,-1.5021742459\H,-1.6321888755,3.4062073133,0.8442269703\H,-1.9412422869,3.664714452,-0.8611624892\H,-3.5186783088,1.9047362234,0.4769428027\H,-2.9298170137,1.4678378711,-1.113992342\H,-1.8711446441,0.5259230265,1.5802876631\C,0.7356935832,0.1286969509,0.5811160122\O,1.7055354047,0.3530078674,-0.2114615977\O,0.5897558582,-0.5537780632,1.5270489448\C,3.0234854535,-0.3956435909,-0.1497384274\C,2.7343778342,-1.8760448034,-0.3413747682\C,3.687812871,-0.0723249738,1.1788906737\C,3.7736936374,0.1994249444,-1.3284986991\H,2.1654224385,-2.0423973217,-1.2484104144\H,3.6789161011,-2.3999875653,-0.4328558903\H,2.1971668346,-2.2960923536,0.4977862102\H,3.1329089703,-0.4721641344,2.016571907\H,4.6759454913,-0.5178493979,1.1868708186\H,3.8037705667,0.9985936015,1.3021880969\H,3.9053430251,1.267911351,-1.2061326988\H,4.7533192067,-0.2587487001,-1.3936316219\H,3.2469398943,0.0132818029,-2.2564716146\C,-2.0491702157,-0.7801379702,-0.1217654326\O,-1.2854349855,-1.2756876561,-0.8843999797\O,-3.1944053591,-1.2499381448,0.2649066115\C,-3.6121540617,-2.5223544093,-0.2589530253\H,-4.5740069285,-2.7102269213,0.1865500345\H,-3.6883766293,-2.4662571283,-1.3340151857\H,-2.9002297391,-3.281

6851293,0.0256284143\\Version=EM64L-G09RevA.02\State=2-A\HF=-781.33502
46\S2=0.775388\S2-1=0.\S2A=0.750532\RMSD=8.801e-09\RMSF=6.389e-06\Dipole=-0.7594278,1.6554612,-0.2080064\Quadrupole=14.9910173,1.1643367,-16
.155354,-0.6596957,-0.3070744,0.0558954\PG=C01 [X(C11H19N1O4)]\\@

tert-butyl piperidine-1-carboxylate cation (4):

1\1\GINC-HER05-12\FOpt\RHF\6-31G(d,p)\C10H18N1O2(1+)\LHAYA\11-Nov-2010
0\#opt freq hf/6-31g(d,p) geom=connectivity\\111110_27\1,1\C,-1.405
2575598,0.88741726,-0.3620647669\C,-1.5740747876,0.1750896079,0.975732
1363\C,-3.0429775977,0.0649222959,1.3508762569\N,-3.852254779,-0.46587
07774,0.2079959724\C,-2.1395175774,0.1032172198,-1.447609812\C,-5.1795
147519,-0.9897364472,0.5645728957\O,-5.5057023109,-0.9364813625,1.6923
292351\O,-5.788764962,-1.4341501088,-0.4731131391\C,-7.1764921837,-2.0
314790255,-0.4274155\C,-7.1395342211,-3.2664746382,0.4593235317\C,-8.1
438288726,-0.9643708577,0.0609066861\C,-7.4111589208,-2.3865061185,-1.
8862749832\H,-1.130829202,-0.8159431479,0.9322321616\H,-1.0696066589,0
.7132184027,1.7689137331\H,-3.202675034,-0.6098491829,2.1747686818\H,-
3.4709418801,1.0229026164,1.6138401834\H,-2.32319242,0.6898221462,-2.3
43074663\H,-1.564963613,-0.7620436387,-1.7804011288\H,-6.9585272841,-3
0.160281721,1.4950675848\H,-8.1001786572,-3.7645364623,0.3956041517\H,
-6.3801887519,-3.9617958984,0.1193048384\H,-8.0771455881,-0.0738528662
, -0.5541328153\H,-9.1530069336,-1.3513599058,-0.0213479788\H,-7.967865
4787,-0.7005044101,1.0941757749\H,-6.6745428689,-3.1003518994,-2.23609
33712\H,-8.3923192741,-2.8333920906,-1.9918694146\H,-7.3726569172,-1.5
02882352,-2.5126697256\H,-1.8062715796,1.8944166928,-0.30161844\H,-0.3
596147648,0.9764533106,-0.6259935792\C,-3.4499763627,-0.4447867502,-1.
0046124476\H,-4.1152155268,-0.8658193897,-1.7356119684\\Version=EM64L-
G09RevA.02\State=1-A\HF=-593.1869734\RMSD=7.585e-09\RMSF=5.852e-06\Dip
ole=1.7046212,0.5637733,-1.1811442\Quadrupole=13.3047811,-5.4123443,-7
.8924369,10.4574688,0.931099,0.4603689\PG=C01 [X(C10H18N1O2)]\\@

tert-butyl pyrrolidine-1-carboxylate cation (5):

1\1\GINC-HER03-30\FOpt\RHF\6-31G(d,p)\C9H16N1O2(1+)\LHAYA\02-Dec-2010\
0\#opt freq hf/6-31g(d,p) maxdisk=2000MB geom=connectivity\\011210_9\
1,1\N,-1.3669960091,-0.1936625965,-0.0063539008\C,-1.7847884548,1.234
5990851,-0.0821586773\C,-3.3001550555,1.1492852057,0.1617594147\C,-3.6
602000348,-0.3275894811,-0.1004817583\C,-2.34333944001,-1.011680864,-0.
0211268622\H,-1.248798521,1.7985701517,0.6634790298\H,-1.5196325916,1.
6067498967,-1.0617798894\H,-3.5275476839,1.4091104766,1.1871950287\H,-
3.8458269299,1.8241955209,-0.4814048349\H,-4.3658474568,-0.7509224919,
0.6041837868\H,-4.0629847673,-0.5049972468,-1.0960514088\H,-2.15573257
03,-2.0707193858,0.0007007792\C,0.0160069033,-0.66746794,0.023156859\O
,0.7987362251,0.3401341408,-0.0184524066\O,0.2135706675,-1.8275399062,
0.0760861218\C,2.3047229364,0.2255788357,-0.0054541791\C,2.7369764645,
-0.5486878745,-1.2412448471\C,2.7239862067,-0.435043858,1.298892521\C,
2.7298709052,1.6830294344,-0.0686064996\H,2.34881452,-0.0847258074,-2.
1410917283\H,3.8192787347,-0.5311585172,-1.2974047693\H,2.4189300621,-
1.5812969171,-1.2038344783\H,2.4062244227,-1.4671134251,1.3505209596\H
,3.8056570142,-0.4115670617,1.364450662\H,2.3264795851,0.106910586,2.1
49720582\H,2.3591795883,2.2329954067,0.7882031528\H,3.8117856247,1.739
3475066,-0.0669293292\H,2.3656006146,2.1547011263,-0.973438328\\Versio
n=EM64L-G09RevA.02\State=1-A\HF=-554.1443234\RMSD=6.349e-09\RMSF=2.761
e-05\Dipole=-2.4931564,0.4361587,-0.1069026\Quadrupole=20.5041148,-10.
0879625,-10.4161523,2.8045952,0.441759,0.1994024\PG=C01 [X(C9H16N1O2)]
\\@

tert-butyl diethylcarbamate cation (6):

1\1\GINC-HER03-29\FOpt\RHF\6-31G(d,p)\C9H18N1O2(1+)\LHAYA\25-Nov-2010\
0\#opt freq hf/6-31g(d,p) maxdisk=2000MB geom=connectivity\\231110_7\
1,1\N,1.6035395543,0.0925280793,-0.2648863523\C,1.8861309862,1.338702
5861,-0.2144939055\C,2.6854907517,-0.8990878641,-0.5984817714\H,2.9055
323172,1.565285257,-0.4805145375\H,3.3590929546,-0.3924495829,-1.27480
46293\H,2.2096051735,-1.7067184752,-1.128335214\C,0.2928525978,-0.5034
722495,0.0375914724\O,-0.6476231551,0.359569714,-0.0691945868\O,0.2637
119143,-1.6493671017,0.2991109826\C,-2.1060566537,0.0111342233,0.13206
01596\C,-2.298023432,-0.4678711216,1.5628888551\C,-2.5011392758,-1.023
9480087,-0.9103718281\C,-2.7868057954,1.3473647937,-0.1154932621\H,-1.
9331650483,0.2695451112,2.2695537452\H,-3.3588297429,-0.6013845761,1.7
41102657\H,-1.8049367889,-1.4122727574,1.7441666272\H,-2.0144119115,-1
.9742912054,-0.7437500163\H,-3.5722770173,-1.1789934647,-0.8510267312\
H,-2.2702308685,-0.6710768848,-1.9092703478\H,-2.5809449793,1.70930091
55,-1.1159338208\H,-3.8583175308,1.2250972213,-0.013872593\H,-2.463932
4668,2.0911492395,0.6036439818\C,3.4027313023,-1.3946155699,0.64732619
63\H,3.8843793715,-0.5799337185,1.1780063961\H,2.7207471931,-1.9024189
842,1.3150570658\H,4.1709210383,-2.0973173556,0.3468624402\C,1.0315898
573,2.5002687834,0.1610079154\H,0.4001994921,2.2864776045,1.0088231788
\H,1.6733079243,3.343948909,0.3710071502\H,0.3909072378,2.7483374822,-
0.6792482272\\Version=EM64L-G09RevA.02\State=1-A\HF=-555.2990973\RMSD=
4.352e-09\RMSF=5.749e-06\Dipole=1.6938115,1.6319861,-0.4593552\Quadrup
ole=13.6497704,-4.1716937,-9.4780768,2.6227631,-2.7366741,0.576226\PG=

C01 [X(C9H18N1O2)]\ \@

1-*tert*-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate cation (7):

1\1\GINC-HERO3-22\FOpt\RFHF\6-31G(d,p)\C11H18N1O4(1+)\LHAYA\15-Dec-2010
\0\#\opt freq hf/6-31g(d,p) maxdisk=2500MB geom=connectivity\151210_1
6\1,1\N,-0.3302004785,0.8866004818,0.2647552337\C,-0.2968825143,1.949
0817815,-0.4362761083\C,-1.6213353115,2.6223107588,-0.5045026357\C,-2.
4236499017,1.8954115509,0.5913949824\C,-1.6860037871,0.5512405162,0.75
63997533\H,0.6138958925,2.2605858965,-0.9127034111\H,-1.5332497151,3.6
925210121,-0.3643688051\H,-2.0157208906,2.4558566875,-1.5050051323\H,-
2.3792438613,2.4498542681,1.5196203967\H,-3.4634352271,1.7578036577,0.
3329184388\H,-1.6333342235,0.1985341029,1.7729554692\C,0.7718384631,-0
.0457553786,0.4633096174\O,1.8287274226,0.3939490769,-0.1112994499\O,0
.556346017,-1.013648228,1.0953469633\C,3.1419646062,-0.3529451305,-0.1
1400427\C,2.9308763171,-1.6911271312,-0.8052702615\C,3.6222788261,-0.4
828291217,1.3231205739\C,4.0277970326,0.5748160338,-0.9285942731\H,2.5
06117455,-1.5513986275,-1.7927985197\H,3.8942562773,-2.1747334321,-0.9
196803827\H,2.2909969603,-2.3465048272,-0.2312541649\H,2.9808952512,-1
.1281334648,1.9069517032\H,4.617263839,-0.9128723564,1.3163868988\H,3.
6821643238,0.4898528072,1.7985153815\H,4.1137125144,1.5456067946,-0.45
45193647\H,5.0197167106,0.1459682438,-1.0047205018\H,3.6365778277,0.70
41102787,-1.9309108971\C,-2.2516216174,-0.5312167229,-0.1563857235\O,-
1.8230691445,-0.7241839465,-1.2471027186\O,-3.2605779532,-1.1279731152
0.4045012554\C,-3.929648737,-2.1572621859,-0.3396315861\H,-4.71645749
73,-2.509903947,0.305362824\H,-4.3344336817,-1.745994331,-1.2519751674
\H,-3.2342271949,-2.9505820027,-0.5670521181\Version=EM64L-G09RevA.02
\State=1-A\HF=-780.7887718\RMSD=6.347e-09\RMSF=1.301e-05\Dipole=-0.576
0517,2.2246636,-0.1092744\Quadrupole=15.801159,0.6190584,-16.4202173,-
2.1450339,-1.2124184,-0.3970967\PG=C01 [X(C11H18N1O4)]\ \@

1.3 Optimized geometries at HF/6-311++G(2df,2p) level:

***tert*-butyl indoline-1-carboxylate (1):**

1\1\GINC-HERO3-49\FOpt\RFHF\6-311++G(2df,2p)\C13H17N1O2\LHAYA\03-Dec-20
10\0\#\opt freq hf/6-311++g(2df,2p) maxdisk=2500MB geom=connectivity\1
261110_5\0,1\N,-0.4661377175,-0.9637809366,-0.0002562627\C,-1.1426346
929,-2.2653916619,-0.0007450189\C,-2.6458120286,-1.9373748901,0.001352
7876\C,-2.6834177239,-0.4319885352,0.0004814425\C,-1.3982702939,0.0895
617808,-0.0002467663\C,-1.198270531,1.4568278143,-0.0009560406\C,-2.31
06321433,2.2843138033,-0.0008965277\C,-3.5917173381,1.7726085279,-0.00
0168772\C,-3.7768497292,0.3994088279,0.0005312936\C,0.8892457625,-0.95
69537563,-0.000257557\O,1.5183194377,-1.9707661475,-0.0006509016\O,1.4
031523244,0.2513884901,0.0001753931\H,-0.8436764914,-2.8313055518,0.86
82178207\H,-3.1405914392,-2.3488808819,-0.868871259\H,-3.1378466932,-2
.3475970037,0.8737561972\H,-0.2187973701,1.8760209395,-0.0015440209\H,
-2.1630024376,3.3474825213,-0.001456452\H,-4.4375697014,2.4320688618,-
0.0001536802\H,-4.7686535684,-0.013182985,0.0011101472\H,-0.8458337617
, -2.829503977,-0.8716609316\C,2.8286887623,0.5041510222,0.0002949831\C
,2.9024851253,2.0257637832,0.0008839105\H,3.9359090208,2.3470334832,0.
0011024259\H,2.4190575935,2.4330267563,-0.8777857985\H,2.4188802437,2.
4323503776,0.8797675041\C,3.4678930772,-0.0551367615,-1.2655424042\H,4
.4989172939,0.2729125397,-1.3184615104\H,3.4472188188,-1.132495791,-1.
2784390219\H,2.9520799782,0.3160624547,-2.1428365692\C,3.4678121431,-0
.0561121686,1.2657402354\H,4.4988497993,0.2718464096,1.3189532408\H,2.
951973721,0.3144499506,2.1432884742\H,3.4470875597,-1.1334812959,1.277
8206387\Version=EM64L-G09RevA.02\State=1-A\HF=-706.6267672\RMSD=2.935
e-09\RMSF=8.534e-06\Dipole=-0.1912692,0.4745223,0.0004493\Quadrupole=5
.230336,-1.6006775,-3.6296585,7.0653065,-0.0004027,-0.0046408\PG=C01 [X
(C13H17N1O2)]\ \@

***tert*-butyl 1*H*-indole-1-carboxylate (2):**

1\1\GINC-HERO3-11\FOpt\RFHF\6-311++G(2df,2p)\C13H15N1O2\URIETA\27-Jan-2
011\0\#\opt freq hf/6-311++g(2df,2p) maxdisk=2500MB geom=connectivity\
\aromatico_17\0,1\C,-2.577797355,0.9485926923,-0.0003247536\C,-1.6991
436379,-0.1321041805,0.0001775493\C,-2.1545076608,-1.441833583,0.00074
2053\C,-3.5177252479,-1.6363163502,0.0007887421\C,-4.4106717946,-0.565
4612145,0.0002911012\C,-3.9492817082,0.7286540579,-0.000266093\C,-1.77
56678442,2.1516221799,-0.0008337917\C,-0.4965341428,1.7771624918,-0.00
06357763\H,-1.4761586362,-2.2659738678,0.0011263281\H,-3.899887099,-2.
6389989074,0.0012205758\H,-5.4662342627,-0.757649198,0.0003455818\H,-4
.6337271322,1.5554236172,-0.0006504915\H,-2.1306201255,3.1593775727,-0
.0012892616\H,0.3878532087,2.3694314787,-0.000874761\C,0.7637038218,-0
.3446304103,0.0003509484\O,0.7825673366,-1.5292497196,0.0008309592\O,1
.8089427523,0.4435847061,-0.000032636\N,-0.4018668025,0.3870253133,-0.
0000074186\C,3.1763967867,-0.0423477705,-0.00002385\C,3.4492814357,-0.
8456444762,1.2657094488\C,3.4496171947,-0.8452921117,-1.2659209889\C,3
.9879762571,1.2457978682,0.0002442309\H,3.1856315422,-0.268118638,2.14
32041007\H,2.8962875229,-1.7708308175,1.2777674682\H,4.5064244567,-1.0
746417989,1.3195471511\H,3.1860719436,-0.267559137,-2.1433107546\H,4.5
0680147,-1.0741407638,-1.3196219968\H,2.8967472383,-1.7705373005,-1.27

83427049\H,5.0457139852,1.0172768598,0.0003269641\H,3.7657296614,1.837
8096106,-0.8780032182\H,3.7655408356,1.8375657967,0.878609294\Version
=EM64L-G09RevA.02\State=1-A\HF=-705.458779\RMSD=4.021e-09\RMSF=6.649e-
06\Dipole=0.8911271,0.708595,-0.000458\Quadrupole=7.3005793,-1.302171,
-5.9984082,0.2276061,-0.001187,-0.0018174\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate (3):

1\1\GINC-LOST\FOpt\RHF\6-311++G(2df,2p)\C13H23N1O2\LUISA\24-Oct-2010\0
\#opt freq hf/6-311++g(2df,2p)\280910_3\0,1\N,-0.3719131961,0.35503
91618,-0.2251204287\C,-0.4905510822,1.742422602,0.2242621957\C,-1.7928
402804,2.216689612,-0.4198333075\C,-2.6238259735,0.9391788102,-0.52637
18224\C,-1.5698929433,-0.0999625858,-0.9452276448\C,-3.3155230334,0.61
69814936,0.8060881365\C,-3.7892648494,-0.8276953411,0.9089636972\C,-2.
6210320349,-1.7796266461,0.6809246492\C,-1.9969186324,-1.5462196375,-0
.6902253748\H,0.3576301254,2.3274192493,-0.0932945708\H,-2.2763650214,
2.9947503166,0.1565354767\H,-1.5890964957,2.614381799,-1.4073322771\H,
-3.3781615392,1.0147094604,-1.3008731712\H,-1.385170228,0.0001838416,-
2.0107042243\H,-2.6319087218,0.8082148709,1.6273599098\H,-4.1462358013
1.3027779329,0.9370415377\H,-4.2409435655,-0.9978750671,1.8801779564\H,
-4.562230349,-1.0191402037,0.1682659943\H,-1.8774323431,-1.633753828
5,1.4591888991\H,-2.9491031417,-2.8104811077,0.7554414367\H,-2.7381376
843,-1.7841557344,-1.4495419742\H,-1.1610549161,-2.205398813,-0.856966
088\H,-0.53139588493,1.7939669724,1.3047669139\C,0.823872322,-0.2442577
03,-0.4090485991\O,0.99132398,-1.2222905402,-1.0742391232\O,1.78312576
65,0.3835482138,0.249866586\C,3.159190788,-0.0451124563,0.2516942656\C
3.2862055322,-1.432552348,0.8717254393\C,3.7412958758,0.0075959578,-1
.1569564597\C,3.8353637088,0.9921105566,1.1399362675\H,2.8165473649,-1
.4517765607,1.847868502\H,2.8305971955,-2.1867102422,0.2510690801\H,4.
3347314561,-1.6737864784,0.9987528568\H,3.5889166254,0.9890465601,-1.5
902267238\H,4.8080188864,-0.175990139,-1.1107640565\H,3.2906636611,-0.
7306098446,-1.799905907\H,4.8928596905,0.7777358971,1.2268838387\H,3.7
20266281,1.9846086045,0.7234652198\H,3.4009954226,0.9859593648,2.13121
88941\Version=EM64L-G09RevA.02\State=1-A\HF=-710.1270599\RMSD=3.509e-
09\RMSF=2.296e-05\Dipole=-0.1600568,0.840833,0.3713326\Quadrupole=4.87
30934,-2.3639833,-2.5091101,0.1801659,2.0152349,-2.3197503\PG=C01 [X(C
13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate (4):

