What defines electrophilicity in carbonyl compounds

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Contents:

Cartesian coordinates (in Å) and total energies (in a.u., noncorrected ZVPE included) of all the stationary points discussed in the text. All calculations have been performed at the M06-2X/6-311+G* level.

1-CH2: E= -309.672580

C	-1.075964746	0.100167117	0.000000000
C	-0.313242819	0.387342776	1.279380000
C	1.065102558	-0.292234474	1.259683000
C	1.848321517	0.078874561	0.000000000
C	1.065102558	-0.292234474	-1.259683000
C	-0.313242819	0.387342776	-1.279380000
H	-0.919977037	0.067845271	2.127187000
H	-0.174822407	1.473705998	1.349963000
H	1.623258815	-0.016121957	2.157542000
H	0.929602112	-1.378949017	1.295446000
H	2.819730769	-0.422367863	0.000000000
H	2.049837861	1.157239534	0.000000000
H	1.623258815	-0.016121957	-2.157542000
H	0.929602112	-1.378949017	-1.295446000
H	-0.919977037	0.067845271	-2.127187000
H	-0.174822407	1.473705998	-1.349963000
O	-2.198169894	-0.341794635	0.000000000

1-NMe: E= -364.983851

C	0.137107000	-0.859512000	1.197234000
C	0.137107000	0.686898000	1.269806000
C	0.736120000	1.252945000	0.000000000
C	0.137107000	0.686898000	-1.269806000
C	0.137107000	-0.859512000	-1.197234000
N	-0.495698000	-1.389700000	0.000000000
H	-0.361114000	-1.275263000	2.075736000
H	1.172781000	-1.213624000	1.217280000
H	0.704895000	1.048496000	2.128006000
H	-0.893307000	1.048054000	1.363225000
O	1.647355000	2.043811000	0.000000000
H	0.704895000	1.048496000	-2.128006000
H	-0.893307000	1.048054000	-1.363225000
H	-0.361114000	-1.275263000	-2.075736000
H	1.172781000	-1.213624000	-1.217280000
C	-1.942585000	-1.258386000	0.000000000
H	-2.348627000	-1.756743000	-0.882291000
H	-2.348627000	-1.756743000	0.882291000
H	-2.309992000	-0.220400000	0.000000000

1-C(O2C2H4): E= -537.462334

C	-0.238209000	1.181354000	-0.700706000
C	-1.509412000	1.304860000	0.148660000
C	-2.306173000	0.013067000	0.151009000
C	-1.503869000	-1.230387000	0.485997000
C	-0.245455000	-1.319542000	-0.385985000

C	0.576954000	-0.040728000	-0.296286000
H	0.387378000	2.070575000	-0.591073000
H	-0.488087000	1.088311000	-1.761525000
H	-2.152595000	2.114199000	-0.196574000
H	-1.218785000	1.512570000	1.184721000
O	-3.486062000	-0.021586000	-0.094243000
H	-2.143852000	-2.104903000	0.369685000
H	-1.199671000	-1.159815000	1.536390000
H	0.379747000	-2.160861000	-0.078016000
H	-0.515714000	-1.471925000	-1.434815000
O	1.725345000	-0.116974000	-1.126882000
C	2.857972000	-0.299639000	-0.293705000
H	3.037305000	-1.365072000	-0.111008000
H	3.723437000	0.139648000	-0.788008000
O	1.051278000	0.095082000	1.042163000
C	2.431306000	0.414264000	0.978194000
H	2.575829000	1.497328000	0.894352000
H	2.911845000	0.048272000	1.884494000

1-O: E= -345.598379

C	0.395062000	1.066498000	0.000000000
C	-0.180283000	0.470486000	-1.268470000
C	-0.180283000	-1.061040000	-1.168646000
O	-0.838604000	-1.498173000	0.000000000
C	-0.180283000	-1.061040000	1.168646000
C	-0.180283000	0.470486000	1.268470000
H	0.393023000	0.820660000	-2.127754000
H	-1.216360000	0.810652000	-1.371195000
H	-0.710300000	-1.505292000	-2.010617000
H	0.852290000	-1.437718000	-1.176023000
H	-0.710300000	-1.505292000	2.010617000
H	0.852290000	-1.437718000	1.176023000
H	0.393023000	0.820660000	2.127754000
H	-1.216360000	0.810652000	1.371195000
O	1.253494000	1.912055000	0.000000000

1-S: E= -668.580510

C	-0.594012000	1.282413000	0.000000000
C	0.017383000	0.768820000	1.291423000
C	0.017383000	-0.762376000	1.356210000
S	0.961511000	-1.518311000	0.000000000
C	0.017383000	-0.762376000	-1.356210000
C	0.017383000	0.768820000	-1.291423000
H	-0.550321000	1.191301000	2.122756000
H	1.050723000	1.125372000	1.353786000
H	0.482335000	-1.104200000	2.281185000
H	-1.004796000	-1.149017000	1.338268000
H	0.482335000	-1.104200000	-2.281185000
H	-1.004796000	-1.149017000	-1.338268000
H	-0.550321000	1.191301000	-2.122756000