1\1\GINC-LOST\FOpt\RHF\6-311++G(2df,2p)\C10H19N1O2\LUISA\04-Dec-2010\0
\#opt freq hf/6-311++g(2df,2p) geom=connectivity\111110_5\0,1\C,-3.
7638634852,0.5437362086,0.1298629151\C,-3.2768834544,-0.8636135056,0.4
62658277\C,-2.053453673,-1.2360025217,-0.3652328767\N,-1.0113721279,-0
.2323560597,-0.2269376507\C,-1.4098239912,1.124962815,-0.5599303709\C,
-2.6222061631,1.5474097867,0.262270644\C,0.2725152506,-0.6371913789,-0
.0873850554\O,0.5965887393,-1.7793342905,0.0479161367\O,1.1210121831,0
.3748838664,-0.1015895124\C,2.5446702318,0.2196252914,0.0706774964\C,2
.857748399,-0.3700132043,1.4415837504\C,3.1343598137,-0.6148688529,-1.
0611836353\C,3.052009034,1.654105881,-0.0138423673\H,-3.0198706853,-0.
9222016546,1.5157246879\H,-4.0605762154,-1.5912432103,0.2837176027\H,-
1.6548231235,-2.1864330158,-0.0607786048\H,-2.3351016471,-1.3168048864
,-1.4143668993\H,-0.5872564786,1.7930507099,-0.3870918428\H,-1.6566505
873,1.1748570123,-1.6197761945\H,-2.9404776983,2.5329337386,-0.0594809
241\H,-2.3277651087,1.629733666,1.3039723773\H,2.5256366254,-1.3922809
929,1.5184118794\H,3.9276896707,-0.3382298572,1.6087926266\H,2.3792601
105,0.2129842574,2.219422282\H,2.8481792573,-0.2014774165,-2.020932754
4\H,4.2155749407,-0.593056993,-0.9957486884\H,2.804917627,-1.639589634
6,-1.0112272347\H,2.6108622769,2.2615893518,0.7659369075\H,4.128009009
8,1.677449956,0.1015225046\H,2.8007996614,2.0918418373,-0.9714279053\H
,-4.1432779127,0.5624087485,-0.889005031\H,-4.5894344794,0.8228223479,
0.7742654605\Version=EM64L-G09RevA.02\State=1-A\HF=-594.1555744\RMSD=
5.944e-09\RMSF=1.024e-05\Dipole=-0.2788986,0.9348614,-0.1170717\Quadru
pole=5.467527,-4.7878354,-0.6796916,1.6844119,0.566978,0.1832697\PG=C0
[X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate (5):

1\1\GINC-LOST\FOpt\RHF\6-311++G(2df,2p)\C9H17N1O2\LUISA\15-Oct-2010\0
\#opt freq hf/6-311++g(2df,2p)\270910_3\0,1\N,-1.2932400019,-0.16069
77241,0.0318171938\C,-1.7045019102,1.2340881815,-0.0351873727\C,-3.204
7003308,1.1620035309,0.2428212277\C,-3.6014515051,-0.2059066473,-0.311
7903973\C,-2.4126628143,-1.0901861581,0.0552768765\H,-1.1744578974,1.8
349550523,0.6878763561\H,-1.5049794329,1.648398101,-1.0175106181\H,-3.
3816559369,1.1931697761,1.3120027031\H,-3.7464908735,1.9830670697,-0.2
059949679\H,-4.5335067293,-0.5778797635,0.0903523233\H,-3.7029047346,-
0.1535282171,-1.3900065299\H,-2.5288328288,-1.5236567615,1.0425782843\H,
-2.252801862,-1.9006668145,-0.6389343426\C,-0.0266952542,-0.60571859
86,0.0451873784\O,0.8378617588,0.3922533443,-0.0243655332\O,0.26525373
16,-1.7630572325,0.1109731695\C,2.267166716,0.2052651441,-0.0215491462
C,2.703408737,-0.5974568794,-1.2424854894\C,2.7193765673,-0.444436067
5,1.2818388467\C,2.7960260989,1.631357988,-0.111458446\H,2.3227968717,
-0.1402134964,-2.1480145422\H,3.7853173816,-0.6046146393,-1.2993622055

\H, 2.3525912198, -1.6153045394, -1.1924045949\H, 2.3691644217, -1.46074878
23, 1.3595403622\H, 3.8019168342, -0.4450765459, 1.3255197296\H, 2.34979429
86, 0.1188807844, 2.1303906759\H, 2.4609365341, 2.2165427374, 0.7352268393\
H, 3.8785119924, 1.6289329325, -0.1195382179\H, 2.4472689483, 2.1108652251,
-1.0169635627\Version=EM64L-G09RevA.02\State=1-A\HF=-555.1071784\RMSD
=3.413e-09\RMSF=1.726e-05\Dipole=-0.3948399, 1.0105606, -0.0682907\Quadr
upole=6.4384998, -5.6370966, -0.8014032, 0.5743359, -0.0350725, 0.398019\PG
=C01 [X(C9H17N1O2)]\@

tert-butyl diethylcarbamate (6):

1\1\GINC-HER05-15\FOpt\RHF\6-311++G(2df,2p)\C9H19N1O2\LHAYA\24-Nov-201
0\0\#opt freq hf/6-311++g(2df,2p) maxdisk=2000MB\191110_29\0,1\N,1.
4095252655, 0.0446520612, -0.4874115218\C, 1.5593613998, 1.4773647851, -0.6
944484912\C, 2.5766138343, -0.8246384175, -0.5514060089\H, 2.4244498196, 1.
6165900535, -1.3286180966\H, 0.7069416515, 1.8428901596, -1.2438017333\H, 3
.3086140912, -0.3332111436, -1.1781268008\H, 2.2899688345, -1.739270179, -1
.0461792805\C, 0.2186319594, -0.5335916177, -0.219073205\O, -0.7659787425,
0.3467562522, -0.1778968081\O, 0.0803997558, -1.7079476014, -0.0424417026\
C, -2.1410557453, -0.0112766747, 0.0699646435\C, -2.2930734637, -0.62412886
91, 1.4579664887\C, -2.6598490378, -0.9371192412, -1.024973072\C, -2.856826
2063, 1.3324596151, 0.0060707961\H, -1.8683733156, 0.0327318525, 2.20774412
76\H, -3.3459134438, -0.7498401927, 1.6803688262\H, -1.8086749414, -1.58463
7562, 1.5217457177\H, -2.1816842346, -1.9021167881, -0.9870201762\H, -3.727
7628373, -1.0727475023, -0.9027994072\H, -2.4869586377, -0.4988786771, -2.0
006778018\H, -2.7243560396, 1.789731009, -0.9660511646\H, -3.9168734383, 1.
1998044887, 0.1803880826\H, -2.4682950107, 2.0082937278, 0.7569985443\C, 3.
1928426446, -1.1575155047, 0.80193708\H, 3.5460283917, -0.2691885195, 1.310
8254409\H, 2.4709726658, -1.654055737, 1.4355335115\H, 4.0383754093, -1.823
0077069, 0.6672282316\C, 1.7282922184, 2.2916551165, 0.5830931801\H, 0.8723
748726, 2.1694197114, 1.2333264724\H, 2.6151506669, 1.9965196045, 1.1290805
022\H, 1.8205966137, 3.3445434975, 0.3401366253\Version=EM64L-G09RevA.02
\State=1-A\HF=-556.271271\RMSD=5.683e-09\RMSF=2.036e-05\Dipole=0.06306
65, 0.9434501, -0.1444223\Quadrupole=5.3815154, -4.4858672, -0.8956482, 0.5
758377, -1.3199182, -0.2521635\PG=C01 [X(C9H19N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate (7):

1\1\GINC-HER03-50\FOpt\RHF\6-311++G(2df,2p)\C11H19N1O4\LHAYA\17-Dec-20
10\0\#opt freq hf/6-311++g(2df,2p) maxdisk=5000MB geom=connectivity\
151210_5\0,1\N, -0.296402994, 0.9137314551, 0.1502806736\C, -0.1156597244
, 2.2311643197, -0.4348509889\C, -1.3295881933, 2.9870477341, 0.0921205216\
C, -2.4197849875, 1.9162900858, 0.1292031515\C, -1.6623547109, 0.6311385509
, 0.522614222\H, 0.8202278184, 2.6651846575, -0.1238285246\H, -0.1214531412
, 2.1792872351, -1.5183041423\H, -1.1264124114, 3.3512976869, 1.0923608693\
H, -1.5952385049, 3.8340706201, -0.5249288391\H, -3.220303814, 2.1377183737
, 0.8192078325\H, -2.8502774001, 1.7996300319, -0.8573518516\H, -1.73903254
79, 0.4323467038, 1.581097927\C, 0.6561770736, -0.0170612349, 0.3496779852\
O, 1.8301797827, 0.3797413116, -0.0947074259\O, 0.4319303542, -1.0639524974
, 0.8804618215\C, 3.0206923669, -0.4354640714, -0.0303064837\C, 2.834082994
2, -1.7118336277, -0.8428124812\C, 3.3896824147, -0.725918846, 1.4201644715
\C, 4.0743568031, 0.4545903304, -0.6768650211\H, 2.5153765296, -1.473065631
2, -1.8499283631\H, 3.7792084992, -2.2379764744, -0.9033887273\H, 2.1028960
35, -2.3639794815, -0.393804134\H, 2.6633856192, -1.366990991, 1.8925482058
\H, 4.3566709758, -1.2132699277, 1.4526070071\H, 3.4604359898, 0.1973350688
, 1.982810244\H, 4.1845538995, 1.3791218985, -0.1247163441\H, 5.031246621, -
0.0511622566, -0.6922377787\H, 3.7969269259, 0.6953366235, -1.6948071225\C
, -2.2290141977, -0.5636147243, -0.2233337912\O, -1.9415405181, -0.86055259
52, -1.3299494792\O, -3.1397224852, -1.1843545502, 0.4949030119\C, -3.77445
52465, -2.3053629901, -0.0871600873\H, -4.4666968409, -2.6718982728, 0.6524
46767\H, -4.3018248618, -2.0200271668, -0.9849297089\H, -3.046703123, -3.06
4886348, -0.3276454168\Version=EM64L-G09RevA.02\State=1-A\HF=-781.8283
93\RMSD=3.945e-09\RMSF=1.233e-05\Dipole=-0.1170396, 0.9371772, 0.1777494
\Quadrupole=7.0088408, 0.717598, -7.7264388, -0.0521218, -1.5758026, 0.5039
049\PG=C01 [X(C11H19N1O4)]\@

tert-butyl indoline-1-carboxylate radical carbocation (1):

1\1\GINC-HER05-17\FOpt\UHF\6-311++G(2df,2p)\C13H17N1O2(1+,2)\LHAYA\17-
Dec-2010\0\#opt freq uhf/6-311++g(2df,2p) maxdisk=5000MB geom=connect
ivity\291110_11\1,2\N, 0.5397247138, -0.9331892485, -0.000169692\C, 1.21
35567528, -2.2569414554, -0.0000393415\C, 2.7089302821, -1.9256257536, -0.0
004408748\C, 2.7339064839, -0.4270719741, -0.0002041269\C, 1.3907874498, 0.
0749921403, -0.0001435316\C, 1.1378161354, 1.4817899328, -0.0000087422\C, 2
.2228824647, 2.3182143374, 0.0000916904\C, 3.5444834492, 1.8231452332, 0.00
00498783\C, 3.7960305219, 0.4430685885, -0.0001013222\C, -0.9081602729, -0.
9480831381, -0.0001123819\O, -1.428453632, -1.9981948217, 0.0006321456\O, -
1.4094772628, 0.2273029452, -0.0004208056\H, 0.889044357, -2.7996399772, -0
.8717644546\H, 3.2049463685, -2.3286552135, 0.8714405817\H, 3.2043678403, -
2.3282915972, -0.872826274\H, 0.142982148, 1.8587346315, 0.0000297213\H, 2.
0631213419, 3.3779477513, 0.0002118969\H, 4.3639754354, 2.5133697602, 0.000
1352787\H, 4.8034840071, 0.0766617627, -0.0001374283\H, 0.889454764, -2.799
2143737, 0.8721099537\C, -2.8864562112, 0.4867003825, -0.0001738991\C, -2.9

461092745,2.0035361859,-0.0009399644\H,-3.9796901933,2.32022907,-0.000
9024446\H,-2.4699622247,2.4122362991,0.8806039325\H,-2.4702932482,2.41
1328219,-0.8830814253\C,-3.4865605396,-0.0937139058,1.2690550939\H,-4.
5234198017,0.2092842006,1.3278142053\H,-3.4505069752,-1.1714295999,1.2
782112619\H,-2.9779242972,0.2885336925,2.1447684978\C,-3.4871733698,-0
.0950168415,-1.2685150673\H,-4.5240727665,0.2078839099,-1.32706156\H,-
2.978986484,0.2863620343,-2.1448675692\H,-3.4510869624,-1.1727411766,-
1.2765962325\Version=EM64L-G09RevA.02\State=2-A\HF=-706.4012039\S2=1.
159677\S2=1=0.\S2A=0.88244\RMSD=4.930e-09\RMSF=1.350e-05\Dipole=1.8294
003,0.5193558,-0.0003775\Quadrupole=18.6142923,-3.3704999,-15.2437924,
-3.7999212,0.0012824,0.0034067\PG=C01 [X(C13H17N1O2)]\@

tert-butyl 1H-indole-1-carboxylate radical carbocation (2):

1\1\GINC-HERO3-12\FOpt\UHF\6-311++G(2df,2p)\C13H15N1O2(1+,2)\URIETA\27
-Jan-2011\0\#opt freq uhf/6-311++g(2df,2p) maxdisk=2500MB geom=connec
tivity\aromatico_18\1,2\C,-2.6067423024,0.9676187118,-0.0000773174\C
,-1.7140656648,-0.142558555,-0.0000154302\C,-2.1578464532,-1.436547863
2,0.0000224515\C,-3.5529977055,-1.6255587346,-0.0000027154\C,-4.462042
1029,-0.5505777461,-0.0000635389\C,-4.0125317933,0.7499891236,-0.00010
14754\C,-1.8461048241,2.1158299191,-0.0001026108\C,-0.4894834059,1.704
3329228,-0.0000564553\H,-1.4880249541,-2.2675697062,0.0000689753\H,-3.
9310754699,-2.6283587838,0.0000258903\H,-5.5134925962,-0.7550685299,-0
.0000801142\H,-4.6881338216,1.5814228015,-0.0001478936\H,-2.1709651165
,3.133858619,-0.0001479825\H,0.3861997188,2.3163628334,-0.0000593606\C
,0.8168521401,-0.368889423,0.0000521458\O,0.7664799566,-1.5393267495,0
.0000804359\O,1.8204557217,0.4269777376,0.0000261217\N,-0.402623648,0.
389829032,-0.000046017\C,3.2455727389,-0.0322108332,0.000043984\C,3.5
034376638,-0.8276294273,1.2682836014\C,3.5034871611,-0.8275960855,-1.2
682068877\C,4.0047804931,1.2819514843,0.0000754644\H,3.2356412105,-0.2
516683472,2.1447367177\H,2.9629416242,-1.7609624981,1.2769962984\H,4.5
606577144,-1.0494981571,1.3261667749\H,3.2357230251,-0.2516122198,-2.1
446549365\H,4.5607098598,-1.0494611461,-1.3260559653\H,2.9629936059,-1
.7609298177,-1.2769648739\H,5.0671507641,1.0813972724,0.0000922475\H,3
.7713283342,1.8652333666,-0.8806308954\H,3.7712961262,1.865209799,0.88
07889459\Version=EM64L-G09RevA.02\State=2-A\HF=-705.2244531\S2=1.1564
49\S2=1=0.\S2A=0.882413\RMSD=6.936e-09\RMSF=7.674e-06\Dipole=-1.363716
9,1.4897453,-0.0000764\Quadrupole=23.2047894,-4.5450227,-18.6597666,-0
.0569521,0.0006532,-0.0004779\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate radical carbocation (3):

1\1\GINC-LOST\FOpt\RHf\6-311++G(2df,2p)\C13H23N1O2\LUISA\24-Oct-2010\0
\#opt freq hf/6-311++g(2df,2p)\280910_3\0,1\N,-0.3719131961,0.35503
91618,-0.2251204287\C,-0.4905510822,1.742422602,0.2242621957\C,-1.7928
402804,2.216689612,-0.4198333075\C,-2.6238259735,0.9391788102,-0.52637
18224\C,-1.569829433,-0.0999625858,-0.9452276448\C,-3.3155230334,0.61
69814936,0.8060881365\C,-3.7892648494,-0.8276953411,0.9089636972\C,-2.
6210320349,-1.7796266461,0.6809246492\C,-1.9969186324,-1.5462196375,-0
.6902253748\H,0.3576301254,2.3274192493,-0.0932945708\H,-2.2763650214,
2.9947503166,0.1565354767\H,-1.5890964957,2.614381799,-1.4073322771\H,
-3.3781615392,1.0147094604,-1.3008731712\H,-1.385170228,0.0001838416,-
2.0107042243\H,-2.6319087218,0.8082148709,1.6273599098\H,-4.1462358013
,1.3027779329,0.9370415377\H,-4.2409435655,-0.9978750671,1.8801779564\H
,-4.562230349,-1.0191402037,0.1682659943\H,-1.8774323431,-1.633753828
5,1.4591888991\H,-2.9491031417,-2.8104811077,0.7554414367\H,-2.73811376
843,-1.7841557344,-1.4495419742\H,-1.1610549161,-2.205398813,-0.856966
088\H,-0.5313958493,1.7939669724,1.3047669139\C,0.823872322,-0.2442577
03,-0.4090485991\O,0.99132398,-1.2222905402,-1.0742391232\O,1.78312576
65,0.3835482138,0.249866586\C,3.159190788,-0.0451124563,0.2516942656\C
,3.2862055322,-1.432552348,0.8717254393\C,3.7412958758,0.0075959578,-1
.1569564597\C,3.8353637088,0.9921105566,1.1399362675\H,2.8165473649,-1
.4517765607,1.847868502\H,2.8305971955,-2.1867102422,0.2510690801\H,4.
3347314561,-1.6737864784,0.9987528568\H,3.5889166254,0.9890465601,-1.5
902267238\H,4.8080188864,-0.175990139,-1.1107640565\H,3.2906636611,-0.
7306098446,-1.799905907\H,4.8928596905,0.7777358971,1.2268838387\H,3.7
20266281,1.9846086045,0.7234652198\H,3.4009954226,0.9859593648,2.13121
88941\Version=EM64L-G09RevA.02\State=1-A\HF=-710.1270599\RMSD=3.509e-
09\RMSF=2.296e-05\Dipole=-0.1600568,0.840833,0.3713326\Quadrupole=4.87
30934,-2.3639833,-2.5091101,0.1801659,2.0152349,-2.3197503\PG=C01 [X(C
13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate radical carbocation (4):

1\1\GINC-HERO3-50\FOpt\UHF\6-311++G(2df,2p)\C10H19N1O2(1+,2)\LHAYA\24-
Nov-2010\0\#opt freq uhf/6-311++g(2df,2p) maxdisk=2000MB\111110_17\
1,2\C,-3.745770044,0.5127125697,0.2793399169\C,-3.2444951406,-0.92701
30686,0.3308636626\C,-2.0926959544,-1.1531977625,-0.6547659399\N,-1.04
77206785,-0.1531829409,-0.4141657586\C,-1.4498159348,1.2553748643,-0.4
81994728\C,-2.6001190948,1.4948091163,0.5038457292\C,0.3034490332,-0.5
973274034,-0.0145688494\O,0.402696666,-1.6776093812,0.4214536226\O,1.1
432401758,0.3286090528,-0.231537323\C,2.6237594857,0.204369422,0.05129
31359\C,2.8076345629,-0.0197902053,1.5411756878\C,3.1782669906,-0.9221

63427,-0.8015339391\C,3.1429880197,1.5589766438,-0.3891672518\H,-2.907
2883157,-1.1792144071,1.3294175837\H,-4.0280542203,-1.626354531,0.0747
459431\H,-1.6549907659,-2.1295215723,-0.5642373298\H,-2.4209335631,-0.
9902520138,-1.6744193694\H,-0.5927292411,1.8696404898,-0.2824934353\H,
-1.7756516059,1.4196152236,-1.5021336755\H,-2.9258125493,2.5174071803,
0.3731705373\H,-2.2220604598,1.4099709771,1.5164978105\H,2.4231822789,
-0.9767661188,1.8584281027\H,3.8663848209,0.0055404386,1.7614034351\H,
2.3308814904,0.766295529,2.1121617425\H,2.9542199426,-0.7603697114,-1.
8477714304\H,4.2541015456,-0.9361738239,-0.6901510418\H,2.798846589,-1.
.8857863538,-0.4984448927\H,2.693632173,2.3550219987,0.1888173169\H,4.
2129102587,1.5937544528,-0.2372751001\H,2.9432802868,1.7295267623,-1.4
380578354\H,-4.2114024105,0.7059590779,-0.681670243\H,-4.507306341,0.6
62813922,1.0317179165\Version=EM64L-G09RevA.02\State=2-A\HF=-593.8945
079\S2=0.778986\S2-1=0.\S2A=0.750678\RMSD=8.855e-09\RMSF=1.961e-06\Dip
ole=-1.2042131,0.6649217,-0.5616012\Quadrupole=17.0223692,-8.5327399,-
8.4896292,0.9511915,1.5272546,1.6496006\PG=C01 [X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate radical carbocation (5):

1\1\GINC-LOST\FOpt\UHF\6-311++G(2df,2p)\C9H17N1O2(1+,2)\LUIA\15-Dec-2
010\0\#opt freq uhf/6-311++g(2df,2p) geom=connectivity\021210_2\1,2
\N,-1.3324362436,-0.1579303645,0.0232619721\C,-1.7508133767,1.24610820
37,0.0142702849\C,-3.2552336108,1.1693390325,0.2668561568\C,-3.6521446
697,-0.1834822518,-0.3305577583\C,-2.4671837848,-1.0852414508,0.005192
9378\H,-1.1724195319,1.7942968821,0.7402793382\H,-1.5043274983,1.62922
08011,-0.9702386724\H,-3.4509151974,1.1902172177,1.330933324\H,-3.7733
800369,2.0013373401,-0.1827204754\H,-4.5716060584,-0.5730164844,0.0762
057481\H,-3.7673488411,-0.1096887858,-1.4040690447\H,-2.5258124566,-1.
5099619219,1.0016957418\H,-2.2595827484,-1.8864992607,-0.6850826102\C,
0.0531108738,-0.6396705647,0.0582894896\O,0.8485767357,0.3468447371,-0.
0290971049\O,0.2118072098,-1.794366484,0.1566375184\C,2.3544807107,0.
2137383273,-0.0276323434\C,2.7605162208,-0.6142421627,-1.233298804\C,2
.7772036409,-0.3994248379,1.2950153566\C,2.7991163303,1.6576826935,-0.
1534963573\H,2.3716102118,-0.1831640472,-2.1465576942\H,3.8401537625,-
0.6141146275,-1.2992575388\H,2.431433419,-1.6387517551,-1.1519812438\H
,2.447024557,-1.4221298194,1.3925865688\H,3.857669831,-0.3904861088,1.
3452188725\H,2.401044533,0.1805831645,2.1276214148\H,2.4489288072,2.24
69459991,0.682911871\H,3.8796056663,1.6951018863,-0.1650242209\H,2.434
8735448,2.0981436422,-1.071449727\Version=EM64L-G09RevA.02\State=2-A\
HF=-554.8444941\S2=0.781694\S2-1=0.\S2A=0.750776\RMSD=8.130e-09\RMSF=1
.608e-05\Dipole=-1.6590434,0.7561072,-0.0576066\Quadrupole=17.7821861,
-9.3384365,-8.4437497,0.6291132,-0.1217487,0.3461672\PG=C01 [X(C9H17N1
O2)]\@

tert-butyl diethylcarbamate radical carbocation (6):

1\1\GINC-LOST\FOpt\UHF\6-311++G(2df,2p)\C9H19N1O2(1+,2)\LUIA\11-Dec-2
010\0\#opt freq uhf/6-311++g(2df,2p) geom=connectivity\191110_41\1,
2\N,1.4841581457,0.0472073542,-0.4971776128\C,1.6740028193,1.460149986
,-0.8509614878\C,2.6369239984,-0.8364528994,-0.2722853728\H,2.45537511
33,1.4762225743,-1.5971435641\H,0.7568657761,1.8165668188,-1.284936716
6\H,3.5181476795,-0.2696277051,-0.5228293939\H,2.5240846216,-1.6528790
825,-0.970262321\C,0.1373773239,-0.5562779052,-0.4345213373\O,-0.69323
05842,0.3040385535,-0.0085901069\O,0.0353115961,-1.6707609024,-0.76931
17213\C,-2.1721095756,0.0337197162,0.1601603458\C,-2.3402026369,-1.078
7183236,1.1789941788\C,-2.7523618084,-0.3030740114,-1.2013776627\C,-2.
6785850546,1.363901342,0.6822330204\H,-1.8414831871,-0.8309292879,2.10
69223583\H,-3.3951548286,-1.1923195081,1.3891166757\H,-1.9691921514,-2
.0236039945,0.8130275786\H,-2.3763528379,-1.2399712993,-1.582429938\H,
-3.8261631899,-0.3884136221,-1.1027601555\H,-2.5463895418,0.4837403467
,-1.9153597691\H,-2.4951309332,2.1570981247,-0.0296037364\H,-3.7452432
055,1.2964220912,0.8455613137\H,-2.2071900315,1.6179836646,1.621649988
8\C,2.6859334275,-1.3510735887,1.1640120045\H,2.7639672263,-0.54072209
68,1.8754416176\H,1.820268963,-1.9530675494,1.3982768625\H,3.563375073
7,-1.9737606081,1.2635793323\C,2.0633049028,2.2870119782,0.3739286833\
H,1.2908819108,2.2517764522,1.1281965245\H,2.9983345957,1.9544424277,0
.802151283\H,2.1858913929,3.3124659539,0.0560991282\Version=EM64L-G09
RevA.02\State=2-A\HF=-556.0093794\S2=0.774842\S2-1=0.\S2A=0.750524\RMS
D=6.928e-09\RMSF=7.310e-06\Dipole=1.5392778,0.8909818,-0.0770007\Quadr
upole=14.1686213,-6.2602847,-7.9083366,0.6020514,-1.6671671,-2.8885641
\PG=C01 [X(C9H19N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate radical carbocation (7):

1\1\GINC-HER03-50\FOpt\RHF\6-311++G(2df,2p)\C11H19N1O4\LHAYA\17-Dec-20
10\0\#opt freq hf/6-311++g(2df,2p) maxdisk=5000MB geom=connectivity\1
51210_5\1\N,-0.296402994,0.9137314551,0.1502806736\C,-0.1156597244
,2.2311643197,-0.4348509889\C,-1.3295881933,2.9870477341,0.0921205216\
C,-2.4197849875,1.9162900858,0.1292031515\C,-1.6623547109,0.6311385509
,0.522614222\H,0.8202278184,2.6651846575,-0.1238285246\H,-0.1214531412
,2.1792872351,-1.5183041423\H,-1.1264124114,3.3512976869,1.0923608693\
H,-1.5952385049,3.8340706201,-0.5249288391\H,-3.220303814,2.1377183737
,0.8192078325\H,-2.8502774001,1.7996300319,-0.8573518516\H,-1.73903254

79,0.4323467038,1.581097927\C,0.6561770736,-0.0170612349,0.3496779852\
O,1.8301797827,0.3797413116,-0.0947074259\O,0.4319303542,-1.0639524974
,0.8804618215\C,3.0206923669,-0.4354640714,-0.0303064837\C,2.834082994
2,-1.7118336277,-0.8428124812\C,3.3896824147,-0.725918846,1.4201644715
\C,4.0743568031,0.4545903304,-0.6768650211\H,2.5153765296,-1.473065631
2,-1.8499283631\H,3.7792084992,-2.2379764744,-0.9033887273\H,2.1028960
35,-2.3639794815,-0.393804134\H,2.6633856192,-1.366990991,1.8925482058
\H,4.3566709758,-1.2132699277,1.4526070071\H,3.4604359898,0.1973350688
,1.982810244\H,4.1845538995,1.3791218985,-0.1247163441\H,5.031246621,-
0.0511622566,-0.6922377787\H,3.7969269259,0.6953366235,-1.6948071225\C
, -2.2290141977,-0.5636147243,-0.2233337912\O,-1.9415405181,-0.86055259
52,-1.3299494792\O,-3.1397224852,-1.1843545502,0.4949030119\C,-3.77445
52465,-2.3053629901,-0.0871600873\H,-4.4666968409,-2.6718982728,0.6524
46767\H,-4.3018248618,-2.0200271668,-0.9849297089\H,-3.046703123,-3.06
4886348,-0.3276454168\Version=EM64L-G09RevA.02\State=1-A\HF=-781.8283
93\RMSD=3.945e-09\RMSF=1.233e-05\Dipole=-0.1170396,0.9371772,0.1777494
\Quadrupole=7.0088408,0.717598,-7.7264388,-0.0521218,-1.5758026,0.5039
049\PG=C01 [X(C11H19N1O4)]\@

tert-butyl piperidine-1-carboxylate cation (4):

1\1\GINC-HER03-38\FOpt\RHF\6-311++G(2df,2p)\C10H18N1O2(1+)\LHAYA\20-No
v-2010\0\#opt freq hf/6-311++g(2df,2p) maxdisk=2500MB\111110_30\1,1
\C,3.8150255315,0.5386744211,0.2999654229\C,3.450180393,-0.7611520163,
-0.4018307032\C,2.0940635127,-1.263726538,0.0569056123\N,1.071333592,-
0.1774707391,0.0133646963\C,2.7564183706,1.5907608545,-0.0071829239\C,
-0.3286907864,-0.626482903,0.049126008\O,-0.528548786,-1.7730673504,0.
1491828892\O,-1.1292628487,0.364293308,-0.0342711787\C,-2.6281772382,0.
2284137608,-0.0182130507\C,-3.0516474349,-0.5994217306,-1.2185417469\
C,-3.0449494816,-0.3801518201,1.3089452947\C,-3.0785278431,1.671638228
8,-0.1424007132\H,3.441520563,-0.6160870552,-1.4768650382\H,4.17655849
92,-1.5338154642,-0.1941496383\H,1.7243563787,-2.0554029689,-0.5688339
433\H,2.1172959848,-1.6279525413,1.073128915\H,2.7714990404,2.42394967
23,0.6860527286\H,2.8974385726,2.0335653856,-0.9919908767\H,-2.7263354
684,-1.6246931322,-1.1382824905\H,-4.1319305494,-0.5926158115,-1.27516
87322\H,-2.6678024141,-0.1724297587,-2.1360592716\H,-2.6582796434,0.19
93129138,2.137369091\H,-4.1249984292,-0.364858889,1.3683780253\H,-2.71
80039551,-1.4034733195,1.405626116\H,-2.7251043894,2.1114183442,-1.065
3877429\H,-4.159030733,1.7085181654,-0.1434456736\H,-2.7220591884,2.26
35735897,0.690016074\H,3.8716097508,0.3792643093,1.3704934951\H,4.7830
950391,0.8955804286,-0.0181802815\C,1.3714864451,1.0579967205,-0.01774
14502\H,0.5522525157,1.7484329356,-0.0624239129\Version=EM64L-G09RevA
.02\State=1-A\HF=-593.3498424\RMSD=6.727e-09\RMSF=2.275e-05\Dipole=1.7
073997,1.2899282,-0.0778116\Quadrupole=18.3019781,-8.1207653,-10.18121
28,0.6370549,-0.0038288,0.2968468\PG=C01 [X(C10H18N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate cation (5):

1\1\GINC-LOST\FOpt\RHF\6-311++G(2df,2p)\C9H16N1O2(1+)\LUIA\05-Dec-201
0\0\#opt freq hf/6-311++g(2df,2p) geom=connectivity\021210_4\1,1\N,
-1.3664695022,-0.1914716867,-0.0007011819\C,-1.7847905867,1.2331593456
, -0.0736138236\C,-3.2986974864,1.1486079494,0.1642844339\C,-3.65486652
69,-0.3246840528,-0.1068300144\C,-2.3398609587,-1.0042800354,-0.024155
8258\H,-1.2545145287,1.7979501139,0.6721114896\H,-1.5183891441,1.60932
87002,-1.0490901237\H,-3.5269756997,1.4000886731,1.1892374261\H,-3.841
4149056,1.8278037869,-0.4723455329\H,-4.3628301407,-0.754416678,0.5875
937413\H,-4.0480463826,-0.4998159308,-1.1044896806\H,-2.1560832885,-2.
0619984874,-0.0082030439\C,0.0161469637,-0.6683827869,0.0282397678\O,0.
798145556,0.332023475,-0.0166393107\O,0.2098298852,-1.8215921552,0.08
35905594\C,2.2991660921,0.2226630838,-0.005885348\C,2.7339842293,-0.55
08635858,-1.2380082252\C,2.7248070197,-0.4326566514,1.2960290614\C,2.7
242308986,1.6771004743,-0.0722757519\H,2.3454750571,-0.092166821,-2.13
80439531\H,3.8140512178,-0.5281546268,-1.2930233232\H,2.4218001279,-1.
5828734627,-1.1991821458\H,2.4131678373,-1.4640663913,1.3510372631\H,3
.804432429,-0.4037670144,1.3567253229\H,2.329366702,0.1072073698,2.146
6482642\H,2.3569460178,2.2286425685,0.7824398059\H,3.8040502354,1.7318
31269,-0.0721084984\H,2.3610138819,2.1470985573,-0.9760123527\Version
=EM64L-G09RevA.02\State=1-A\HF=-554.2983406\RMSD=3.584e-09\RMSF=1.459e
-05\Dipole=-2.4405223,0.4806878,-0.1098032\Quadrupole=20.6475113,-10.2
452999,-10.4022114,2.5818945,0.4382128,0.2449898\PG=C01 [X(C9H16N1O2)]
\@

tert-butyl diethylcarbamate cation (6):

1\1\GINC-HER05-15\FOpt\RHF\6-311++G(2df,2p)\C9H19N1O2\LHAYA\24-Nov-201
0\0\#opt freq hf/6-311++g(2df,2p) maxdisk=2000MB\191110_29\0,1\N,1.
4095252655,0.0446520612,-0.4874115218\C,1.5593613998,1.4773647851,-0.6
944484912\C,2.5766138343,-0.8246384175,-0.5514060089\H,2.42444498196,1.
6165900535,-1.3286180966\H,0.7069416515,1.8428901596,-1.2438017333\H,3
.3086140912,-0.3332111436,-1.1781268008\H,2.2899688345,-1.739270179,-1
.0461792805\C,0.2186319594,-0.5335916177,-0.219073205\O,-0.7659787425,
0.3467562522,-0.1778968081\O,0.0803997558,-1.7079476014,-0.0424417026\
C,-2.1410557453,-0.0112766747,0.0699646435\C,-2.2930734637,-0.62412886

91,1.4579664887\C,-2.6598490378,-0.9371192412,-1.024973072\C,-2.856826
2063,1.3324596151,0.0060707961\H,-1.8683733156,0.0327318525,2.20774412
76\H,-3.3459134438,-0.7498401927,1.6803688262\H,-1.8086749414,-1.58463
7562,1.5217457177\H,-2.1816842346,-1.9021167881,-0.9870201762\H,-3.727
7628373,-1.0727475023,-0.9027994072\H,-2.4869586377,-0.4988786771,-2.0
006778018\H,-2.7243560396,1.789731009,-0.9660511646\H,-3.9168734383,1.
1998044887,0.1803880826\H,-2.4682950107,2.0082937278,0.7569985443\C,3.
1928426446,-1.1575155047,0.80193708\H,3.5460283917,-0.2691885195,1.310
8254409\H,2.4709726658,-1.654055737,1.4355335115\H,4.0383754093,-1.823
0077069,0.6672282316\C,1.7282922184,2.2916551165,0.5830931801\H,0.8723
748726,2.1694197114,1.2333264724\H,2.6151506669,1.9965196045,1.1290805
022\H,1.8205966137,3.3445434975,0.3401366253\\Version=EM64L-G09RevA.02
\State=1-A\HF=-556.271271\RMSD=5.683e-09\RMSF=2.036e-05\Dipole=0.06306
65,0.9434501,-0.1444223\Quadrupole=5.3815154,-4.4858672,-0.8956482,0.5
758377,-1.3199182,-0.2521635\PG=C01 [X(C9H19N1O2)]\@\

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate cation (7):

1\1\GINC-HER05-18\FOpt\RHF\6-311++G(2df,2p)\C11H18N1O4(1+)\LHAYA\22-Jan-2011\0\#\opt freq hf/6-311++g(2df,2p) maxdisk=2500MB geom=connectivity\151210_21\1,1\N,-0.3386307521,0.8768529363,0.2518795872\C,-0.3023
898111,1.9504888206,-0.421769535\C,-1.6205221202,2.6272643568,-0.48823
81139\C,-2.4403201979,1.8695330226,0.5704088728\C,-1.6923905868,0.5324
49941,0.7326198047\H,0.6089941682,2.2753646839,-0.8834595687\H,-1.5295
659555,3.6896700375,-0.3128403406\H,-1.9967784743,2.4979561602,-1.4986
567055\H,-2.4285656146,2.4061299432,1.5071054789\H,-3.4687819903,1.726
6891699,0.2821685171\H,-1.6437246969,0.1816149014,1.7470155834\C,0.769
0380175,-0.0493733506,0.4530569252\O,1.8218417342,0.3925966334,-0.1132
221779\O,0.5564305884,-1.0125888359,1.0800988298\C,3.138290428,-0.3372
621844,-0.1118611852\C,2.9477123537,-1.6752141029,-0.8040492041\C,3.61
69787628,-0.4649136469,1.3233663852\C,4.0194834478,0.59585953,-0.92027
12917\H,2.5272696982,-1.5417621934,-1.7921028616\H,3.9161618719,-2.144
7945035,-0.9131177096\H,2.3150246806,-2.3383709932,-0.2351989603\H,2.9
840468879,-1.117570212,1.9040846737\H,4.6146708487,-0.8829809472,1.316
0761245\H,3.6659878665,0.5048660996,1.8014993384\H,4.0971181687,1.5652
860914,-0.4465096388\H,5.0126706624,0.1746591307,-0.9913150167\H,3.633
9310025,0.7225921351,-1.9229154078\C,-2.2572005137,-0.5534577092,-0.17
50031637\O,-1.8557975876,-0.7236969042,-1.273330908\O,-3.2304385521,-1
.180789535,0.4029164786\C,-3.9013957255,-2.2116207139,-0.3297335983\H,
-4.6577121474,-2.589371851,0.3341700084\H,-4.3451253476,-1.7989857886,
-1.221164504\H,-2.1998591142,-2.9866701217,-0.5909697164\\Version=EM64
L-G09RevA.02\State=1-A\HF=-781.0180454\RMSD=6.041e-09\RMSF=1.038e-05\D
ipole=-0.5428645,2.1910048,-0.0450374\Quadrupole=15.9826882,0.7545439,
-16.7372321,-2.1100996,-1.4826881,-0.3151357\PG=C01 [X(C11H18N1O4)]\@\