H	1.050723000	1.125372000	-1.353786000
O	-1.524149000	2.049282000	0.000000000

1-PMe: E= -651.603624

C	0.257249000	-0.609785000	1.402406000
C	0.257249000	0.924606000	1.288023000
C	0.907472000	1.392420000	0.000000000
C	0.257249000	0.924606000	-1.288023000
C	0.257249000	-0.609785000	-1.402406000
P	-0.521968000	-1.553761000	0.000000000
H	-0.240022000	-0.915273000	2.326985000
H	1.288087000	-0.968831000	1.482498000
H	0.799646000	1.374081000	2.121678000
H	-0.771406000	1.298956000	1.317138000
O	1.899844000	2.078423000	0.000000000
H	0.799646000	1.374081000	-2.121678000
H	-0.771406000	1.298956000	-1.317138000
H	-0.240022000	-0.915273000	-2.326985000
H	1.288087000	-0.968831000	-1.482498000
C	-2.225557000	-0.822244000	0.000000000
H	-2.763251000	-1.182947000	-0.879169000
H	-2.763251000	-1.182947000	0.879169000
H	-2.260809000	0.268158000	0.000000000

1-C(Me2): E= -388.224670

C	-0.354997000	-1.250404000	-0.395865000
C	1.018945000	-1.279397000	0.290436000
C	1.788709000	-0.000043000	0.026302000
C	1.018978000	1.279369000	0.290372000
C	-0.355428000	1.250974000	-0.394934000
C	-1.185346000	0.000000000	-0.057749000
H	-0.918150000	-2.150896000	-0.130077000
H	-0.204769000	-1.286692000	-1.481293000
H	1.621713000	-2.122412000	-0.049080000
H	0.893051000	-1.378853000	1.374853000
O	2.925256000	-0.000028000	-0.377840000
H	1.621835000	2.122224000	-0.049382000
H	0.893885000	1.378828000	1.374927000
H	-0.918476000	2.151060000	-0.127543000
H	-0.206029000	1.288716000	-1.480415000
C	-2.453622000	0.000039000	-0.913635000
H	-3.064626000	0.883744000	-0.708731000
H	-2.210180000	-0.000038000	-1.979733000
H	-3.064852000	-0.883463000	-0.708602000
C	-1.595147000	-0.000546000	1.419565000
H	-2.198680000	0.881985000	1.650120000
H	-2.197394000	-0.883982000	1.649951000
H	-0.741929000	0.000042000	2.100762000

1-TS-CH2: E= -402.524952 (i = -214 cm-1)

C	1.214599000	-0.438580000	-1.260771000
C	0.175272000	0.682340000	-1.282324000
C	-0.666530000	0.837480000	0.000042000
C	0.175214000	0.682121000	1.282421000
C	1.214552000	-0.438786000	1.260729000
C	2.079715000	-0.366843000	0.000001000
H	1.846540000	-0.380212000	-2.155470000
H	0.704099000	-1.405720000	-1.290035000
H	-0.514818000	0.581695000	-2.122552000
H	0.684166000	1.650838000	-1.398229000
O	-1.559765000	1.706058000	0.000098000
H	-0.514920000	0.581322000	2.122595000
H	0.684092000	1.650603000	1.398524000
H	1.846461000	-0.380544000	2.155458000
H	0.704063000	-1.405936000	1.289833000
H	2.819839000	-1.175460000	-0.000052000
H	2.642696000	0.577447000	0.000088000
C	-1.479176000	-0.985513000	-0.000102000
N	-2.100854000	-1.967972000	-0.000131000

1-TS-NMe: E= -457.838463 (i = -219 cm-1)

C	0.804572000	0.691725000	1.199908000
C	-0.046140000	-0.580120000	1.278803000
C	-0.850419000	-0.892455000	-0.000022000
C	-0.046218000	-0.579963000	-1.278865000
C	0.804598000	0.691816000	-1.199895000
N	1.643512000	0.775564000	0.000030000
H	1.457666000	0.775202000	2.076626000
H	0.146453000	1.564393000	1.198026000
H	-0.743042000	-0.535464000	2.118432000
H	0.591813000	-1.459315000	1.440468000
O	-1.572588000	-1.907385000	-0.000066000
H	-0.743215000	-0.535091000	-2.118405000
H	0.591638000	-1.459185000	-1.440766000
H	1.457756000	0.775203000	-2.076576000
H	0.146563000	1.564548000	-1.198075000
C	-1.973769000	0.748956000	0.000074000
N	-2.770993000	1.594763000	0.000069000
C	2.720655000	-0.195768000	0.000012000
H	3.345354000	-0.040365000	-0.884891000
H	3.345423000	-0.040328000	0.884862000
H	2.396979000	-1.247951000	0.000041000

1-TS-C(O2C2H4): E= -630.317065 (i = -216 cm-1)

C	-0.026126000	0.359846000	1.395072000
C	-1.137919000	-0.685766000	1.306872000
C	-1.850280000	-0.788861000	-0.056644000
C	-0.859168000	-0.724780000	-1.237170000
C	0.238968000	0.328704000	-1.107402000

C	0.944518000	0.229158000	0.243100000
H	0.543403000	0.261448000	2.324083000
H	-0.449661000	1.366117000	1.356359000
H	-1.898134000	-0.514439000	2.070601000
H	-0.715701000	-1.683243000	1.481199000
O	-2.804235000	-1.583995000	-0.149861000
H	-1.436248000	-0.586078000	-2.152886000
H	-0.406847000	-1.723914000	-1.280022000
H	0.972664000	0.224188000	-1.916691000
H	-0.186614000	1.332212000	-1.180592000
C	-2.506796000	1.083909000	-0.163160000
N	-3.053099000	2.105897000	-0.252138000
O	1.968205000	1.215014000	0.360600000
C	3.107677000	0.702718000	-0.293548000
H	3.196648000	1.109829000	-1.306987000
H	3.989665000	0.993479000	0.280580000
O	1.656575000	-1.003386000	0.362759000
C	2.877991000	-0.829106000	-0.316402000
H	3.648167000	-1.386882000	0.219423000
H	2.816809000	-1.209987000	-1.342400000