1.4 Optimized geometries at B3LYP/6-31G(d) level:

tert-butyl indoline-1-carboxylate (1):

1\1\GINC-HER05-18\FOpt\RB3LYP\6-31G(d)\C13H17N1O2\LHAYA\29-Nov-2010\0\#\b3lyp/6-31g(d) opt freq maxdisk=2000MB geom=connectivity\291110_2\0,1\N,1.4128678022,0.2688026267,0.4172940047\C,2.8178020797,0.69075419
81,0.6168087823\C,3.6527608579,-0.6040090664,0.4612551144\C,2.62128422
12,-1.6736209503,0.1795585116\C,1.3309620008,-1.1194514589,0.163416832
8\C,0.2132930042,-1.922150359,-0.0785743729\C,0.4171885232,-3.28772671
84,-0.3031134659\C,1.6956845946,-3.8466534695,-0.28882495\C,2.80664944
71,-3.030991818,-0.0451744625\C,0.4452315121,1.2406077364,0.5052059029
\O,0.7271677329,2.407317912,0.7377056744\O,-0.7964016422,0.7464089975,
0.307594855\H,2.9224010314,1.1484722482,1.6044547073\H,4.3789966872,-0
.5153661048,-0.3553283408\H,4.2253626955,-0.8217886028,1.3705363153\H,
-0.7805356587,-1.4993222601,-0.0917576752\H,-0.4456311866,-3.921125640
8,-0.4923465656\H,1.8293782698,-4.9099982152,-0.4659025411\H,3.8081156
2,-3.4549278137,-0.0315425274\H,3.0756635317,1.4546560246,-0.122052442
4\C,-1.9755322494,1.6310369365,0.360589299\C,-3.1294879756,0.662775030
1,0.0864269417\H,-4.0822974588,1.2025080352,0.0981128007\H,-3.01367678
82,0.1887742096,-0.8938591745\H,-3.1678809774,-0.1212024103,0.84994154
48\C,-1.8867798719,2.6918988514,-0.7413815137\H,-2.819526083,3.2664054
497,-0.7717911361\H,-1.0569630249,3.3766897129,-0.5618491802\H,-1.7499
514691,2.214758416,-1.7181340918\C,-2.1077202003,2.2478461094,1.756946
3958\H,-3.0493471498,2.8045786908,1.8230824706\H,-2.1239940147,1.46148
16546,2.5197032871\H,-1.2809417609,2.9278307486,1.9662925696\\Version=
EM64L-G09RevA.02\State=1-A\HF=-710.8601085\RMSD=3.091e-09\RMSF=1.958e-
05\Dipole=-0.1123907,-0.41426,-0.0835128\Quadrupole=7.945905,-4.536740
5,-3.4091645,-3.1167797,0.4478021,-0.4851448\PG=C01 [X(C13H17N1O2)]\@\

tert-butyl 1H-indole-1-carboxylate (2):

1\1\GINC-HER03-29\FOpt\RB3LYP\6-31G(d)\C13H15N1O2\URIETA\24-Jan-2011\0\#\opt freq b3lyp/6-31g(d) maxdisk=2500MB geom=connectivity\aromatico_4\0,1\C,-2.6133579083,0.968479187,-0.0005962781\C,-1.7134197551,-0.1
26660756,0.000252543\C,-2.1560894165,-1.451073736,0.0012142573\C,-3.5
336358913,-1.6626667789,0.0013085687\C,-4.4434903719,-0.5909141872,0.0
004749383\C,-3.9939135453,0.7250367262,-0.0004777025\C,-1.8205595261,2

.1752857528,-0.00145474\C,-0.5127308941,1.8111811905,-0.001128419\H,-1.4525595349,-2.2725586381,0.0018557925\H,-3.9096222197,-2.6821208265,0.002046662\H,-5.5107211385,-0.7954328151,0.0005782195\H,-4.6975999594,1.5533615863,-0.001122105\H,-2.1925271553,3.1911283924,-0.0022242754\H,0.3857293908,2.4061083454,-0.0015299174\C,0.7724363199,-0.332173948,0.0005359979\O,0.7976341051,-1.5469080951,0.0013139237\O,1.8315210825,0.4949932103,-0.000172318\N,-0.4109054923,0.4094542435,-0.000071406\C,3.2130025209,-0.0351750712,-0.0000129321\C,3.457097547,-0.8484350534,1.2746086352\C,3.4570091244,-0.8496626998,-1.2738723201\C,4.0530151851,1.2437902627,-0.0006681254\H,3.2251817229,-0.247405581,2.1606156919\H,2.8479663738,-1.7534319737,1.2908383149\H,4.5133987556,-1.1350569226,1.3262547815\H,3.22496144,-0.2495065469,-2.1604369377\H,4.5133255907,-1.1362605203,-1.3253560659\H,2.8479403542,-1.7547139481,-1.2891644697\H,5.1181904305,0.9906921237,-0.0005881285\H,3.840702208,1.8466272352,-0.8894965551\H,3.840773657\H,1.847488842,0.8875926583\Version=EM64L-G09RevA.02\State=1-A\HF=-709.6513899\RMSD=3.497e-09\RMSF=9.187e-06\Dipole=0.8402074,0.6138582,-0.000536\Quadrupole=6.6501344,-1.3265315,-5.3236029,0.2882296,-0.0007785,-0.0028013\PG=C01 [X(C13H15N1O2)]\@\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate (3):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C13H23N1O2\LUISA\06-Sep-2010\0\#\opt=calcfreq b3lyp/6-31g(d) geom=connectivity\060910_3\0,1\N,0.0773297231,-0.9429625488,-1.0904429916\C,-1.0948702715,-0.1924079378,-0.6033975371\C,-0.9299982544,-0.2235223461,0.9251507296\C,0.5956627746,-0.2853818012,1.1203615901\C,1.0321633997,-1.2618150061,-0.00099017\C,1.2279870859,1.1188439346,1.00082014\C,2.7363904969,1.090283304,0.7292978935\C,3.030001358,0.2725817895,-0.5339383268\C,2.5198063474,-1.1637465041,-0.3790354417\H,-2.0212736719,-0.6631596168,-0.9400449022\H,-1.3892529735,0.6444072264,1.4104406531\H,-1.4028872397,-1.1251027517,1.3328738301\H,0.8631058947,-0.7137215334,2.094141651\H,0.8413419277,-2.2946157859,0.3282364163\H,0.7435103931,1.6696388159,0.1822854588\H,1.007540405,1.6795598958,1.9188031155\H,3.1161025245,2.1151357585,0.6295677713\H,3.2630472502,0.6423065252,1.585430976\H,2.5472183285,0.7494573653,-1.3985516035\H,4.1067119441,0.2586903955,-0.7443796378\H,3.0818358439,-1.6514837457,0.4311998417\H,2.6937901374,-1.7522070102,-1.2820918321\H,-1.0889561959,0.8323374819,-0.996179688\C,0.0650519543,-1.668331109,-2.2487375069\O,0.8850209025,-2.5313468912,-2.535799708\O,-0.9768509398,-1.2830977817,-3.0350182322\C,-1.2038152202,-1.9038522473,-4.3471628213\C,-0.0116134482,-1.6343448662,-5.2721058907\C,-1.4854925533,-3.4020045013,-0.1485675317\C,-2.4518552904,-1.1714252067,-4.8488841759\H,0.1831132753,-0.5578891008,-5.3355621994\H,0.886206691,-2.1357525135,-4.9082507199\H,-0.2381435724,-1.9987283008,-6.2807111752\H,-2.3165333245,-3.5586674103,-3.4874830888\H,-1.7698333217,-3.8308578737,-5.1523421833\H,-0.6057502032,-3.9271347985,-3.8101383955\H,-2.7354850186,-1.5443282614,-5.8387727945\H,-3.2933826802,-1.3279189761,-4.1658731634\H,-2.2643444788,-0.0953360661,-4.9240483493\Version=EM64L-G09RevA.02\State=1-A\HF=-714.4816977\RMSD=6.279e-09\RMSF=2.556e-06\Dipole=-0.592044,0.5275517,0.3902175\Quadrupole=-0.6830733,-3.2624717,3.945545,1.9875251,2.0567494,0.3499482\PG=C01 [X(C13H23N1O2)]\@\@

tert-butyl piperidine-1-carboxylate (4):

1\1\GINC-HER05-12\FOpt\RB3LYP\6-31G(d)\C10H19N1O2\LUISA\11-Nov-2010\0\#\opt=calcfreq b3lyp/6-31g(d) geom=connectivity\111110_7\0,1\C,-1.2803077337,0.4978081215,-0.357984364\C,-1.7588007905,0.1164200409,1.050963506\C,-3.2312452796,0.4941414712,1.2541124061\N,-4.0634148535,-0.0738918666,0.1942424997\C,-3.6704483607,0.2722520386,-1.1715399838\C,-2.2040726034,-0.1054693007,-1.4266404518\C,-5.1838817126,-0.7863411331,0.5356426195\O,-5.5168955934,-1.0193575986,1.6902085831\O,-5.8589013581,-1.2003299603,-0.568381651\C,-7.0892290725,-1.9950312179,-0.4462038962\C,-6.7945926342,-3.3284103719,0.2503479216\C,-8.170705818,-1.1864300951,0.2788651547\C,-7.4786530879,-2.2270959499,-1.9092017894\H,-1.6465452365,-0.9658257513,1.199967084\H,-1.1485773548,0.6141723881,1.8150640216\H,-3.6159722616,0.1306035073,2.2066469274\H,-3.3354108413,1.5916822143,1.241892776\H,-4.3355680274,-0.2349840994,-1.867428847\H,-3.7985969911,1.3581293697,-1.3146957947\H,-1.9132258491,0.2358168498,-2.4282658691\H,-2.1144354863,-1.2000808243,-1.4173915409\H,-6.4993273721,-3.1717158456,1.288559602\H,-7.6896506026,-3.9605836834,0.227453042\H,-5.9906490502,-3.8597338768,-0.2713836198\H,-8.331837203,-0.2283178075,-0.2279518153\H,-9.1160479936,-1.7408777541,0.2658130571\H,-7.8870195271,-0.9954448951,1.3146016165\H,-6.6867176431,-2.7665153946,-2.4392857907\H,-8.3980525931,-2.8194826247,-1.9650126026\H,-7.649359021,-1.2737740209,-2.4201013482\H,-1.2806595081,1.5938156033,-0.456372381\H,-0.2459848301,0.168976067,-0.5159570619\Version=EM64L-G09RevA.02\State=1-A\HF=-597.7489198\RMSD=3.679e-09\RMSF=1.334e-05\Dipole=0.3556895,0.1643433,-0.8096126\Quadrupole=3.3686581,0.6737189,-4.042377,2.6500232,1.8674997,0.7583129\PG=C01 [X(C10H19N1O2)]\@\@

tert-butyl pyrrolidine-1-carboxylate (5):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C9H17N1O2\LUISA\06-Jul-2010\0\#\opt=calcfreq b3lyp/6-31g(d) geom=connectivity\carbamat02\0,1\N,0.8380441252

, -0.5528496833, -0.4395436055\C, 0.6228914938, -1.424876509, 0.7209913099\C, 0.1052861527, -2.7251875062, 0.0843258522\C, -0.6220082604, -2.2388903097, -1.1820812541\C, 0.2630279934, -1.0858397927, -1.6787446436\H, 1.5501782198, -1.5618012145, 1.284607057\H, -0.1176048972, -0.9865833327, 1.4046687628\H, 0.9504091612, -3.3675722409, -0.1913912716\H, -0.5384679973, -3.2932342545, 0.7626908157\H, -0.7488466609, -3.0227124262, -1.9347440853\H, -1.6178394701, -1.8604143952, -0.921067473\H, 1.0565381555, -1.4426536962, -2.35022261\H, -0.2887345823, -0.3056793594, -2.2104648213\C, 1.456950681, 0.6588709245, -0.4263893797\O, 1.8646137364, 0.9664878067, 0.8351931951\O, 1.6097617725, 1.3527951013, -1.4231436734\C, 2.5752026345, 2.221709525, 1.1106607057\C, 1.676938638, 3.4199989687, 0.7831840248\C, 3.8985283121, 2.2609931079, 0.337740886\C, 2.8320664369, 2.1348759856, 2.6179075286\H, 0.7265055949, 3.3402383341, 1.3227557871\H, 2.1693210849, 4.3474250637, 1.0975063078\H, 1.472568497, 3.4726529271, -0.2870535104\H, 3.7213817647, 2.295005217, -0.7381543291\H, 4.4713011681, 3.1481302278, 0.6313851202\H, 4.5007901132, 1.3756106109, 0.5707516851\H, 3.43668133, 1.2537270031, 2.8568164877\H, 3.3674398371, 3.026394926, 2.9613537536\H, 1.8876139653, 2.0640229612, 3.167401198
\Version=EM64L-G09RevA.02\State=1-A\HF=-558.4310432\RMSD=4.684e-09\RM
SF=1.092e-05\Dipole=-0.2581741, -0.7305257, 0.6666267\Quadrupole=0.70892
84, 2.7108345, -3.4197629, 2.6993785, 1.5456651, 3.6280773\PG=C01 [X(C9H17N
1O2)]\@\@

tert-butyl diethylcarbamate (6):

1\1\GINC-HERO3-04\FOpt\RB3LYP\6-31G(d)\C9H19N1O2\LHAYA\20-Nov-2010\0\#\
#opt freq b3lyp/6-31g(d)maxdisk=2500MB\191110_31\0,1\N, -1.5138257991
, -0.1385413827, 0.6968174486\C, -1.818498612, 1.2600780123, 1.0132376891\C
, -2.5673840282, -1.1575321787, 0.7537563234\H, -2.6550596722, 1.252411458,
1.7209682057\H, -0.9590032204, 1.6886245108, 1.5339871347\H, -3.303250422,
-0.821244139, 1.4924964017\H, -2.1153983205, -2.0792562015, 1.1290797018\C
, -0.2802708074, -0.5464912322, 0.2618226837\O, 0.5923289236, 0.495627425, 0
.2168852322\O, -0.0161706801, -1.703853963, -0.0382990392\C, 1.9917614713,
0.2915030283, -0.1845626347\C, 2.0584597314, -0.2121771414, -1.6305655114\
C, 2.6889028648, -0.6596343197, 0.7945748866\C, 2.5767854414, 1.7026403653,
-0.075693392\H, 1.5213213332, 0.4724011091, -2.2966638816\H, 3.1035812971,
-0.2537705258, -1.958040641\H, 1.6199746222, -1.2070466647, -1.7169752806\
H, 2.2634969191, -1.622879859, 0.7348938287\H, 3.7579366158, -0.7124493076
, 0.5587014679\H, 2.5856171786, -0.2904239243, 1.8211231528\H, 2.491714897,
2.0794494194, 0.9489303074\H, 3.6358669657, 1.6942982049, -0.3543353679\H,
2.0491579151, 2.3929803397, -0.7421396261\C, -3.247314447, -1.4378582153,
-0.590153371\H, -3.7453218359, -0.5466508271, -0.9869949526\H, -2.507429115
7, -1.7800578671, -1.3194349934\H, -4.0021207203, -2.224771668, -0.47358520
97\C, -2.1674195627, 2.1275407901, -0.2014800357\H, -1.3349726343, 2.140417
1968, -0.9111819205\H, -3.0585379242, 1.757642277, -0.7196169325\H, -2.3633
546841, 3.1590215172, 0.1154513553\Version=EM64L-G09RevA.02\State=1-A\H
F=-559.6387494\RMSD=3.758e-09\RMSE=7.283e-06\Dipole=-0.2132703, 0.80004
03, 0.1955027\Quadrupole=4.7871188, -4.0064949, -0.7806239, 0.7343673, -1.6
327784, -0.2175914\PG=C01 [X(C9H19N1O2)]\@\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate (7):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C11H19N1O4\LUIA\06-Jul-2010\0\#\op
t freq b3lyp/6-31g(d)\carb2_01\0,1\N, -1.2537175232, -0.184505671, 0.01
28451518\C, -1.7282567587, 1.1887483991, -0.1749021521\C, -3.19225424, 1.09
47821446, 0.2737960867\C, -3.601510592, -0.3220457426, -0.1638870004\C, -2.
3273907498, -1.172010667, 0.0750386325\H, -1.1331843788, 1.8835376598, 0.42
1806214\H, -1.6479939735, 1.4894060334, -1.2288023894\H, -3.2551590342, 1.1
907421645, 1.3641780058\H, -3.8199533523, 1.8728964589, -0.1709724978\H, -4
.462967395, -0.7180696353, 0.380265189\H, -3.8404411979, -0.3249621976, -1.
233224048\H, -2.3424922911, -1.6672507072, 1.0515674537\C, 0.0438505002, -0
.5954043794, 0.0949781519\O, 0.8880085898, 0.4573995088, -0.0242118127\O, 0
.3599062122, -1.766306202, 0.2640594458\C, 2.3458794867, 0.2643868374, 0.02
22367577\C, 2.7932289081, -0.6332603968, -1.136456329\C, 2.7589546386, -0.2
971316341, 1.3870678012\C, 2.8748182405, 1.6894739262, -0.1610557242\H, 2.4
45064001, -0.2232175215, -2.0907612674\H, 3.8879863839, -0.6795320402, -1.1
642014937\H, 2.3994406404, -1.6442471475, -1.0235372861\H, 2.3644071706, -1
.3039637704, 1.5310146365\H, 3.8523092767, -0.3314922429, 1.4556592657\H, 2
.3887024362, 0.3480686896, 2.1917494975\H, 2.5196118484, 2.3413121529, 0.64
39870064\H, 3.9698266043, 1.6887134688, -0.1484046114\H, 2.5393101976, 2.10
6173328, -1.1162961916\C, -2.1718148534, -2.2413262115, -1.0075965466\O, -1
.8392406054, -2.0209976196, -2.1502731211\O, -2.5322198245, -3.4513753139,
-0.5391464414\C, -2.448547083, -4.5251167031, -1.4903735443\H, -2.78790759
64, -5.4146437665, -0.9588082743\H, -3.0867078569, -4.3247238045, -2.355359
9647\H, -1.4167624188, -4.6493733774, -1.8287947601\Version=EM64L-G09Rev
A.02\State=1-A\HF=-786.3031962\RMSD=7.677e-09\RMSE=1.070e-05\Dipole=-0
.5185614, 0.5611698, 0.3352002\Quadrupole=4.7665122, 1.9364898, -6.703002,
2.2501631, -0.7632419, 2.438455\PG=C01 [X(C11H19N1O4)]\@\@

tert-butyl indoline-1-carboxylate radical carbocation (1):

1\1\GINC-HERO3-26\FOpt\UB3LYP\6-31G(d)\C13H17N1O2(1+,2)\LHAYA\30-Nov-2
010\0\#\opt freq ub3lyp/6-31g(d) maxdisk=2500MB geom=connectivity\291
110_13\1,2\N, 1.4439441942, 0.2245935366, 0.4125584736\C, 2.8467845385, 0.

6659691094,0.6148747648\C,3.6844649042,-0.6162394602,0.4612130362\C,2.6682853075,-1.6846694691,0.1815646947\C,1.3496205331,-1.1087376419,0.167388536\C,0.1978539004,-1.9065612325,-0.0760653249\C,0.3965390398,-3.2523583862,-0.29760196\C,1.6959214357,-3.8218374119,-0.2840206842\C,2.8334083313,-3.0371332723,-0.044137315\C,0.4192315907,1.2525507762,0.5047524851\O,0.7770022935,2.3810554115,0.7373449986\O,-0.7786919961,0.7559144844,0.3104637737\H,2.9240563613,1.1305705763,1.6013266411\H,4.4110078412,-0.5315934433,-0.3556118581\H,4.2584265655,-0.837894518,1.3687811015\H,-0.7874962733,-1.4658149341,-0.0847963931\H,-0.4581397982,-3.8937055471,-0.4870235271\H,1.8081048473,-4.8867338595,-0.4633109217\H,3.8211569252,-3.4871523173,-0.0368386371\H,3.0765809311,1.4370692993,-0.1250781819\C,-2.0179722409,1.6515581085,0.3603072532\C,-3.1358528192,0.6512980872,0.0830832829\H,-4.0970381896,1.1740106699,0.0908827342\H,-3.0138759598,0.1837966121,-0.8992411121\H,-3.1691273577,-0.1278474929,0.8513354033\C,-1.9043205054,2.6980666375,-0.7446812653\H,-2.8407007405,3.2639340169,-0.7864395361\H,-1.0911788338,3.4018316013,-0.5579429891\H,-1.7570735949,2.2226964688,-1.7198986367\C,-2.1261826497,2.2520617034,1.7591865495\H,-3.0729052268,2.7971620149,1.8321966303\H,-2.1326286806,1.4670071282,2.5223201115\H,-1.3150625741,2.9524014437,1.9664014512\Version=EM64L-G09RevA.02\State=2-A\HF=-710.6008455\S2=0.766987\S2-1=0.\S2A=0.7502\RMSD=8.422e-09\RMSF=1.128e-05\Dipole=1.115836,-1.7969547,-0.2208491\Quadrupole=11.315316,4.2976322,-15.6129482,-11.6036034,0.3598661,2.5987414\PG=C01 [X(C13H17N1O2)]\@

tert-butyl 1H-indole-1-carboxylate radical carbocation (2):

1\1\GINC-HERO3-28\FOpt\UB3LYP\6-31G(d)\C13H15N1O2(1+,2)\URIETA\24-Jan-2011\0\#opt freq b3lyp/6-31g(d) maxdisk=2500MB geom=connectivity\aromatico_10\1,2\C,-2.6395832776,0.9780762262,-0.0004839859\C,-1.7324542664,-0.1245467633,0.0001366112\C,-2.1662508348,-1.4291427629,0.0009647655\C,-3.5754679986,-1.6373224073,0.0011813583\C,-4.4913049056,-0.5782167349,0.0005879415\C,-4.040784493,0.7387035292,-0.0002495143\C,-1.8751370212,2.1563777281,-0.0012556909\C,-0.5142267224,1.7679698481,-0.0010999887\H,-1.4758110978,-2.2621592686,0.0014313158\H,-3.9419299136,-2.6592573878,0.001832049\H,-5.5553558034,-0.7880103224,0.0007835213\H,-4.7376807324,1.5711094433,-0.0007170808\H,-2.2274700158,3.1795335803,-0.0018624773\H,0.3746843488,2.3817318475,-0.0015307882\C,0.813340929,-0.3548328614,0.0001141366\O,0.756797038,-1.5583020364,0.0009093899\O,1.8326571374,0.4656848462,-0.0003592788\N,-0.4202794703,0.4236629216,-0.0002843779\C,3.2740102924,-0.0473681209,-0.0000037749\C,3.4969619575,-0.85232798,1.2769527524\C,3.4970426233,-0.8538666342,-1.2759749278\C,4.0650302005,1.2561610162,-0.0007645514\C,3.2551836607,-0.2554544526,2.1622844479\H,2.9081661954,-1.77167711,1.2879815911\H,4.5553824862,-1.1259018132,1.3370591671\H,3.2553315392,-0.2580572639,-2.1620415124\H,4.5554650158,-1.1275213111,-1.3356773008\H,2.9082397931,-1.7732231853,-1.2859378103\H,5.135069509,1.02768808,-0.0005960015\H,3.8446145622,1.8514431175,-0.8921670834\H,3.8445622646,1.8525152319,0.8899080979\Version=EM64L-G09RevA.02\State=2-A\HF=-709.3826802\S2=0.763408\S2-1=0.\S2A=0.750119\RMSD=8.051e-09\RMSF=3.011e-05\Dipole=-1.7918639,1.0327302,-0.0005719\Quadrupole=26.0771295,-6.3069669,-19.7701627,0.4949758,-0.0019107,-0.0084709\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate radical carbocation (3):

1\1\GINC-LOST\FOpt\UB3LYP\6-31G(d)\C13H23N1O2(1+,2)\LUISA\07-Sep-2010\0\#opt freq ub3lyp/6-31g(d) geom=connectivity\070910_5\1,2\N,-0.0001795886,-1.1511695975,-0.9194219154\C,-1.1884780885,-0.4901772978,-0.3813406793\C,-0.8931981374,-0.3591942792,1.1205045149\C,0.64559977,-0.266031095,1.1752805785\C,1.0848116085,-1.2470894918,0.0579834303\C,1.1570040711,1.1726724574,0.9372604763\C,2.6400837209,1.22770999429,0.5519046891\C,2.9046282725,0.3907541652,-0.7040370991\C,2.5243729762,-1.0816795657,-0.4833683157\H,-2.082381487,-1.0588691085,-0.6567233468\H,-1.3878125574,0.5139193552,1.5527291089\H,-1.2571686865,-1.2486734536,1.646249152\H,1.0326581124,-0.6327989357,2.1310030196\H,0.9986741791,-2.289293094,0.4265229157\H,0.5699130231,1.6503970234,0.1388498294\H,0.967122454,1.7567616094,1.8446572094\H,2.9380500304,2.2683577996,0.3855803568\H,3.2580775173,0.8545412377,1.3803481241\H,2.3397202206,0.8032582001,-1.5528485832\H,3.9632560453,0.4325568666,-0.9829920123\H,3.175344612,-1.5129468137,0.2864098337\H,2.6619564547,-1.6878231459,-1.3809986717\H,-1.2718168591,0.4834290732,-0.8904067479\C,-0.0020006511,-1.8716093986,-2.1915927033\O,0.7363192988,-2.8182125721,-2.3204931452\O,-0.883455816,-1.3301753394,-2.9858429917\C,-1.1490536273,-1.8844842216,-4.3966758019\C,0.1493278671,-1.8047691581,-5.1926576915\C,-1.688143737,-3.3038149029,-4.2474335723\C,-2.2046858788,-0.9148170316,-4.9134743117\H,0.538429491,-0.7816938812,-5.2077089474\H,0.9134138462,-2.479555417,-4.8007673806\H,-0.0600211121,-2.0971570602,-6.2267555736\H,-2.578900766,-3.3205888662,-3.6113516433\H,-1.9789895363,-3.6703464285,-5.2373165575\H,-0.9381394378,-3.986333503,-3.8421393835\H,-2.4876182923,-1.2028332117,-5.9304905375\H,-3.1037859098,-0.9391373161,-4.2904879603\H,-1.8203334024,0.1090161559,-4.9438576661\Version=EM64L-G09RevA.02\State=2-A\HF=-714.1955486\S2=0.75647\S2-1=0.\S2A=0.750031\RMSD=9.392e-09\RMS

F=3.566e-06\Dipole=-0.7066312,0.3414017,0.682517\Quadrupole=-1.7312848
-9.3513913,11.0826761,3.8998079,7.0213819,5.9962174\PG=C01 [X(C13H23N
102)]\ \@

tert-butyl piperidine-1-carboxylate radical carbocation (4):

1\1\GINC-HERO5-15\FOpt\UB3LYP\6-31G(d)\C10H19N1O2(1+,2)\LHAYA\12-Nov-2
010\0\#opt freq ub3lyp/6-31g(d) geom=connectivity\111110_19\1,2\C,-
1.3336938328,0.1913955343,-0.2852116479\C,-1.9304455102,0.0924700635,1
.1192210757\C,-3.3210875964,0.8262320654,1.1761423933\N,-4.1545478583,
0.2822310479,0.131415967\C,-3.6879008533,0.4430349449,-1.2273999362\C,
-2.3086585867,-0.3005776488,-1.3562208163\C,-5.2142271378,-0.672542936
7,0.511673555\O,-5.3244529432,-0.9665496548,1.6770322361\O,-5.87297745
52,-1.0424144917,-0.5492454908\C,-7.0647430381,-2.0150510974,-0.458769
4145\C,-6.545805644,-3.3473047045,0.0726136816\C,-8.1290543118,-1.3753
181757,0.4266707018\C,-7.4994980342,-2.1014239963,-1.9163900387\H,-2.0
839864333,-0.9493211072,1.4210309731\H,-1.2964997972,0.5692820804,1.87
34879599\H,-3.8093061406,0.6780047541,2.1377596661\H,-3.1683625825,1.8
911628741,0.9673358474\H,-4.4288539011,0.0491277334,-1.9187482856\H,-3
.5283349067,1.5131860659,-1.4040426232\H,-1.9431143152,-0.1060962452,-
2.3695911846\H,-2.4887177741,-1.3780142249,-1.2685071943\H,-6.20127800
93,-3.2706132348,1.1059750575\H,-7.3645453423,-4.0735484959,0.04289982
08\H,-5.7362148136,-3.7322269661,-0.5556972314\H,-8.414186933,-0.38915
41497,0.0469903284\H,-0.9203257924,-2.0110734967,0.4081050391\H,-7.801
9923483,-1.2856703459,1.4647237948\H,-6.6981164936,-2.4992434131,-2.54
64133799\H,-8.3577316867,-2.7757865329,-1.9933751209\H,-7.801593095,-1
.1217745688,-2.2984060919\H,-1.0354617854,1.2263288589,-0.4955340149\H
,-0.4190713376,-0.4146269358,-0.328943616\Version=EM64L-G09RevA.02\Sta
te=2-A\HF=-597.4596668\S2=0.755962\S2-1=0.\S2A=0.750026\RMSD=5.498e-0
9\RMSF=2.249e-05\Dipole=1.2671916,0.93164,-0.6086439\Quadrupole=11.138
6212,-2.4288818,-8.7097394,10.7375199,2.0218234,1.9396989\PG=C01 [X(C1
0H19N1O2)]\ \@

tert-butyl pyrrolidine-1-carboxylate radical carbocation (5):

1\1\GINC-LOST\FOpt\UB3LYP\6-31G(d)\C9H17N1O2(1+,2)\LUIA\06-Jul-2010\0
\#opt freq b3lyp/6-31g(d) geom=connectivity\intermedio2\1,2\N,0.792
492531,-0.5767921614,-0.4483687797\C,0.630508777,-1.4745281233,0.68674
69608\C,0.1078792707,-2.7781502389,0.0640097076\C,-0.6296390648,-2.298
4620652,-1.2030095765\C,0.2124271911,-1.103836024,-1.6731956504\H,1.56
85935249,-1.5277157883,1.2498336322\H,-0.1039265489,-0.9983624901,1.36
10611195\H,0.9505566084,-3.4281383725,-0.1943937287\H,-0.538108304,-3.
324073791,0.7541412613\H,-0.700772407,-3.0687902117,-1.9730242701\H,-1
.6452215437,-1.964940784,-0.9647309907\H,1.0576388328,-1.4094984001,-2
.3169533978\H,-0.2991998219,-0.2997161167,-2.2130536977\C,1.4753611955
,0.7219491747,-0.427981069\O,1.854397132,0.9830103643,0.7905821289\O,1
.5822900778,1.3177061965,-1.4718181263\C,2.6027613904,2.2876944223,1.1
397001472\C,1.6897585883,3.4592197365,0.7948516894\C,3.9201530735,2.29
08675708,0.3712841098\C,2.8053978173,2.1297931519,2.640950708\H,0.7282
669872,3.3736131736,1.3108771123\H,2.1701670092,4.3823458391,1.1353414
508\H,1.520569751,3.546111797,-0.2806154124\H,3.7672872224,2.365894233
1,-0.7074915323\H,4.5023678883,3.1617667835,0.6897602147\H,4.508969033
5,1.3959438459,0.59600072\H,3.4024365478,1.2417362303,2.8688740873\H,3
.339500395,3.0052700011,3.0224246486\H,1.8476258451,2.0607260169,3.165
1363531\Version=EM64L-G09RevA.02\State=2-A\HF=-558.1379167\S2=0.75649
8\S2-1=0.\S2A=0.750032\RMSD=6.453e-09\RMSF=5.946e-06\Dipole=-0.8148718
, -1.610346,0.0963055\Quadrupole=-2.5488364,8.1388407,-5.5900043,10.339
5157,4.7196047,7.7094832\PG=C01 [X(C9H17N1O2)]\ \@

tert-butyl diethylcarbamate radical carbocation (6):

1\1\GINC-HERO3-34\FOpt\UB3LYP\6-31G(d)\C9H19N1O2(1+,2)\LHAYA\20-Nov-20
10\0\#opt freq ub3lyp/6-31g(d)maxdisk=2500MB\191110_43\1,2\N,-1.559
2430587,-0.1437224944,0.6714022767\C,-1.9245463152,1.2585305812,0.8228
121852\C,-2.5256837001,-1.204635475,0.8977898876\H,-2.8561842187,1.295
6111974,1.390004447\H,-1.1225377354,1.735701143,1.3954552837\H,-3.1257
562003,-0.9131845673,1.7652473096\H,-1.9710312998,-2.1210030248,1.1003
04448\C,-0.2283071827,-0.5400696112,0.1636069884\O,0.5979853791,0.4599
509115,0.263950456\O,-0.0969137754,-1.6660841826,-0.251072456\C,2.0821
100654,0.327087803,-0.147661829\C,2.1306592769,0.0320741572,-1.6428970
256\C,2.7107343661,-0.7636004988,0.7125397908\C,2.6167763527,1.7126966
867,0.1902810712\H,1.6116513554,0.8074687167,-2.2154602984\H,3.1787908
587,0.0311592243,-1.9596186334\H,1.7063142806,-0.9449883384,-1.8831690
499\H,2.3026012924,-1.7516098501,0.4887681616\H,3.78534422903,-0.789457
5167,0.5043080676\H,2.582358966,-0.5468740866,1.7776834716\H,2.5073700
141,1.9311752077,1.2566626127\H,3.6819104327,1.7528447541,-0.057084300
2\H,2.1053596756,2.4883240928,-0.3876580239\C,-3.4480611612,-1.4233745
831,-0.3341311541\H,-4.0414140103,-0.5342646281,-0.5597488715\H,-2.854
9735468,-1.7124486437,-1.2041599365\H,-4.1286371637,-2.2411074911,-0.0
799851341\C,-2.0776173948,1.989380593,-0.5353776387\H,-1.1409757693,1.
9830700441,-1.0956759174\H,-2.8717807764,1.5451519175,-1.1394811763\H,
-2.3447296074,3.0267860718,-0.3146319828\Version=EM64L-G09RevA.02\Sta
te=2-A\HF=-559.3453162\S2=0.756443\S2-1=0.\S2A=0.750031\RMSD=6.017e-09

\RMSF=5.945e-06\Dipole=-1.5237093,0.5897082,0.6004608\Quadrupole=14.44
27862,-6.2917963,-8.1509899,2.460444,-3.6461919,-1.282506\PG=C01 [X(C9
H19N1O2)]\ \@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate radical carbocation (7):

1\1\GINC-LOST\FOpt\UB3LYP\6-31G(d)\C11H19N1O4(1+,2)\LUISA\08-Jul-2010\0\#\
opt freq b3lyp/6-31g(d) geom=connectivity\carb2_02\1,2\N,-0.4334
862254,0.9425412075,-0.0684935217\C,-0.3138536234,2.0977073423,-0.9455
938296\C,-1.4872891165,2.9845530971,-0.5091244336\C,-2.5694961469,1.96
29512258,-0.0971444514\C,-1.7743368476,0.7256227245,0.3890357789\H,0.6
878772313,2.5238620768,-0.8711018693\H,-0.4467353187,1.7240207049,-1.9
788827081\H,-1.1832244854,3.6057704962,0.3392649203\H,-1.8184212914,3.
6456119137,-1.3123961012\H,-3.235578649,2.3365110694,0.6826730964\H,-3
.1793540054,1.6850003949,-0.9615432875\H,-1.7592422247,0.564963474,1.4
749616493\C,0.622582634,-0.0034506001,0.2552505478\O,1.7574678073,0.43
08607889,-0.2206187646\O,0.3267367086,-0.9998889337,0.8737511501\C,3.0
583197703,-0.3674248125,-0.0527482656\C,2.8863441965,-1.706899566,-0.7
629139694\C,3.3440181996,-0.4998517333,1.4401099759\C,4.0658203044,0.5
33824889,-0.7563194423\H,2.6112305039,-1.561784626,-1.8123797294\H,3.8
439425055,-2.2372153967,-0.7383902897\H,2.1394250982,-2.336483326,-0.2
749006709\H,2.6013586144,-1.1197295377,1.946683345\H,4.3225790098,-0.9
751609141,1.5644189698\H,3.3867346184,0.4832872856,1.9194792462\H,4.12
55708557,1.5136282545,-0.2729799344\H,5.0557074737,0.0701286395,-0.708
0836349\H,3.8052334263,0.6712809478,-1.81000419\C,-2.3549544536,-0.624
2426641,-0.2051173239\O,-2.3299758013,-0.84965331,-1.3888362885\O,-2.8
906698287,-1.3429525709,0.7573113534\C,-3.5183141215,-2.5986697903,0.3
542423992\H,-3.9408727868,-3.0026656207,1.2717721936\H,-4.2937517915,-
2.4003467513,-0.3872466941\H,-2.75815924,-3.2648343789,-0.0566582257\\
Version=EM64L-G09RevA.02\State=2-A\HF=-786.0092713\S2=0.756053\S2-1=0.
\S2A=0.750027\RMSD=5.425e-09\RMSF=1.982e-06\Dipole=-0.5302232,1.092565
4,0.0550543\Quadrupole=14.9489519,0.5863,-15.5352518,-0.0456511,-2.659
8746,-2.467189\PG=C01 [X(C11H19N1O4)]\ \@

tert-butyl piperidine-1-carboxylate cation (4):