1-TS-O: E= -438.456850 (i = -213 cm-1)

C	-1.238887000	0.478468000	-1.171824000
C	-0.228832000	-0.656875000	-1.269876000
C	0.620505000	-0.855877000	0.000050000
C	-0.228764000	-0.656672000	1.269990000
C	-1.238823000	0.478655000	1.171810000
O	-2.035517000	0.373361000	0.000022000
H	-1.939308000	0.456565000	-2.011219000
H	-0.723134000	1.446735000	-1.175524000
H	0.440945000	-0.519864000	-2.121564000
H	-0.764997000	-1.604210000	-1.411008000
O	1.477426000	-1.757067000	0.000100000
H	0.441058000	-0.519525000	2.121621000
H	-0.764919000	-1.603986000	1.411301000
H	-1.939201000	0.456888000	2.011246000
H	-0.723070000	1.446922000	1.175327000
C	1.507768000	0.935368000	-0.000115000
N	2.182793000	1.881674000	-0.000196000

1-TS-S: E= -761.441775 (i = -209 cm.1)

C	-0.936683000	0.319168000	-1.365915000
C	0.156743000	-0.738906000	-1.295472000
C	0.989536000	-0.806760000	0.000049000
C	0.156784000	-0.738691000	1.295586000
C	-0.936640000	0.319395000	1.365887000
S	-2.137470000	0.174583000	0.000018000
H	-1.520565000	0.217257000	-2.283974000
H	-0.508685000	1.322258000	-1.342283000
H	0.865594000	-0.604602000	-2.116888000

H	-0.292330000	-1.733980000	-1.403751000
O	1.959052000	-1.586974000	0.000099000
H	0.865660000	-0.604253000	2.116957000
H	-0.292286000	-1.733748000	1.404042000
H	-1.520492000	0.217636000	2.283983000
H	-0.508642000	1.322480000	1.342075000
C	1.626044000	1.087633000	-0.000115000
N	2.157735000	2.121198000	-0.000194000

1-TS-PMe: E= -744.461905 (i = -208 cm-1)

C	0.551226000	-0.553038000	-1.407267000
C	-0.316011000	0.701890000	-1.299574000
C	-1.115838000	0.917416000	0.000191000
C	-0.317358000	0.699840000	1.300480000
C	0.551428000	-0.554254000	1.406893000
P	1.722181000	-0.865244000	-0.000428000
H	1.145288000	-0.532646000	-2.328397000
H	-0.087213000	-1.438490000	-1.465246000
H	-1.042628000	0.731809000	-2.115434000
H	0.302592000	1.602644000	-1.405581000
O	-1.928232000	1.860906000	0.000562000
H	-1.045243000	0.726644000	2.115312000
H	0.299700000	1.601259000	1.409703000
H	1.146251000	-0.533141000	2.327536000
H	-0.085925000	-1.440440000	1.465542000
C	-2.083666000	-0.839073000	-0.001040000
N	-2.782223000	-1.768228000	-0.000620000
C	2.683701000	0.729509000	0.000505000
H	3.331039000	0.755150000	0.880760000
H	3.325692000	0.759390000	-0.883543000
H	2.058264000	1.623088000	0.004491000

1-TS-C(Me2): E= -481.078350 (i = -218 cm-1)

C	-0.647031000	0.276781000	-1.253179000
C	0.520199000	-0.709513000	-1.281936000
C	1.375019000	-0.764320000	0.000018000
C	0.520205000	-0.709502000	1.281972000
C	-0.646920000	0.276897000	1.253212000
C	-1.532014000	0.146085000	0.000076000
H	-1.272390000	0.148091000	-2.147761000
H	-0.247864000	1.295376000	-1.287781000
H	1.190843000	-0.500486000	-2.117803000
H	0.154241000	-1.735273000	-1.423765000
O	2.365052000	-1.522308000	0.000011000
H	1.190861000	-0.500600000	2.117860000
H	0.154101000	-1.735223000	1.423726000
H	-1.272204000	0.148423000	2.147875000
H	-0.247673000	1.295470000	1.287586000
C	1.957531000	1.134532000	-0.000016000
N	2.446100000	2.189294000	-0.000083000

C	-2.568010000	1.272108000	0.000014000
H	-3.210911000	1.216962000	0.885574000
H	-2.076218000	2.248959000	0.000455000
H	-3.210112000	1.217357000	-0.886179000
C	-2.274887000	-1.195433000	-0.000006000
H	-2.913391000	-1.282904000	0.886144000
H	-2.914698000	-1.281829000	-0.885348000
H	-1.592256000	-2.046725000	-0.001020000

Me_2S=CH-CN: E= -609.339470

C	-0.724267000	0.000776000	-1.074065000
H	-0.892399000	0.000630000	-2.136483000
C	-1.734623000	0.000190000	-0.108057000
N	-2.500221000	-0.000393000	0.764165000
S	0.874037000	0.000148000	-0.555776000
C	1.055731000	1.362928000	0.638130000
H	0.979300000	2.287868000	0.071041000
H	0.242736000	1.300386000	1.362308000
H	2.026034000	1.294088000	1.129031000
C	1.055485000	-1.363571000	0.637106000
H	2.025905000	-1.295066000	1.127791000
H	0.242639000	-1.301347000	1.361472000
H	0.978780000	-2.288121000	0.069418000

Me_2S=CH-CO_2Me: E= -744.916589

C	0.121475000	-1.299746000	0.000099000
H	0.206709000	-2.373825000	-0.000259000
S	1.593014000	-0.485782000	-0.000050000
C	1.639487000	0.711608000	-1.370315000
H	2.575865000	1.267214000	-1.319467000
H	1.594920000	0.130180000	-2.288648000
H	0.777687000	1.370120000	-1.292936000
C	1.639751000	0.711549000	1.370240000
H	2.576015000	1.267303000	1.319057000
H	0.777785000	1.369863000	1.293145000
H	1.595624000	0.130124000	2.288597000
C	-1.166429000	-0.692671000	0.000057000
O	-2.235989000	-1.260713000	-0.000045000
O	-1.104772000	0.691424000	0.000144000
C	-2.370235000	1.339797000	0.000007000
H	-2.945454000	1.066120000	-0.884763000
H	-2.944382000	1.068442000	0.886221000
H	-2.161192000	2.408058000	-0.001467000

Me_2S=CH-*p*(NO_2)C_6H_4: E= -952.508270

C	1.871671000	-1.197570000	-0.000088000
H	2.089321000	-2.255434000	-0.000391000
S	3.284747000	-0.293564000	0.000010000

C	3.320501000	0.903517000	-1.381867000
H	4.250810000	1.467780000	-1.318148000
H	3.303289000	0.311433000	-2.294129000
H	2.463921000	1.572073000	-1.356239000
C	3.320064000	0.903169000	1.382139000
H	4.250229000	1.467704000	1.318763000
H	2.463308000	1.571506000	1.356562000
H	3.302820000	0.310828000	2.294236000
C	0.522641000	-0.738763000	-0.000077000
C	-0.516029000	-1.707661000	-0.000067000
C	0.120171000	0.619190000	-0.000103000
C	-1.845129000	-1.353091000	-0.000035000
C	-1.212880000	0.983189000	-0.000066000
C	-2.192374000	-0.001495000	-0.000031000
H	-0.246951000	-2.758215000	-0.000060000
H	0.855945000	1.412740000	-0.000186000
H	-2.625485000	-2.103017000	-0.000012000
H	-1.507519000	2.024703000	-0.000086000
N	-3.594699000	0.382541000	0.000022000
O	-3.862038000	1.570838000	0.000041000
O	-4.428534000	-0.504060000	0.000027000

[Cl-CH-SO_2Ph]$^-$: E= -1278.957760

C	-2.034909000	0.036078000	-0.844159000
H	-1.655981000	-0.167263000	-1.844826000
Cl	-1.885283000	1.818897000	-0.557236000
S	-1.073561000	-0.850337000	0.260077000
O	-1.440693000	-0.556556000	1.649637000
O	-1.069700000	-2.248122000	-0.202826000
C	0.667890000	-0.343501000	0.166743000
C	1.520838000	-0.977305000	-0.732144000
C	1.113085000	0.738343000	0.920799000
C	2.829922000	-0.529545000	-0.873244000
C	2.422283000	1.187544000	0.769727000
C	3.282338000	0.555733000	-0.124482000
H	1.147046000	-1.825769000	-1.295298000
H	0.431434000	1.203436000	1.623360000
H	3.501637000	-1.030146000	-1.563649000
H	2.773576000	2.031353000	1.355103000
H	4.303536000	0.905860000	-0.236844000

Me_2S=CH-CN, TS(1-CH_2): E= -919.001503 (i = -240 cm-1)

C	2.462546000	1.204571000	0.367624000
C	1.544198000	0.403243000	1.291378000
C	0.728178000	-0.699200000	0.606914000
C	1.558423000	-1.495048000	-0.417273000
C	2.497005000	-0.673462000	-1.302159000
C	3.350400000	0.279291000	-0.464596000
H	3.074318000	1.889175000	0.961887000
H	1.872222000	1.837196000	-0.306062000

H	0.864698000	1.052500000	1.851346000
H	2.148207000	-0.127226000	2.037768000
O	-0.027576000	-1.407157000	1.364763000
H	0.882081000	-2.125810000	-1.005089000
H	2.149331000	-2.184936000	0.197010000
H	3.132722000	-1.344778000	-1.887137000
H	1.929936000	-0.083651000	-2.034041000
H	4.012756000	0.863120000	-1.110126000
H	3.993909000	-0.305665000	0.204018000
C	-0.433642000	0.243078000	-0.533912000
H	-0.160177000	0.104267000	-1.579997000
C	-0.715421000	1.618906000	-0.246700000
N	-0.961159000	2.706054000	0.054710000
S	-1.921325000	-0.759174000	-0.269626000
C	-2.559224000	-0.184743000	1.320091000
H	-1.818467000	-0.503265000	2.050159000
H	-2.679676000	0.897791000	1.290327000
H	-3.516173000	-0.683454000	1.469357000
C	-3.120694000	0.062058000	-1.356268000
H	-4.096888000	-0.388126000	-1.177604000
H	-3.148366000	1.132297000	-1.152520000
H	-2.821118000	-0.119945000	-2.386944000