1\1\GINC-HER05-21\FOpt\RB3LYP\6-31G(d)\C10H18N1O2(1+)\LHAYA\11-Nov-201
0\#\opt freq b3lyp/6-31g(d)\111110_31\1,1\C,-1.352914476,0.8778645
301,-0.3544367238\C,-1.5640654139,0.1959212409,1.001564824\C,-3.047504
0318,0.1064497769,1.3443719698\N,-3.8363539374,-0.4498394178,0.2007214
973\C,-2.0967404329,0.1002139165,-1.447530053\C,-5.1937393623,-0.99907
65993,0.5661168044\O,-5.513569648,-0.9661297144,1.7212911304\O,-5.7995
194946,-1.4243737005,-0.5037014543\C,-7.213924866,-2.0440287736,-0.437
8956708\C,-7.1398792935,-3.2926451486,0.4330423844\C,-8.1686853758,-0.
9811738499,0.0931560421\C,-7.4682770181,-2.3721320722,-1.9035505139\H,
-1.1263308088,-0.8102796823,0.9943872419\H,-1.0665791936,0.7521240881,
1.8016157607\H,-3.2462235919,-0.5448983949,2.1954934221\H,-3.481291358
3,1.0854284234,1.5731145953\H,-2.2758264021,0.6989441756,-2.3519495538
\H,-1.5138572218,-0.7646381267,-1.8087379633\H,-6.9212787399,-3.051995
6165,1.4754483218\H,-8.1115828284,-3.7961376092,0.399510665\H,-6.38831
0444,-3.9925509605,0.0543211969\H,-8.1339776733,-0.077545375,-0.523622
4737\H,-9.1880737743,-1.3780038559,0.046504251\H,-7.9559419842,-0.7215
81789,1.1321541877\H,-6.7317826695,-3.086462492,-2.2840340352\H,-8.460
0381553,-2.8240363021,-2.0010804189\H,-7.4450282291,-1.4695301999,-2.5
217460903\H,-1.7264444761,1.9079438388,-0.3177566911\H,-0.2900449338,0
.9343537582,-0.6029378363\C,-3.4048450204,-0.4544158401,-1.0193687312\
H,-4.0661664647,-0.9085241782,-1.7527259953\Version=EM64L-G09RevA.02\
State=1-A\HF=-596.8985101\RMSD=8.004e-09\RMSF=9.973e-06\Dipole=1.52187
29,0.5121355,-1.0206533\Quadrupole=13.8091658,-5.7092738,-8.099892,10.
8354521,0.8484407,0.7577306\PG=C01 [X(C10H18N1O2)]\ \@

tert-butyl pyrrolidine-1-carboxylate cation (5):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C9H16N1O2(1+)\LUISA\07-Jul-2010\0\#\
opt freq b3lyp/6-31g(d) geom=connectivity\producto2\1,1\N,-1.365446
0398,-0.1335944227,-0.0785833562\C,-1.7608183924,1.3089546356,-0.08076
67946\C,-3.2950719831,1.2449116427,0.096271876\C,-3.6722481861,-0.2313
88805,-0.201674212\C,-2.3709556503,-0.9396957143,-0.1472673907\H,-1.23
23819189,1.8190811312,0.7250525176\H,-1.4367054512,1.7387012199,-1.032
4650918\H,-3.5688419568,1.5030577984,1.1220029628\H,-3.8049526371,1.94
26277884,-0.5696081104\H,-4.3921343395,-0.6684152761,0.499891101\H,-4.
1025287254,-0.3831724975,-1.2039237027\H,-2.1912625869,-2.0117186172,-
0.1790198379\C,0.0394340705,-0.6496682988,-0.0565720684\O,0.8371813152
,0.3749170809,-0.0425530586\O,0.2141903167,-1.8372330438,-0.0560477061
\C,2.3714273317,0.200881123,-0.0199748845\C,2.7789846783,-0.5397349392
, -1.288694391\C,2.740654203,-0.5337654722,1.2639012265\C,2.8406540316,
1.6500973352,-0.0162788576\H,2.4263941367,-0.013781092,-2.1815584037\H
,3.8724064954,-0.5748391527,-1.3323671924\H,2.4085069465,-1.5669493551
, -1.3003984268\H,2.3663466738,-1.5596577726,1.2714671337\H,3.832291443
6,-0.5725453384,1.3382761789\H,2.3652503775,-0.0013123647,2.1435208899
\H,2.4750669171,2.1825626631,0.8668105518\H,3.9345063175,1.6707496709,
0.0026699052\H,2.5058586126,2.1772760729,-0.9145798579\Version=EM64L-
G09RevA.02\State=1-A\HF=-557.5778608\RMSD=9.807e-09\RMSF=3.110e-05\Dip

ole=-2.201552,0.5145363,-0.1035714\Quadrupole=20.7700514,-10.1739615,-
10.5960899,1.5642086,0.908551,0.222966\PG=C01 [X(C9H16N1O2)]\ \@

tert-butyl diethylcarbamate radical cation (6):

1\1\GINC-HERO3-29\FOpt\RB3LYP\6-31G(d)\C9H18N1O2(1+)\LHAYA\26-Nov-2010
\0\#opt freq b3lyp/6-31g(d) maxdisk=2000MB geom=connectivity\231110_
9\1,1\N,1.6104382044,0.1336031173,-0.2340380441\C,1.942740664,1.37665
21235,-0.0943829906\C,2.6270352804,-0.8734658797,-0.7040503041\H,2.961
9457026,1.6043707059,-0.4091838868\H,3.2565710817,-0.3533634073,-1.430
2842075\H,2.0701697826,-1.6534829594,-1.2233984272\C,0.2765704581,-0.4
639774174,0.138576609\O,-0.6755410256,0.3840447969,-0.1222872677\O,0.2
695368993,-1.5884489278,0.5551263631\C,-2.1609558619,0.0064341263,0.09
55961808\C,-2.3666536791,-0.2798550325,1.5786348383\C,-2.4791415086,-1
.1798693908,-0.8076421032\C,-2.86657351,1.2790757691,-0.3555445628\H,-
2.0675557403,0.5762716817,2.1923799926\H,-3.4334661885,-0.4546893606,1
.7525583739\H,-1.8226059603,-1.1687423753,1.9043112688\H,-1.9500333427
,-2.0838938957,-0.4998964234\H,-3.5537599096,-1.380903,-0.7475826762\H
,-2.2405266405,-0.9530791316,-1.8515379485\H,-2.6421422414,1.507326604
7,-1.4016156405\H,-3.9476848508,1.138099919,-0.2626330722\H,-2.5839306
38,2.1345448525,0.2656902562\C,3.4437071939,-1.4472999287,0.4510526129
\H,4.0057395906,-0.6643746419,0.9711868132\H,2.8036452737,-1.969345636
1,1.1647899414\H,4.1625866454,-2.1648020683,0.0435244492\C,1.148128601
1,2.5060661444,0.4394952005\H,0.2822575258,2.2049846856,1.0238057593\H
1,1.8134474662,3.1486153361,1.0262018512\H,0.8000957276,3.1129941901,-0
.4103219558\Version=EM64L-G09RevA.02\State=1-A\HF=-558.7787065\RMSD=2
.735e-09\RMSF=3.255e-06\Dipole=1.5010723,1.4246095,-0.4355584\Quadrupo
le=13.6228388,-3.605923,-10.0169157,2.594521,-2.4409551,1.8135809\PG=C
01 [X(C9H18N1O2)]\ \@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate cation (7):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d)\C11H18N1O4(1+)\LUIA\07-Jul-2010\0\
\#opt freq b3lyp/6-31g(d) geom=connectivity\carb2_03\1,1\N,-1.242703
0092,-0.3106219966,0.2145644636\C,-1.7234141432,0.8360299538,-0.131353
8374\C,-3.2050239369,0.8251062863,-0.2233696512\C,-3.5822079273,-0.525
2439211,0.4359818477\C,-2.2858620685,-1.3678864788,0.3303670128\H,-1.0
551351621,1.6676316339,-0.3324464055\H,-3.6500556321,1.7067281451,0.25
02195781\H,-3.4719725773,0.8751098303,-1.2904151642\H,-3.840281047,-0.
3751951823,1.4876375769\H,-4.4265197513,-1.0158891921,-0.0506676291\H,
-2.0819499339,-1.9948625143,1.1973499366\C,0.1959604942,-0.6821653526,
0.305980849\O,0.9227127996,0.3773711828,0.1048534739\O,0.4552572977,-1
.8299968812,0.5419264312\C,2.4649078614,0.3100735386,0.1139431276\C,2.
8995569078,-0.6331177773,-1.00200563\C,2.9075712777,-0.1361430649,1.50
27067823\C,2.833633311,1.7597603941,-0.1746358444\H,2.4903655845,-0.31
57436588,-1.9662181395\H,3.9916699889,-0.6036180512,-1.0751625424\H,2.
6022506876,-1.6650452038,-0.8042560696\H,2.6065373803,-1.1635879565,1.
7177335414\H,4.0003656615,-0.0873531994,1.5498772038\H,2.5098863257,0.
5298763655,2.2749892656\H,2.4509676222,2.4284114621,0.6024279534\H,3.9
236318436,1.8532144652,-0.1960255861\H,2.446767748,2.0810244247,-1.146
4757598\C,-2.2301509773,-2.1958355553,-0.966547643\O,-1.8161928851,-1.
7400575177,-2.009538773\O,-2.7437546031,-3.3988577527,-0.7628437156\C
,-2.8084065934,-4.2768159713,-1.9205514224\H,-3.2598446102,-5.19614718
52,-1.5527230304\H,-3.4223619007,-3.820398969,-2.6991890037\H,-1.80088
86228,-4.4579292803,-2.2987623977\Version=EM64L-G09RevA.02\State=1-A\
HF=-785.4488928\RMSD=4.965e-09\RMSF=2.223e-06\Dipole=-1.2996677,1.3941
991,0.4297327\Quadrupole=14.531817,0.1985357,-14.7303527,5.2119145,1.4
785206,5.4808965\PG=C01 [X(C11H18N1O4)]\ \@

1.5 Optimized geometries at B3LYP/6-31G(d,p) level:

tert-butyl indoline-1-carboxylate (1):

1\1\GINC-HERO5-29\FOpt\RB3LYP\6-31G(d,p)\C13H17N1O2\LHAYA\29-Nov-2010\
\0\#opt freq b3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\291110_
_3\0,1\N,1.4116003824,0.2681030953,0.4169877021\C,2.816437569,0.69101
8537,0.6166046709\C,3.651701825,-0.6030152102,0.4614163979\C,2.6213865
552,-1.6731925398,0.1796636241\C,1.3306607106,-1.1200339817,0.16324133
66\C,0.2134412979,-1.9230421399,-0.0787989117\C,0.4184527064,-3.288257
9336,-0.3031475905\C,1.6970488278,-3.8462262038,-0.2886192763\C,2.8075
806588,-3.0303052834,-0.0449213598\C,0.443370137,1.2390847169,0.504666
4235\O,0.7247973082,2.4061555111,0.7371587388\O,-0.7979464225,0.744697
0534,0.3071001031\H,2.9211041552,1.1491362844,1.603546165\H,4.37717073
6,-0.5150967733,-0.3548011986\H,4.2233678962,-0.8212425066,1.370169668
8\H,-0.7796948161,-1.4998782256,-0.0919061639\H,-0.443167764,-3.922175
0135,-0.4923971488\H,1.8309778246,-4.9088788975,-0.4655357688\H,3.8086
472691,-3.4534576513,-0.031132977\H,3.0742721077,1.4548026039,-0.12170
64899\C,-1.976698439,1.6308469246,0.3604800566\C,-3.1312157078,0.66397
4989,0.0865093635\H,-4.0824273892,1.2042518696,0.0985034059\H,-3.01603
85369,0.19071625,-0.8929755311\H,-3.1700352217,-0.1190944822,0.8493475
007\C,-1.8855847992,2.6915485016,-0.7408803572\H,-2.8158903882,3.26791
33033,-0.7702658068\H,-1.0540565708,3.3726050421,-0.5606890327\H,-1.75
09427773,2.2146866697,-1.7168004062\C,-2.1063796079,2.2475195678,1.756

6802913\H,-3.0454598411,2.8063080922,1.8230075477\H,-2.1246863177,1.46
16866738,2.5183124785\H,-1.2776512676,2.9241098568,1.9644761142\Ver
sion=EM64L-G09RevA.02\State=1-A\HF=-710.8847758\RMSD=2.394e-09\RMSF=1.85
6e-05\Dipole=-0.106328,-0.4025594,-0.0808289\Quadrupole=7.9716992,-4.5
961333,-3.3755659,-3.0749532,0.454394,-0.4979116\PG=C01 [X(C13H17N1O2)
]\@

tert-butyl 1H-indole-1-carboxylate (2):

1\1\GINC-HER05-27\FOpt\RB3LYP\6-31G(d,p)\C13H15N1O2\URIETA\24-Jan-2011
\0\#opt freq b3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\aroma
tico_5\0,1\C,2.6102604431,0.9661241893,-0.0000388153\C,1.7104971798,-
0.1289335402,-0.0000999798\C,2.1524765264,-1.453445134,0.0000972196\C,
3.5297849444,-1.6649712449,0.0003576737\C,4.4396274796,-0.5934907765,0
.0004193646\C,3.9907637499,0.7224808022,0.0002216511\C,1.8177366411,2.
1729583983,-0.000281023\C,0.5099086731,1.8089868655,-0.0004690572\H,1.
4477039107,-2.2732849144,0.000043781\H,3.9057522354,-2.6837581764,0.00
05140553\H,5.5061132261,-0.7984718758,0.0006240177\H,4.6942167602,1.55
01179614,0.0002698773\H,2.1888806974,3.1882571066,-0.0003053794\H,-0.3
880472385,2.4036556383,-0.0006716869\C,-0.7749675997,-0.3341230471,-0.
0005380158\O,-0.8002344586,-1.5490829775,-0.0001056009\O,-1.8340772434
,0.492632673,-0.0003706983\N,0.4083588338,0.4072680958,-0.0003931089\C
, -3.2152388673,-0.0400402256,0.000018895\C,-3.4566529356,-0.8547459414
, -1.2737124409\C,-3.4560648575,-0.854455539,1.2740482586\C,-4.05727484
91,1.2370409092,0.000674114\H,-3.2274538563,-0.2537964453,-2.15910308
03\H,-2.8443738741,-1.7564992243,-1.2886099127\H,-4.5109328731,-1.1446
303603,-1.3245440361\H,-3.2264515095,-0.2533048424,2.1591949625\H,-4.5
103215412,-1.1443268177,1.3254388484\H,-2.8437814861,-1.7562071499,1.2
888645403\H,-5.1208283335,0.9819127834,0.0003399424\H,-3.8460459812,1.
8399958285,0.8877129357\H,-3.8464537963,1.8397949813,-0.8878115991\Ver
sion=EM64L-G09RevA.02\State=1-A\HF=-709.6740207\RMSD=9.198e-09\RMSF=1.
358e-05\Dipole=-0.8466336,0.6131944,-0.0000826\Quadrupole=6.5696255,-
1.3402634,-5.2293621,-0.2783558,0.0006879,-0.0005231\PG=C01 [X(C13H15N
1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate (3):

1\1\GINC-LOST\FOpt\RB3LYP\6-31G(d,p)\C13H23N1O2\LUISA\15-Sep-2010\0\#
opt=calcfreq b3lyp/6-31g(d,p) geom=connectivity\140910_5\0,1\N,0.
0776875524,-0.9395156676,-1.0924548839\C,-1.0934438189,-0.187064837,-0
.6054947495\C,-0.9306326564,-0.222824275,0.9227675985\C,0.5946119153,
-0.2858370257,1.1196738107\C,1.031464833,-1.2608405035,-0.0025607638\C
,1.2287596139,1.1175554352,1.0031047739\C,2.7367903437,1.0881962762,0.
7316358305\C,3.0300089121,0.2721871925,-0.5323927678\C,2.5188343016,-1
.1636443899,-0.3801942877\H,-2.0201693642,-0.6538674422,-0.944940206\H
, -1.3895913201,0.6437745859,1.4096412139\H,-1.4041486628,-1.1239755639
,1.3271516532\H,0.86033459237,-0.7161210931,2.0922987338\H,0.8400274151
, -2.2934379233,0.3255282879\H,0.7452608383,1.6695382219,0.1859172535\H
,1.0084171608,1.6767158816,1.9209190605\H,3.1172911439,2.1119328553,0.
633969508\H,3.2626298351,0.6389648673,1.5865597519\H,2.5473886347,0.75
00473141,-1.3955197733\H,4.1056121142,0.2583177605,-0.7434460981\H,3.0
797141538,-1.6533832187,0.4284261198\H,2.6909342569,-1.7506724377,-1.2
837321076\H,-1.0847632663,0.8384957408,-0.9947698726\C,0.064052215,-1.
665123623,-2.2502620079\O,0.8847967383,-2.5275136153,-2.5382310701\O,-
0.979302486,-1.2821370378,-3.0352753321\C,-1.2046250288,-1.9047558566,
-4.3475126701\C,-0.012197179,-1.6332037541,-5.2709022702\C,-1.48164066
34,-3.4031260085,-4.1826548812\C,-2.4539284018,-1.1760575357,-4.850076
5549\H,0.1786320873,-0.5572890968,-5.3359836204\H,0.8852735648,-2.1309
298639,-4.9039016243\H,-0.2360129041,-1.9998943083,-6.2780438221\H,-2.
312218387,-3.5608083429,-3.4870265186\H,-1.7632666701,-3.8338489128,-5
.1491151204\H,-0.6008093323,-3.9232133807,-3.8064314029\H,-2.735731718
7,-1.5502143102,-5.8387773514\H,-3.2943905478,-1.3341821922,-4.1679145
042\H,-2.269061146,-0.1006857624,-4.9258793349\Version=EM64L-G09RevA.
02\State=1-A\HF=-714.5139948\RMSD=6.861e-09\RMSF=3.259e-06\Dipole=-0.5
929939,0.526155,0.3875822\Quadrupole=-0.6576233,-3.2417379,3.8993613,1.
.9726786,2.0418762,0.3480272\PG=C01 [X(C13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate (4):

1\1\GINC-HER05-12\FOpt\RB3LYP\6-31G(d,p)\C10H19N1O2\LHAYA\12-Nov-2010\
0\#opt freq b3lyp/6-31g(d,p) geom=connectivity\111110_9\0,1\C,-1.28
04230381,0.5042430545,-0.3569780168\C,-1.7572596135,0.1183058925,1.050
9192034\C,-3.2311947241,0.4878512752,1.2546637306\N,-4.0602068529,-0.0
821294389,0.1930931996\C,-3.6684507083,0.2664543502,-1.1725934878\C,-2
.2001513936,-0.1027022015,-1.4265321279\C,-5.1833786075,-0.7903041449,
0.5333736756\O,-5.5183719176,-1.0214411397,1.6880538122\O,-5.858858178
1,-1.2027894523,-0.5705835901\C,-7.0912882486,-1.9951428619,-0.4470179
153\C,-6.7980761647,-3.3272870837,0.2515944591\C,-8.169363075,-1.18307
51676,0.2784002187\C,-7.4818031746,-2.2279380139,-1.9091121664\H,-1.63
95665451,-0.9628323398,1.1978819679\H,-1.1502843395,0.6170509411,1.815
5916967\H,-3.6144498538,0.1200853371,2.205732737\H,-3.3403282047,1.584
3887691,1.2457951839\H,-4.3295575063,-0.2444725606,-1.8689181924\H,-3.
8024447511,1.3509391185,-1.3167848729\H,-1.9107691768,0.2402569421,-2.