Me_2S=CH-CN, TS(1-S): E= -1277.911178 (i = -240 cm-1)

C	2.195377000	1.261496000	0.367712000
C	1.271988000	0.528566000	1.334389000
C	0.447141000	-0.625836000	0.754808000
C	1.253288000	-1.586357000	-0.141158000
C	2.208486000	-0.976539000	-1.161853000
S	3.413434000	0.153840000	-0.405949000
H	2.772917000	2.022597000	0.894429000
H	1.640961000	1.775893000	-0.422093000
H	0.582487000	1.233301000	1.810677000
H	1.868409000	0.078307000	2.134149000
O	-0.346080000	-1.209921000	1.572134000
H	0.544130000	-2.263506000	-0.633195000
H	1.824672000	-2.200557000	0.561654000
H	2.792972000	-1.759186000	-1.648637000
H	1.683553000	-0.435666000	-1.955428000
C	-0.662309000	0.213943000	-0.522985000
H	-0.349478000	0.001370000	-1.545552000
C	-0.953171000	1.606365000	-0.347374000
N	-1.201544000	2.713615000	-0.134612000
S	-2.160508000	-0.769984000	-0.249366000
C	-2.896385000	-0.061014000	1.240613000
H	-2.199735000	-0.299386000	2.040901000
H	-3.023651000	1.012446000	1.104295000
H	-3.856269000	-0.557756000	1.377087000
C	-3.296575000	-0.066548000	-1.476480000
H	-4.280353000	-0.505532000	-1.312361000
H	-3.338041000	1.017785000	-1.375409000

H	-2.936989000	-0.342186000	-2.466290000

Me_2S=CH-CO_2Me, TS(1-CH2): E= -1054.571550 (i = -258 cm-1)

C	2.548809000	1.336778000	0.103214000
C	1.646288000	0.710306000	1.169239000
C	0.996370000	-0.630841000	0.796177000
C	1.967173000	-1.556427000	0.032723000
C	2.866815000	-0.888797000	-1.007403000
C	3.574783000	0.328388000	-0.413156000
H	3.054371000	2.211341000	0.524256000
H	1.952858000	1.701027000	-0.738584000
H	0.865223000	1.399906000	1.506525000
H	2.242260000	0.476439000	2.060360000
O	0.320911000	-1.207800000	1.720305000
H	1.402014000	-2.395491000	-0.387902000
H	2.591757000	-1.987589000	0.824378000
H	3.595953000	-1.614459000	-1.380878000
H	2.287077000	-0.564494000	-1.880510000
H	4.223088000	0.794607000	-1.160768000
H	4.221973000	0.003847000	0.411369000
C	-0.236457000	-0.200159000	-0.564044000
H	0.191055000	-0.427841000	-1.539607000
S	-1.422970000	-1.516284000	-0.269799000
C	-2.407811000	-1.173422000	1.213137000
H	-2.841492000	-2.132138000	1.495114000
H	-1.693936000	-0.840323000	1.962301000
H	-3.168341000	-0.432589000	0.987445000
C	-2.680676000	-1.198705000	-1.535155000
H	-3.489979000	-1.915525000	-1.396311000
H	-3.053782000	-0.179628000	-1.438798000
H	-2.224238000	-1.344993000	-2.512208000
C	-0.748722000	1.181579000	-0.564950000
O	-0.338476000	2.059362000	-1.284271000
O	-1.683723000	1.409154000	0.385970000
C	-2.070669000	2.774192000	0.542210000
H	-1.204367000	3.382992000	0.800328000
H	-2.511675000	3.156919000	-0.378219000
H	-2.797420000	2.785464000	1.350499000

Me_2S=CH-CO_2Me, TS(1-S): E= -1413.481470 (i = -253 cm-1)

C	2.305023000	1.331666000	0.198929000
C	1.392663000	0.678424000	1.233774000
C	0.726350000	-0.652571000	0.850638000
C	1.676422000	-1.641682000	0.140697000
C	2.608999000	-1.095852000	-0.934672000
S	3.669338000	0.240888000	-0.310623000
H	2.773868000	2.223968000	0.617555000
H	1.761553000	1.639916000	-0.695072000
H	0.605360000	1.373160000	1.549170000

H	1.974155000	0.445147000	2.131570000
O	0.010455000	-1.189778000	1.766142000
H	1.073991000	-2.468703000	-0.254158000
H	2.278626000	-2.063143000	0.951443000
H	3.280776000	-1.880268000	-1.287780000
H	2.068795000	-0.720260000	-1.808814000
C	-0.460348000	-0.208730000	-0.548150000
H	-0.018815000	-0.451194000	-1.514163000
S	-1.685568000	-1.496139000	-0.277112000
C	-2.704044000	-1.121704000	1.175572000
H	-3.163990000	-2.069676000	1.452103000
H	-2.005944000	-0.796021000	1.942609000
H	-3.443319000	-0.368385000	0.922502000
C	-2.898158000	-1.162442000	-1.581040000
H	-3.725299000	-1.861890000	-1.460344000
H	-3.253033000	-0.135445000	-1.502120000
H	-2.416853000	-1.325705000	-2.543334000
C	-0.941644000	1.184885000	-0.569840000
O	-0.479902000	2.050835000	-1.272129000
O	-1.908189000	1.435674000	0.340811000
C	-2.272776000	2.809862000	0.477557000
H	-1.405269000	3.400999000	0.770069000
H	-2.666712000	3.197882000	-0.461644000
H	-3.032028000	2.838648000	1.254770000

Me_2S=CH-*p*(NO_2)C_6H_4, TS(1-CH2): E= -1262.173388 (i = -245 cm-1)

C	-1.936539000	-2.629328000	-0.390685000
C	-1.517331000	-1.909908000	0.891878000
C	-1.993422000	-0.455696000	1.028780000
C	-3.466243000	-0.295086000	0.603806000
C	-3.880255000	-1.023849000	-0.675440000
C	-3.440029000	-2.489731000	-0.641322000
H	-1.668712000	-3.687677000	-0.320263000
H	-1.379751000	-2.239934000	-1.251301000
H	-0.437001000	-1.947735000	1.052245000
H	-1.968205000	-2.417701000	1.754321000
O	-1.639208000	0.159251000	2.079009000
H	-3.729856000	0.767555000	0.572964000
H	-4.030046000	-0.709355000	1.449666000
H	-4.966282000	-0.964734000	-0.795499000
H	-3.456915000	-0.531009000	-1.558597000
C	-1.031754000	0.342315000	-0.491676000
H	-1.392799000	-0.075073000	-1.431005000
S	-1.567285000	2.034961000	-0.601338000
C	-1.312354000	2.818402000	1.010269000
H	-1.828328000	3.776714000	0.973133000
H	-1.734398000	2.136727000	1.753575000
H	-0.246328000	2.957620000	1.182880000
C	-0.307979000	2.921163000	-1.558899000
H	-0.555117000	3.982559000	-1.544699000
H	0.672552000	2.742059000	-1.118452000

H	-0.340165000	2.542888000	-2.579087000
C	0.422546000	0.147681000	-0.323821000
C	1.168412000	-0.469206000	-1.340965000
C	1.077104000	0.499427000	0.869880000
C	2.525714000	-0.707856000	-1.196548000
C	2.437629000	0.274080000	1.022815000
C	3.142727000	-0.316063000	-0.016542000
H	0.673108000	-0.762251000	-2.261222000
H	0.489797000	0.871990000	1.699600000
H	3.107654000	-1.177965000	-1.978163000
H	2.951370000	0.531073000	1.939879000
N	4.589244000	-0.543739000	0.138260000
O	5.113427000	-0.158199000	1.161613000
O	5.171199000	-1.100427000	-0.769346000
H	-3.980347000	-2.999773000	0.165657000
H	-3.721083000	-2.992243000	-1.571430000

Me_2S=CH-*p*(NO_2)C_6H_4, TS(1-S): E= -1621.083492 (i = -240 cm-1)

C	-1.832676000	-2.396302000	-0.154475000
C	-1.463371000	-1.616518000	1.101401000
C	-1.832979000	-0.127209000	1.143308000
C	-3.294507000	0.148271000	0.744436000
C	-3.810823000	-0.488013000	-0.540533000
S	-3.604277000	-2.296407000	-0.567157000
H	-1.641271000	-3.460571000	-0.005534000
H	-1.237421000	-2.090433000	-1.017520000
H	-0.392264000	-1.705466000	1.305137000
H	-1.982414000	-2.053186000	1.961765000
O	-1.407855000	0.517024000	2.144927000
H	-3.455201000	1.232497000	0.723506000
H	-3.883902000	-0.226226000	1.588785000
H	-4.886891000	-0.328261000	-0.632648000
H	-3.353440000	-0.050457000	-1.431095000
C	-0.836296000	0.498628000	-0.456094000
H	-1.246055000	0.059072000	-1.365823000
S	-1.238266000	2.219361000	-0.656001000
C	-0.863887000	3.071568000	0.896011000
H	-1.286353000	4.071539000	0.809043000
H	-1.327814000	2.485027000	1.692643000
H	0.215091000	3.116910000	1.034765000
C	0.054135000	2.942348000	-1.702874000
H	-0.107893000	4.019161000	-1.747616000
H	1.031638000	2.711234000	-1.280281000
H	-0.042468000	2.507866000	-2.696251000
C	0.603386000	0.200398000	-0.303209000
C	1.283278000	-0.506907000	-1.308007000
C	1.305172000	0.549314000	0.864060000
C	2.622469000	-0.838385000	-1.176836000
C	2.648760000	0.231087000	1.003183000
C	3.288527000	-0.448491000	-0.023425000
H	0.751821000	-0.795621000	-2.209449000

H	0.764499000	0.998682000	1.687471000
H	3.153858000	-1.378372000	-1.949286000
H	3.197769000	0.485357000	1.900376000
N	4.718097000	-0.775901000	0.116791000
O	5.286717000	-0.393470000	1.116989000
O	5.240589000	-1.405234000	-0.778999000

[Cl-CH-SO_2Ph]$^-$, TS(1-CH2): E= -1588.635571 (i = -185 cm-1)