4269618047\H,-2.104649578,-1.1960213125,-1.418016821\H,-6.5005897358,-
3.1677514152,1.2877767003\H,-7.6937169268,-3.9567696217,0.2317153418\H
, -5.9972206408, -3.860743949, -0.2703291993\H, -8.3288557479, -0.226493492
1, -0.2293822797\H, -9.1149249616, -1.7349551468, 0.2676132987\H, -7.882518
6071, -0.9917948463, 1.3122454357\H, -6.6919862998, -2.7691456003, -2.43822
58279\H, -8.4015434993, -2.8178528912, -1.9634397187\H, -7.6506097216, -1.2
756986342, -2.4202711518\H, -1.2870291219, 1.5995474867, -0.4537918143\H, -
0.2449153752, 0.182341747, -0.5149296646\Version=EM64L-G09RevA.02\State
=1-A\HF=-597.7755153\RMSD=8.823e-09\RMSF=1.313e-05\Dipole=0.3536055,0.
1651746,-0.8073682\Quadrupole=3.3668365,0.6409621,-4.0077986,2.6308524
,1.8735281,0.7667214\PG=C01 [X(C10H19N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate (5):

1\1\GINC-HER05-17\FOpt\RB3LYP\6-31G(d,p)\C9H17N1O2\LHAYA\02-Dec-2010\
\#opt freq b3lyp/6-31g(d,p) maxdisk=2000MB geom=connectivity\011210_
3\0,1\N,-1.3053175945,-0.1554391776,0.0441982218\C,-1.7270560801,1.24
82601769,-0.0319662447\C,-3.2388575915,1.1685150276,0.2338341416\C,-3.
6265729662,-0.2150772202,-0.3174494326\C,-2.4293185178,-1.0972132,0.06
51388133\H,-1.1929249514,1.8578148708,0.7016694585\H,-1.5133542472,1.6
654998648,-1.0254509583\H,-3.430130325,1.2095494276,1.3122323723\H,-3.
7874218904,1.990661251,-0.2336017925\H,-4.5696320431,-0.5920370437,0.0
870187187\H,-3.7241737407,-0.1702147268,-1.4082311607\H,-2.5502460326,
-1.532712698,1.0663957781\H,-2.2501869141,-1.9217037053,-0.6296690881\
C,-0.0215784648,-0.6057202865,0.0473754847\O,0.8457095753,0.4405638602
, -0.0233762008\O,0.2810790625,-1.7906305669,0.1053832801\C,2.297077242
9,0.2133383048,-0.0214955018\C,2.703968338,-0.6043747572,-1.2522109725
\C,2.7241602576,-0.4591614583,1.2878351656\C,2.8568956246,1.6357227882
, -0.10730423\H,2.3514062423,-0.1147969482,-2.1656652516\H,3.7954691185
, -0.674196609,-1.3039575133\H,2.2858669429,-1.6098571932,-1.2053872536
\H,2.3034527761,-1.4617206128,1.3651576373\H,3.816216673,-0.5276722339
,1.327737683\H,2.3898664343,0.1339122099,2.1451448788\H,2.52896969,2.2
318759865,0.74927978\H,3.9506459839,1.6102209654,-0.1136194075\H,2.516
0973974,2.1299376041,-1.0217284058\Version=EM64L-G09RevA.02\State=1-A
\HF=-558.4547006\RMSD=7.468e-09\RMSF=1.186e-05\Dipole=-0.4951217,0.890
9439,-0.0593306\Quadrupole=6.113547,-5.0166099,-1.0969371,0.562833,-0.
0172203,0.3281744\PG=C01 [X(C9H17N1O2)]\@

tert-butyl diethylcarbamate (6):

1\1\GINC-HER03-40\FOpt\RB3LYP\6-31G(d,p)\C9H19N1O2\LHAYA\20-Nov-2010\
\#opt freq b3lyp/6-31g(d,p) maxdisk=2500MB\191110_33\0,1\N,-1.51378
92098,-0.1399865735,0.6978404036\C,-1.8219768761,1.2582525523,1.012603
3454\C,-2.5642596205,-1.1621298764,0.7547310145\H,-2.6605435,1.2499760
503,1.7169601583\H,-0.9653729644,1.6885752444,1.5358544641\H,-3.301506
9599,-0.8286241778,1.4924615444\H,-2.1093889995,-2.0820372269,1.129951
5409\C,-0.2794872979,-0.5444944788,0.2627935469\O,0.590413217,0.499566
3716,0.2170326076\O,-0.0124953864,-1.7016032374,-0.03687912\C,1.990617
7009,0.2963880151,-0.1844986455\C,2.0564384836,-0.209678283,-1.6292894
888\C,2.6871995421,-0.6534952784,0.7956384434\C,2.5742413175,1.7077194
509,-0.077436411\H,1.5200174479,0.4735411443,-2.2954963578\H,3.1004175
476,-0.2521204527,-1.9565215282\H,1.6173809796,-1.2035675386,-1.712513
7489\H,2.2601197487,-1.6545110283,0.7371337619\H,3.7549075947,-0.70754
2575,0.5592983168\H,2.5849567884,-0.2825154645,1.8204447568\H,2.488595
3822,2.0852950509,0.9456595591\H,3.6323279263,1.6995601952,-0.35548206
59\H,2.0467978443,2.3958646257,-0.7444597511\C,-3.241398598,-1.4457242
301,-0.5893862079\H,-3.7419360036,-0.557677837,-0.9873223569\H,-2.4994
743952,-1.785238472,-1.3163427261\H,-3.9926290425,-2.2346499762,-0.473
9896886\C,-2.1669582623,2.1244288215,-0.2035242045\H,-1.3322950345,2.1
37129703,-0.9090181182\H,-3.0552562824,1.7547076465,-0.7244342679\H,-2
.3640893979,3.1551799446,0.1111942536\Version=EM64L-G09RevA.02\State=
1-A\HF=-559.6652703\RMSD=6.465e-09\RMSF=1.028e-05\Dipole=-0.2158684,0.
798221,0.1906179\Quadrupole=4.7415775,-3.9712568,-0.7703207,0.7644077,
-1.5908816,-0.2253817\PG=C01 [X(C9H19N1O2)]\@

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate (7):

1\1\GINC-HER03-24\FOpt\RB3LYP\6-31G(d,p)\C11H19N1O4\URIETA\15-Dec-2010
\#opt freq b3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\15121
0_3\0,1\N,0.3302035817,0.9351633713,-0.1558959366\C,0.1514137083,2.28
28464867,0.3903749602\C,1.4041121132,3.0098544694,-0.1138479116\C,2.47
73178749,1.9082496828,-0.0977763472\C,1.7103491832,0.629561677,-0.5210
820524\H,-0.7817243474,2.720264483,0.0303987494\H,0.1148638389,2.25869
31363,1.4879013138\H,1.2407208725,3.3684724292,-1.1361573029\H,1.67085
48636,3.8693262447,0.5070739197\H,3.3249217767,2.1111784337,-0.7561672
744\H,2.8576878019,1.7769115998,0.920597726\H,1.7948703655,0.436860805
3,-1.5954645266\C,-0.634132952,-0.0157986522,-0.3120875981\O,-1.834214
1235,0.4438108513,0.1161346123\O,-0.4061200063,-1.1205340971,-0.789070
708\C,-3.0320549531,-0.4096405251,0.0564592789\C,-2.8341690078,-1.6507
680249,0.9326489298\C,-3.3485440582,-0.7689171653,-1.398967752\C,-4.11
6172126,0.4995952577,0.6402068492\H,-2.5690621654,-1.3562811315,1.9527
695029\H,-3.7667970961,-2.2229826435,0.9744970395\H,-2.0451431246,-2.2
882278824,0.5338788802\H,-2.5652999581,-1.3965379393,-1.8240947316\H,-

4.3004458707,-1.3079644867,-1.4459572878\H,-3.4432779294,0.1395557062,
-2.0024203448\H,-4.2267084089,1.4060950797,0.0378741183\H,-5.076482693
3,-0.0241869755,0.6568963812\H,-3.863638466,0.7932286426,1.6631016221\
C,2.2326793981,-0.5955500718,0.2306917642\O,2.0209385869,-0.8291258288
1,3.992609154\O,3.0270784343,-1.3396598697,-0.5624112864\C,3.593677954
9,-2.5043580637,0.0610073272\H,4.2165003084,-2.9729960729,-0.700526481
7\H,4.192913655,-2.2240454282,0.9308569194\H,2.8012289688,-3.184849498
,0.3808347322\Version=EM64L-G09RevA.02\State=1-A\HF=-786.3295045\RMSD
=4.311e-09\RMSF=1.158e-05\Dipole=0.1490175,0.8009238,-0.1803296\Quadru
pole=5.8321216,1.4287983,-7.26092,-0.1919794,-1.6121473,-0.5854114\PG=
C01 [X(C11H19N1O4)]\@

tert-butyl indoline-1-carboxylate radical carbocation (1):

1\1\GINC-HERO3-26\FOpt\UB3LYP\6-31G(d,p)\C13H17N1O2(1+,2)\LHAYA\30-Nov
-2010\0\#opt freq ub3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\
\291110_15\1,2\N,1.442771698,0.2237930225,0.4121623117\C,2.8451107325
,0.6659162155,0.6145787616\C,3.6830736218,-0.6154293854,0.4612615986\C
,2.6683206631,-1.6843220025,0.1816760205\C,1.3492401069,-1.1096184119,
0.1671421168\C,0.198110165,-1.9078676342,-0.0763316008\C,0.3982070168,
-3.2532262863,-0.2975655143\C,1.697816115,-3.8216487507,-0.2836745533\
C,2.8345638114,-3.0367366629,-0.0438170042\C,0.4176742314,1.2510594054
,0.5040781549\O,0.7751816536,2.3798547197,0.7366190102\O,-0.7800502314
,0.7543869372,0.3099077163\H,2.922329236,1.131201943,1.6003012416\H,4.
4090200663,-0.531500383,-0.355156995\H,4.2563991517,-0.8374777021,1.36
8226658\H,-0.7868319839,-1.4671833669,-0.0851146117\H,-0.4553690079,-3
.8951851282,-0.4869976709\H,1.8103633876,-4.8861091738,-0.4627770343\H
3,8.22121801,-3.4857738306,-0.0362805512\H,3.0747915922,1.4372478336,-
0.1246201598\C,-2.0191910285,1.6517877816,0.3602520543\C,-3.1374938946
,0.6528292226,0.0831280153\H,-4.0970478506,1.1762922524,0.0913378838\H
,-3.0163614358,0.1863015661,-0.8985332957\H,-3.1714023008,-0.125391630
1,0.8507161774\C,-1.9031552823,2.6979914518,-0.7440558516\H,-2.8372908
068,3.2655426412,-0.7846765368\H,-1.0886890858,3.3985156452,-0.5567901
607\H,-1.7581090076,2.2229128017,-1.7184912629\C,-2.1249242705,2.25184
31459,1.7589446918\H,-3.0693651922,2.7987033255,1.8320360972\H,-2.1332
783602,1.467222299,2.5209035862\H,-1.3123932112,2.9493368389,1.9649042
773\Version=EM64L-G09RevA.02\State=2-A\HF=-710.6254707\S2=0.766857\S2
-1=0.\S2A=0.750197\RMSD=6.453e-09\RMSF=1.171e-05\Dipole=1.1189376,-1.7
790985,-0.2171823\Quadrupole=11.3894044,4.2311265,-15.6205309,-11.5873
243,0.3698477,2.5894876\PG=C01 [X(C13H17N1O2)]\@

tert-butyl 1H-indole-1-carboxylate radical carbocation (2):

1\1\GINC-HERO5-22\FOpt\UB3LYP\6-31G(d,p)\C13H15N1O2(1+,2)\URIETA\26-Ja
n-2011\0\#opt freq ub3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\
\aromatico_12\1,2\C,-2.6349235821,0.9683787432,0.0001437451\C,-1.724
0318359,-0.1309245763,-0.0001698518\C,-2.1523209474,-1.4371357143,-0.0
00304994\C,-3.5606733582,-1.6502494951,-0.0001164713\C,-4.4801201913,-
0.5947608192,0.0001897575\C,-4.035076165,0.7238657348,0.0003232296\C,-
1.8749927978,2.149513804,0.0002101632\C,-0.5125897618,1.7661247062,-0.
0000563375\H,-1.4574258217,-2.2660523976,-0.0005457052\H,-3.9235553976
, -2.6730240581,-0.0002182379\H,-5.5427976333,-0.8087668344,0.000323036
3\H,-4.7349064018,1.5531968815,0.000561317\H,-2.2310106932,3.170793461
8,0.0004254281\H,0.3743038728,2.382274012,-0.0000941857\C,0.8220849231
, -0.3513911819,-0.0006147243\O,0.7702718791,-1.555326293,-0.0004998968
\O,1.8386506523,0.4723593003,-0.0002619031\N,-0.414169483,0.4221542192
, -0.0002977333\C,3.2818231026,-0.0386150217,0.0000382332\C,3.504248140
4,-0.8439651866,1.2762443259\C,3.5046307716,-0.8442928839,-1.275892694
6\C,4.0703959609,1.2657682403,-0.000087981\H,3.2628135562,-0.24785751
45,2.1608055056\H,2.9158363669,-1.762363119,1.2858789381\H,4.561717594
1,-1.1169894705,1.3358656445\H,3.2634938184,-0.2484033705,-2.160682028
9\H,4.5621114487,-1.1173613476,-1.3351067862\H,2.9161960269,-1.7626773
953,-1.2854798983\H,5.1396300771,1.0386454913,0.0001823791\H,3.8495052
452,1.8602733875,-0.8904499675\H,3.8492346335,1.8605016975,0.890212511
3\Version=EM64L-G09RevA.02\State=2-A\HF=-709.4049636\S2=0.763304\S2-1
=0.\S2A=0.750117\RMSD=5.964e-09\RMSF=1.503e-05\Dipole=-1.7834323,1.026
9415,0.0002243\Quadrupole=26.0381795,-6.311683,-19.7264965,0.583258,-0.
0012035,0.0013789\PG=C01 [X(C13H15N1O2)]\@

tert-butyl (S,S)-octahydro-1H-indole-1-carboxylate radical carbocation (3):

1\1\GINC-LOST\FOpt\UB3LYP\6-31G(d,p)\C13H23N1O2(1+,2)\LUISA\16-Sep-201
0\0\#opt=calcfc freq ub3lyp/6-31g(d,p) geom=connectivity\140910_9\1
,2\N,-0.0016053253,-1.145693923,-0.9246689856\C,-1.1870741262,-0.47818
39103,-0.3900613118\C,-0.8983826595,-0.355114604,1.1132965411\C,0.6404
743717,-0.2722067711,1.1758216138\C,1.0785712974,-1.2511098772,0.05659
76377\C,1.162968392,1.1636814241,0.9466317042\C,2.6477909138,1.2102417
105,0.568412576\C,2.9128132885,0.3765935398,-0.6892038361\C,2.52132030
9,-1.0937774751,-0.4771018413\H,-2.08410914,-1.0368259352,-0.673451157
3\H,-1.3893113841,0.5184394364,1.5467018305\H,-1.2700922599,-1.2440488
357,1.6328393466\H,1.0203483707,-0.6457916349,2.1311083771\H,0.9841616
475,-2.2940232447,0.420559789\H,0.5833587695,1.6481775378,0.1480392706
\H,0.9724405047,1.7449107061,1.8546471107\H,2.9536932998,2.2485996656,

0.4081721862\H,3.2588298381,0.8298902234,1.3976856187\H,2.3552801506,0.7959707513,-1.5384273886\H,3.9720685673,0.4122971807,-0.9630422063\H,3.1648149279,-1.5330129126,0.293371278\H,2.6580433048,-1.6969049013,-1.3758699569\H,-1.2599015768,0.4980822457,-0.8950946009\C,-0.0031503723,-1.8630842307,-2.1982385058\O,0.7378288935,-2.8072510361,-2.3312699184\O,-0.8873797093,-1.3227150151,-2.990146645\C,-1.1510100027,-1.8767177111,-4.4022387718\C,0.1474346393,-1.7920183398,-5.1966565125\C,-1.6847148977,-3.2976014322,-4.2533641708\C,-2.2093901059,-0.9103895566,-4.9180364804\H,0.531908536,-0.7683702781,-5.2113847057\H,0.9125161758,-2.4636115926,-4.804147455\H,-0.0601982955,-2.0848466052,-6.2298322965\H,-2.575651809,-3.3172976675,-3.6195268245\H,-1.9722578714,-3.6645481865,-5.2428579978\H,-0.9329974864,-3.9761412448,-3.8473405264\H,-2.490750559,-1.1986491089,-5.934262901\H,-3.1075650903,-0.9384375683,-4.2958095489\H,-1.8285235264,0.1135891771,-4.9477503347\Version=EM64L-G09RevA.02\State=2-A\HF=-714.2279793\S2=0.756453\S2-1=0.\S2A=0.750031\RMSD=7.668e-09\RMSF=2.408e-06\Dipole=-0.7094972,0.3474696,0.6801312\Quadrupole=-1.70796,-9.3705785,11.0785386,3.8557283,7.0543188,5.9867246\PG=C01[X(C13H23N1O2)]\@

tert-butyl piperidine-1-carboxylate radical carbocation (4):

1\1\GINC-LOST\FOpt\UB3LYP\6-31G(d,p)\C13H23N1O2(1+,2)\LUISA\16-Sep-2010\0\#opt=calcfreq ub3lyp/6-31g(d,p) geom=connectivity\140910_9\1,2\N,-0.0016053253,-1.145693923,-0.9246689856\C,-1.1870741262,-0.4781839103,-0.3900613118\C,-0.8983826595,-0.355114604,1.1132965411\C,0.6404743717,-0.2722067711,1.1758216138\C,1.0785712974,-1.2511098772,0.0565976377\C,1.162968392,1.1636814241,0.9466317042\C,2.6477909138,1.2102417105,0.568412576\C,2.9128132885,0.3765935398,-0.6892038361\C,2.521320309,-1.0937774751,-0.4771018413\H,-2.08410914,-1.0368259352,-0.6734511573\H,-1.3893113841,0.5184394364,1.5467018305\H,-1.2700922599,-1.2440488357,1.6328393466\H,1.0203483707,-0.6457916349,2.1311083771\H,0.9841616475,-2.2940232447,0.420559789\H,0.5833587695,1.6481775378,0.1480392706\H,0.9724405047,1.7449107061,1.8546471107\H,2.9536932998,2.2485996656,0.4081721862\H,3.2588298381,0.8298902234,1.3976856187\H,2.3552801506,0.7959707513,-1.5384273886\H,3.9720685673,0.4122971807,-0.9630422063\H,3.1648149279,-1.5330129126,0.293371278\H,2.6580433048,-1.6969049013,-1.3758699569\H,-1.2599015768,0.4980822457,-0.8950946009\C,-0.0031503723,-1.8630842307,-2.1982385058\O,0.7378288935,-2.8072510361,-2.3312699184\O,-0.8873797093,-1.3227150151,-2.990146645\C,-1.1510100027,-1.8767177111,-4.4022387718\C,0.1474346393,-1.7920183398,-5.1966565125\C,-1.6847148977,-3.2976014322,-4.2533641708\C,-2.2093901059,-0.9103895566,-4.9180364804\H,0.531908536,-0.7683702781,-5.2113847057\H,0.9125161758,-2.4636115926,-4.804147455\H,-0.0601982955,-2.0848466052,-6.2298322965\H,-2.575651809,-3.3172976675,-3.6195268245\H,-1.9722578714,-3.6645481865,-5.2428579978\H,-0.9329974864,-3.9761412448,-3.8473405264\H,-2.490750559,-1.1986491089,-5.934262901\H,-3.1075650903,-0.9384375683,-4.2958095489\H,-1.8285235264,0.1135891771,-4.9477503347\Version=EM64L-G09RevA.02\State=2-A\HF=-714.2279793\S2=0.756453\S2-1=0.\S2A=0.750031\RMSD=7.668e-09\RMSF=2.408e-06\Dipole=-0.7094972,0.3474696,0.6801312\Quadrupole=-1.70796,-9.3705785,11.0785386,3.8557283,7.0543188,5.9867246\PG=C01[X(C13H23N1O2)]\@

tert-butyl pyrrolidine-1-carboxylate radical carbocation (5):