C	2.888730000	1.705101000	0.393770000
C	2.754176000	0.378592000	1.145129000
C	2.311605000	-0.838276000	0.301530000
C	3.019425000	-0.845371000	-1.084045000
C	3.186473000	0.499776000	-1.794931000
C	3.766151000	1.553463000	-0.849910000
H	3.309421000	2.465761000	1.061877000
H	1.900019000	2.072431000	0.105360000
H	2.097878000	0.468378000	2.013444000
H	3.739992000	0.085138000	1.532456000
O	2.274114000	-1.952577000	0.885009000
H	2.526201000	-1.586823000	-1.717973000
H	4.014495000	-1.250656000	-0.857012000
H	3.834510000	0.378554000	-2.671718000
H	2.224803000	0.858198000	-2.180897000
H	3.871352000	2.514823000	-1.366482000
H	4.776130000	1.244238000	-0.547520000
C	0.545001000	-0.364504000	-0.274310000
H	0.499097000	0.394610000	-1.056602000
Cl	-0.146557000	-1.863065000	-0.955148000
S	-0.553607000	0.258576000	0.983494000
O	-0.660678000	-0.653717000	2.113473000
O	-0.177593000	1.659468000	1.211102000
C	-2.203475000	0.321532000	0.251100000
C	-2.578220000	1.441129000	-0.481017000
C	-3.063987000	-0.756954000	0.413825000
C	-3.838952000	1.478496000	-1.067743000
C	-4.322448000	-0.713070000	-0.177524000
C	-4.709091000	0.401347000	-0.917521000
H	-1.887607000	2.272979000	-0.566973000
H	-2.736754000	-1.607553000	1.000558000
H	-4.145282000	2.350195000	-1.636189000
H	-5.002627000	-1.549842000	-0.060396000
H	-5.691531000	0.431502000	-1.377117000

[Cl-CH-SO_2Ph]$^-$, TS(1-S): E= -1947.551581 (i = -190 cm-1)

C	-2.679872000	1.407711000	-0.815411000
C	-2.534594000	-0.028847000	-1.307290000
C	-2.064703000	-1.088048000	-0.287463000
C	-2.815846000	-0.984587000	1.068228000
C	-3.014415000	0.388168000	1.702418000
S	-3.840559000	1.566393000	0.584626000

H	-3.087170000	2.044611000	-1.604156000
H	-1.719384000	1.833629000	-0.528564000
H	-1.862041000	-0.064025000	-2.168347000
H	-3.511681000	-0.389538000	-1.649790000
O	-1.936853000	-2.259289000	-0.719427000
H	-2.316504000	-1.659546000	1.769290000
H	-3.799504000	-1.418670000	0.856784000
H	-3.660711000	0.314881000	2.580906000
H	-2.072437000	0.828175000	2.038083000
C	-0.331277000	-0.421024000	0.270952000
H	-0.338950000	0.470029000	0.901134000
Cl	0.388797000	-1.738570000	1.236479000
S	0.787505000	0.009200000	-1.046491000
O	0.997103000	-1.096828000	-1.968989000
O	0.339942000	1.311390000	-1.557552000
C	2.392908000	0.320674000	-0.282709000
C	2.665836000	1.581601000	0.232997000
C	3.320837000	-0.710169000	-0.202964000
C	3.892128000	1.812778000	0.847281000
C	4.544284000	-0.471520000	0.414869000
C	4.829188000	0.786324000	0.939617000
H	1.925478000	2.367717000	0.131787000
H	3.073011000	-1.676325000	-0.627170000
H	4.119435000	2.794828000	1.247955000
H	5.276663000	-1.268367000	0.486127000
H	5.784742000	0.968256000	1.420258000

2-NMe2: E= -479.266390

C	3.294272000	0.328609000	-0.009121000
H	3.682565000	1.368066000	-0.014422000
O	4.061596000	-0.603446000	-0.012293000
C	1.829365000	0.215563000	0.001260000
C	1.202869000	-1.035108000	0.006832000
C	1.032253000	1.359694000	0.001484000
C	-0.171673000	-1.141459000	0.015348000
C	-0.348727000	1.275964000	0.009799000
C	-0.988505000	0.016713000	0.021136000
H	1.821797000	-1.925968000	0.003097000
H	1.502725000	2.339299000	-0.006377000
H	-0.620792000	-2.125467000	0.017089000
H	-0.930131000	2.187777000	0.006339000
N	-2.354517000	-0.084227000	0.037880000
C	-2.984926000	-1.387742000	-0.022357000
H	-4.065142000	-1.262868000	-0.009051000
H	-2.715169000	-1.927588000	-0.936727000
H	-2.707387000	-2.005024000	0.837266000
C	-3.166066000	1.114335000	-0.019214000
H	-2.984476000	1.684889000	-0.936957000
H	-4.217266000	0.836783000	0.005410000
H	-2.971046000	1.767846000	0.836518000

2-tBu: E= -502.497414

C	3.589483000	0.311748000	0.000013000
H	3.995274000	1.343590000	0.000074000
O	4.333450000	-0.634806000	-0.000103000
C	2.112256000	0.218987000	0.000014000
C	1.475746000	-1.025115000	0.000045000
C	1.344497000	1.377181000	0.000034000
C	0.095051000	-1.092346000	0.000058000
C	-0.046068000	1.302615000	-0.000020000
C	-0.697421000	0.068527000	-0.000107000
H	2.082427000	-1.924052000	0.000045000
H	1.833624000	2.347388000	0.000086000
H	-0.380529000	-2.067161000	0.000079000
H	-0.615858000	2.222946000	0.000041000
C	-2.220831000	-0.062573000	-0.000018000
C	-2.662224000	-0.833520000	-1.255177000
H	-3.751108000	-0.931899000	-1.271667000
H	-2.353079000	-0.309523000	-2.162916000
H	-2.237208000	-1.838658000	-1.286698000
C	-2.662171000	-0.832615000	1.255699000
H	-2.353022000	-0.307932000	2.163043000
H	-3.751048000	-0.931263000	1.272469000
H	-2.236854000	-1.837597000	1.288067000
C	-2.921361000	1.298697000	-0.000503000
H	-4.003894000	1.151970000	-0.000940000
H	-2.669385000	1.885772000	0.886291000
H	-2.668677000	1.885345000	-0.887376000