1\1\GINC-HER05-22\FOpt\UB3LYP\6-31G(d,p)\C9H17N1O2(1+,2)\LHAYA\02-Dec-2010\0\#opt freq ub3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\011210_7\1,2\N,-1.344085485,-0.1504361341,0.0134719091\C,-1.7680439588,1.2414976117,-0.0254466455\C,-3.2806712925,1.1810289215,0.2338364688\C,-3.6785704846,-0.2105205874,-0.2988455518\C,-2.4603209612,-1.080877616,0.0392673469\H,-1.1607805279,1.8305098751,0.6696541559\H,-1.5229211528,1.6161040763,-1.0353129767\H,-3.4742464176,1.2599660563,1.3081270187\H,-3.8079482193,1.9964338221,-0.2630779871\H,-4.5897796994,-0.5983089484,0.1582194781\H,-3.8279969523,-0.1886787252,-1.3828369216\H,-2.5063550756,-1.4906575359,1.0647905499\H,-2.2433098674,-1.9337853036,-0.6120748791\C,0.0432804038,-0.6265568314,0.0421601331\O,0.8452389718,0.3973929141,-0.0279366304\O,0.2284727132,-1.8162468953,0.1236847877\C,2.379842699,0.2188699408,-0.0222421983\C,2.7587053295,-0.6136679071,-1.2415712016\C,2.7692664613,-0.4248618892,1.3037725028\C,2.8541705527,1.6614937728,-0.1309722013\H,2.3928393321,-0.1508817922,-2.1622384011\H,3.8500215075,-0.6581560409,-1.3015571435\H,2.3844978028,-1.6362921418,-1.1724149942\H,2.3923279335,-1.4450523605,1.3912256663\H,3.8610368676,-0.463848853,1.3588893213\H,2.4140587618,0.1708460527,2.1491345682\H,2.5087145569,2.2566815229,0.7181894917\H,3.9471934439,1.6768659979,-0.1339756159\H,2.5052897571,2.1242369977,-1.0576010505\Version=EM64L-G09RevA.02\State=2-A\HF=-558.1618662\S2=0.756467\S2-1=0.\S2A=0.750032\RMSD=7.728e-09\RMSF=6.927e-06\Dipole=-1.6667176,0.7055364,-0.0371746\Quadrupole=17.929758,-9.002557,-8.927201,0.7211387,-0.1665822,0.0152831\PG=C01[X(C9H17N1O2)]\@

tert-butyl diethylcarbamate radical carbocation (6):

1\1\GINC-HER03-04\FOpt\UB3LYP\6-31G(d,p)\C9H19N1O2(1+,2)\LHAYA\20-Nov-2010\0\#opt freq ub3lyp/6-31g(d,p) maxdisk=2500MB\191110_45\1,2\N,-

1.5580453738,-0.1463413687,0.6737862812\C,-1.9246108702,1.2550836722,0.8260267509\C,-2.5222388237,-1.2088603973,0.9007145281\H,-2.8552471608,1.2915928678,1.3938973356\H,-1.1216593296,1.7325094557,1.3965633574\H,-3.1212051219,-0.9197100496,1.769166662\H,-1.9654122693,-2.1243314986,1.0993099332\C,-0.2256500647,-0.5408230686,0.1690802947\O,0.5955044287,0.4645469304,0.2574409772\O,-0.0878973036,-1.670710368,-0.2333097976\C,2.0809014197,0.331695514,-0.1531438275\C,2.1292208202,0.016697412,-1.6437350311\C,2.7119950268,-0.7456629449,0.7210199879\C,2.6104637185,1.722985185,0.1663769517\H,1.6094096667,0.7827345797,-2.2259127819\H,3.1764163096,0.0136164096,-1.9598420369\H,1.7072251922,-0.9636469143,-1.8696334481\H,2.3062009041,-1.7363238044,0.5100843574\H,3.7854512759,-0.771358646,0.5124919014\H,2.5838567675,-0.5150154954,1.7821270724\H,2.5003970998,1.9547913733,1.2287441054\H,3.674467062,1.7627990669,-0.0812108205\H,2.0973709666,2.4882850123,-0.4216677338\C,-3.4463171723,-1.4266812556,-0.3294990819\H,-4.043575372,-0.540183522,-0.5500766657\H,-2.8543988293,-1.710060295,-1.2010106046\H,-4.1221422403,-2.2474943076,-0.0770553196\C,-2.0785971677,1.9861339352,-0.5315206875\H,-1.1426185017,1.9798950897,-1.0909553811\H,-2.8721381993,1.5420011124,-1.1346584678\H,-2.3455528983,3.02242443,-0.3105957897\Version=EM64L-G09RevA.02\State=2-A\HF=-559.3719692\S2=0.756441\S2-1=0.\S2A=0.750031\RMSD=5.501e-09\RMSF=6.923e-06\Dipole=-1.5256586,0.5900086,0.5892303\Quadrupole=14.4278433,-6.2935213,-8.134322,2.5340284,-3.6287025,-1.2664794\PG=C01 [X(C9H19N1O2)]\@\

1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate radical carbocation (7):

1\1\GINC-HER03-42\FOpt\UB3LYP\6-31G(d,p)\C11H19N1O4(1+,2)\URIETA\15-Dec-2010\0\#opt freq ub3lyp/6-31g(d,p) maxdisk=2500MB geom=connectivity\151210_11\1,2\N,0.3772433656,0.9194748223,-0.164000574\C,0.2467528744,2.2208602644,-0.473530729\C,1.4185172277,3.0138033736,-0.1187019013\C,2.5072292288,1.9381339146,-0.3197425568\C,1.7201819343,0.6286457614,-0.5715167433\H,-0.7566320818,2.6180720155,0.3148474094\H,0.3753625118,2.0542599715,1.5597289802\H,1.1172425957,3.4575105392,-1.0720814612\H,1.7410601494,3.8187418098,0.5432459851\H,3.1813203576,2.1605778548,-1.147779971\H,3.1063513058,1.8291742875,0.5880873611\H,1.7087213942,0.2697906543,-1.6090871062\H,-0.6731738314,-0.0758963601,-0.3050653706\O,-1.8109455706,0.4335189195,0.0808749275\O,-0.3717075337,-1.1689718433,-0.7263862059\C,-3.1068511248,-0.3914938951,0.0642379433\C,-2.9257462667,-1.5733192758,1.0113521347\C,-3.3874385348,-0.801915896,-1.3776592547\C,-4.1212534333,0.6178169846,0.5866064178\H,-2.6549893541,-1.2330823198,2.0146625016\H,-3.8782560145,-2.1060457899,1.0847158882\H,-2.1733115393,-2.2755265965,0.6494979153\H,-2.6391622984,-1.4988147533,-1.7578965194\H,-4.3610819243,-1.2993427337,-1.4116711571\H,-3.4367072518,0.073561626,-2.0310099987\H,-4.1869804807,1.4886508683,-0.0707563931\H,-5.1066662205,0.1462767056,0.6251642068\H,-3.8637187624,0.9507486777,1.5953061106\C,2.3063639983,-0.5866098273,0.2588599012\O,2.2851253154,-0.5909407177,1.4638954581\O,2.8430321577,-1.46835764,-0.5565383932\C,3.475848302,-2.626664331,0.0696998662\H,3.9058595957,-3.1879464816,-0.7563538958\H,4.2454752539,-2.2936742587,0.7668231298\H,2.7182836547,-3.2126853306,0.5911906364\Version=EM64L-G09RevA.02\State=2-A\HF=-786.0358095\S2=0.756045\S2-1=0.\S2A=0.750027\RMSD=5.254e-09\RMSF=3.064e-06\Dipole=0.5170955,1.0706888,-0.258184\Quadrupole=14.9168689,1.0213907,-15.9382596,-0.3806746,-2.6611479,-0.6410195\PG=C01 [X(C11H19N1O4)]\@\

tert-butyl piperidine-1-carboxylate cation (4):

1\1\GINC-HER05-20\FOpt\RB3LYP\6-31G(d,p)\C10H18N1O2(1+)\LHAYA\11-Nov-2010\0\#opt freq b3lyp/6-31g(d,p)\111110_33\1,1\C,-1.3497865259,0.8721498777,-0.3545694829\C,-1.5690624418,0.2003133514,1.0048926557\C,-3.0538871661,0.1187502458,1.3412811376\N,-3.837776335,-0.446776213,0.199332735\C,-2.0936178306,0.0923111588,-1.4454782123\C,-5.1932036042,-0.9994281742,0.5642432204\O,-5.5112199851,-0.9740031011,1.7203277319\O,-5.8011612335,-1.4188633199,-0.5065885898\C,-7.2142671029,-2.043178198,-0.4387234365\C,-7.1325880202,-3.2953251571,0.425482191\C,-8.1684742416,-0.9856459826,0.1023515781\C,-7.4732109077,-2.3638181165,-1.9046771488\H,-1.1357158226,-0.8069137716,1.0064515553\H,-1.0732305793,0.7594810948,1.8026688651\H,-3.2600464786,-0.5223693828,2.197812861\H,-3.4847583322,1.101437259,1.5576055218\H,-2.2705654726,0.6866682817,-2.352258157\H,-1.5136156035,-0.7749311258,-1.803712859\H,-6.9097033382,-3.0586928704,1.4668291789\H,-8.1025099811,-3.8000312476,0.3941342828\H,-6.3823081041,-3.9909517003,0.0395766233\H,-8.1391657066,-0.0799679457,-0.5096961296\H,-9.1859032952,-1.3848549587,0.0587109101\H,-7.9507293241,-0.7317647415,1.1406404053\H,-6.7371411889,-3.0735714943,-2.2913696466\H,-8.463195661,-2.8174791387,-2.0001912519\H,-7.4550874685,-1.4586273993,-2.5172642764\H,-1.7180509352,1.9035360319,-0.3255741329\H,-0.2866727415,0.9223762335,-0.5996075511\C,-3.4020131556,-0.4599379106,-1.0193184505\H,-4.0601287368,-0.9206461268,-1.7515725761\Version=EM64L-G09RevA.02\State=1-A\HF=-596.9240657\RMSD=5.310e-09\RMSF=1.442e-05\Dipole=1.5229357,0.5144687,-1.0204041\Quadrupole=13.8460617,-5.739358,-8.1067037,10.8720076,0.8181845,0.8265317\PG=C01 [X(C10H18N1O2)]\@\

tert-butyl pyrrolidine-1-carboxylate cation (5):

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1\1\GINC-HER05-21\FOpt\RB3LYP\6-31G(d,p)\C9H16N1O2(1+)\LHAYA\02-Dec-20
10\0\#b3lyp/6-31g(d,p) opt freq maxdisk=2000MB geom=connectivity\011
210_11\1,1N,-1.3863526772,-0.186464714,-0.0037094678\C,-1.8168960547
,1.2444785885,-0.0647502957\C,-3.34521277,1.1509823952,0.1431143368\C,
-3.6899737022,-0.344442336,-0.0896227396\C,-2.3723854731,-1.0188595323
,-0.0224268746\H,-1.2873748189,1.80453181,0.7057473712\H,-1.5211448407
,1.6370819082,-1.0410010893\H,-3.6066925351,1.4417060468,1.1625415534\
H,-3.8837996813,1.8091366423,-0.5389810862\H,-4.3914789014,-0.76966002
05,0.6361798778\H,-4.1256932792,-0.5481327927,-1.0795490479\H,-2.16594
14919,-2.0864707242,-0.0101410898\C,0.0306620247,-0.6673690788,0.02138
8813\O,0.8037093689,0.375155217,-0.0164885221\O,0.233968696,-1.8496293
21,0.068320992\C,2.3424091938,0.2355953509,-0.0066132955\C,2.749697764
6,-0.5473398541,-1.2491297996\C,2.7418813227,-0.4386584627,1.300523626
1\C,2.7791303673,1.6930596963,-0.0673628949\H,2.3764416015,-0.06536284
97,-2.1569268487\H,3.8419548506,-0.5620846812,-1.3046313173\H,2.400357
8057,-1.5803214482,-1.2139371694\H,2.3893527612,-1.4698350301,1.353194
6081\H,3.8338418665,-0.4519114128,1.3618709177\H,2.3665292289,0.120876
4133,2.161778916\H,2.4131812951,2.2521008994,0.7976063127\H,3.87135979
61,1.7375141777,-0.0635010948\H,2.4223842821,2.1753571126,-0.980959691
6\Version=EM64L-G09RevA.02\State=1-A\HF=-557.6005147\RMSD=3.874e-09\R
MSF=9.437e-06\Dipole=-2.2119306,0.4615127,-0.0960613\Quadrupole=20.729
5385,-10.0463134,-10.6832251,2.3051958,0.4258269,0.1809249\PG=C01 [X(C
9H16N1O2)]\@\
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tert-butyl diethylcarbamate cation (6):

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1\1\GINC-HER03-29\FOpt\RB3LYP\6-31G(d,p)\C9H18N1O2(1+)\LHAYA\26-Nov-20
10\0\#opt freq b3lyp/6-31g(d,p) geom=connectivity\231110_11\1,1N,1
.6099845354,0.1359120132,-0.2370575116\C,1.9435109246,1.3793698821,-0.
1018675708\C,2.6282192249,-0.8734312687,-0.6987482987\H,2.9645339992,1
.6036435235,-0.4134585668\H,3.262599359,-0.3562296897,-1.422042836\H,2
.0735422239,-1.6538552726,-1.2189306098\C,0.2758635784,-0.4618514614,0
.1329929533\O,-0.6772059989,0.3870123226,-0.1211748669\O,0.2685441833,
-1.5890413731,0.5428038641\C,-2.1623512195,0.0046248071,0.0977477726\C
,-2.3627034077,-0.2927730253,1.5787662134\C,-2.4786906975,-1.175990139
7,-0.8126738291\C,-2.8712933815,1.2784427303,-0.3427829133\H,-2.064537
2515,0.5588616109,2.1971470392\H,-3.4276528233,-0.4712099404,1.7536786
923\H,-1.8159972795,-1.1820544392,1.8952927846\H,-1.9458309911,-2.0790
827814,-0.5124234552\H,-3.5514102643,-1.3806086136,-0.7505601423\H,-2.
2444371966,-0.9409170886,-1.8545594111\H,-2.6494062962,1.5145211506,-1
.3865026587\H,-3.9507702311,1.1337237046,-0.2491268015\H,-2.5905113036
,2.1291056796,0.2839414235\C,3.4362872812,-1.4457690785,0.462267961\H,
3.9958866539,-0.6633679088,0.9835849267\H,2.7906519805,-1.9644384753,1
.1719403515\H,4.1558330573,-2.1648631874,0.0616339076\C,1.151677424,2.
5123503025,0.4237735375\H,0.2642237971,2.2192793091,0.9765114834\H,1.8
113485971,3.1354657433,1.0362144622\H,0.8441365224,3.1366619644,-0.427
8569011\Version=EM64L-G09RevA.02\State=1-A\HF=-558.804303\RMSD=6.363e
-09\RMSF=4.348e-06\Dipole=1.5004176,1.4305832,-0.4281919\Quadrupole=13
.6046514,-3.5363863,-10.068265,2.6012067,-2.4099036,1.7541292\PG=C01 [
X(C9H18N1O2)]\@\
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1-tert-butyl 2-methyl (S)-pyrrolidine-1,2-dicarboxylate cation (7):

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1\1\GINC-HER03-42\FOpt\RB3LYP\6-31G(d,p)\C11H18N1O4(1+)\URIETA\15-Dec-20
2010\0\#opt freq b3lyp/6-31g(d,p) maxdisk=3000MB geom=connectivity\1
51210_18\1,1N,-0.3549255217,0.9064553896,0.2795139378\C,-0.345159379
9,1.9898504185,-0.4218138865\C,-1.6760808815,2.6434330241,-0.471346472
5\C,-2.4771064917,1.8808730819,0.6131774131\C,-1.7139427453,0.54143535
45,0.7678956879\H,0.5703148296,2.3153374587,-0.9060732182\H,-1.6059065
358,3.7245414771,-0.3156903187\H,-2.0762664913,2.4998378172,-1.4864052
236\H,-2.4540247773,2.4297576037,1.5574317586\H,-3.521173004,1.7239588
061,0.341077589\H,-1.6532061122,0.1693123458,1.7895909066\C,0.77354967
,-0.0468068235,0.4598584705\O,1.836978106,0.4399119356,-0.1087437701\O
,0.5509337767,-1.0565118166,1.0695380499\C,3.1735989343,-0.3342311704,
-0.1104655073\C,2.9497566709,-1.6513631992,-0.8435250603\C,3.618108706
2,-0.5048257765,1.3370808103\C,4.0742725667,0.6173336557,-0.8865900105
\H,2.5544413011,-1.4788514226,-1.8482410465\H,3.9135923196,-2.15861104
38,-0.9451376114\H,2.2759174549,-2.3128451026,-0.2971295737\H,2.945205
1536,-1.1562675165,1.8966390533\H,4.6119312897,-0.9617387413,1.3412367
474\H,3.6934169669,0.4626006009,1.8412439257\H,4.163753986,1.580951731
4,-0.3782401695\H,5.0732022846,0.1797901376,-0.9620489978\H,3.69821799
9,0.7798042088,-1.9000728623\C,-2.2500088349,-0.5505954794,-0.17558307
19\O,-1.8630853322,-0.6701739223,-1.3169955407\O,-3.1967102593,-1.2511
878165,0.4293289662\C,-3.8366277399,-2.2890116884,-0.3644581917\H,-4.5
774844456,-2.7346781251,0.2954056427\H,-4.3079930302,-1.8477056462,-1.
2438602329\H,-3.093141433,-3.0251557561,-0.6727721929\Version=EM64L-G
09RevA.02\State=1-A\HF=-785.4742574\RMSD=7.690e-09\RMSF=8.679e-06\Dipo
le=-0.4778347,1.8964871,-0.0443845\Quadrupole=16.2784975,0.2345667,-16
.5130642,-2.1281131,-1.1963394,-0.0528031\PG=C01 [X(C11H18N1O4)]\@\
```

1.6 Optimized geometries at B3LYP/6-311++G(2df,2p) level:

104623,-0.9278782201\H,2.3039991178,-2.3261275026,-0.2671734394\H,2.96
67285245,-1.1353214593,1.9000568028\H,4.6200817252,-0.9225624887,1.336
4287142\H,3.6864482619,0.4876041056,1.821171225\H,4.1522135798,1.57140
44322,-0.4119413362\H,5.0627915317,0.171735165,-0.9744909879\H,3.68890
01075,0.7484762466,-1.9148504243\C,-2.2606047976,-0.5644738965,-0.1907
453582\O,-1.8784375145,-0.7059674469,-1.3234820209\O,-3.2061598662,-1.
2509803645,0.4212822443\C,-3.8584215796,-2.2987558125,-0.3464535505\H,
-4.5899718105,-2.7289405676,0.3267946117\H,-4.3371098717,-1.8703157877
, -1.2228291137\H,-3.1230714878,-3.0390112987,-0.6487912625\\Version=EM
64L-G09RevA.02\State=1-A\HF=-785.7160747\RMSD=6.424e-09\RMSF=6.796e-06
\Dipole=-0.4408695,1.9246246,0.0061311\Quadrupole=16.7862704,0.4435216
, -17.229792,-2.1812105,-1.3925581,-0.0026938\PG=C01 [X(C11H18N1O4)]\@