2-Me: E= -384.675747

C	-2.512204000	0.365752000	0.001118000
H	-2.874121000	1.413747000	0.001815000
O	-3.295417000	-0.548464000	0.001410000
C	-1.039904000	0.210788000	0.000042000
C	-0.460458000	-1.061372000	-0.000921000
C	-0.225571000	1.339228000	-0.000504000
C	0.916823000	-1.189915000	-0.002384000
C	1.158746000	1.203095000	-0.001915000
C	1.747202000	-0.060341000	-0.002072000
H	-1.108350000	-1.931014000	-0.001283000
H	-0.675554000	2.328032000	-0.000535000
H	1.367458000	-2.177857000	-0.003809000
H	1.788404000	2.086753000	-0.002989000
C	3.243173000	-0.225071000	0.002929000
H	3.575347000	-0.722257000	0.917722000
H	3.571116000	-0.839618000	-0.838580000
H	3.752197000	0.736943000	-0.061381000

2-H: E= -345.397271

C	-1.943735362	0.499939050	0.000000000

H	-2.220008667	1.573494049	0.000000000
O	-2.796287507	-0.348823108	0.000000000
C	-0.485940141	0.225841057	0.000000000
C	-0.017124795	-1.089634265	0.000000000
C	0.412441069	1.290868071	0.000000000
C	1.347927865	-1.332430699	0.000000000
C	1.781527033	1.046811259	0.000000000
C	2.246137206	-0.264403258	0.000000000
H	-0.736787312	-1.900726795	0.000000000
H	0.037527391	2.310351708	0.000000000
H	1.718942960	-2.350912692	0.000000000
H	2.482858877	1.873070052	0.000000000
H	3.313078605	-0.457971847	0.000000000

2-Br: E= -2918.980694

C	3.745450443	-0.335364032	0.000000000
H	4.144501452	-1.369082526	0.000000000
O	4.491085966	0.608122261	0.000000000
C	2.265745153	-0.230048384	0.000000000
C	1.650410050	1.023057992	0.000000000
C	1.490532005	-1.386823577	0.000000000
C	0.268344864	1.119983405	0.000000000
C	0.103123708	-1.305252130	0.000000000
C	-0.490854053	-0.049133179	0.000000000
H	2.271075383	1.912159860	0.000000000
H	1.971937922	-2.360270067	0.000000000
H	-0.221937490	2.085355956	0.000000000
H	-0.508583145	-2.198355407	0.000000000
Br	-2.381506596	0.078326497	0.000000000

2-CF3: E= -682.444151

C	3.536552000	0.314159000	0.010020000
H	3.941952000	1.344941000	0.016096000
O	4.273011000	-0.635043000	0.012512000
C	2.052268000	0.215609000	-0.001093000
C	1.435179000	-1.037130000	-0.010309000
C	1.286715000	1.377498000	-0.006820000
C	0.053603000	-1.121814000	-0.024269000
C	-0.101691000	1.298665000	-0.019456000
C	-0.706526000	0.048566000	-0.030083000
H	2.053980000	-1.927086000	-0.008698000
H	1.775365000	2.346938000	-0.002813000
H	-0.440378000	-2.086580000	-0.037281000
H	-0.706948000	2.196619000	-0.028503000
C	-2.205875000	-0.066021000	0.000315000
F	-2.808304000	1.066854000	-0.380143000
F	-2.643655000	-1.044210000	-0.804323000
F	-2.649087000	-0.352831000	1.234606000

2-CN: E= -437.636378

C	-2.793125000	0.333141000	0.000055000
H	-3.180225000	1.370722000	0.000102000
O	-3.544993000	-0.603593000	0.000084000
C	-1.310300000	0.207282000	0.000028000
C	-0.718175000	-1.056988000	0.000017000
C	-0.522210000	1.355738000	0.000009000
C	0.660858000	-1.172184000	-0.000012000
C	0.861818000	1.251731000	-0.000023000
C	1.449307000	-0.014744000	-0.000032000
H	-1.354659000	-1.934420000	0.000030000
H	-0.992347000	2.334228000	0.000017000
H	1.138343000	-2.144438000	-0.000020000
H	1.487991000	2.135372000	-0.000039000
C	2.882198000	-0.131376000	-0.000064000
N	4.028374000	-0.224045000	-0.000089000

2-NO2: E= -549.882421

C	-3.208416371	0.365426580	0.000000000
H	-3.595666821	1.402697583	0.000000000
O	-3.958716516	-0.571914742	0.000000000
C	-1.724056596	0.238553448	0.000000000
C	-1.134632091	-1.027005811	0.000000000
C	-0.936726014	1.387715878	0.000000000
C	0.245522056	-1.146366183	0.000000000
C	0.448682906	1.285562652	0.000000000
C	1.005627168	0.016915621	0.000000000
H	-1.771925973	-1.903598244	0.000000000
H	-1.406331044	2.366187232	0.000000000
H	0.737832117	-2.109553503	0.000000000
H	1.089847876	2.156579791	0.000000000
N	2.483335217	-0.103962263	0.000000000
O	2.949907605	-1.220632497	0.000000000
O	3.125645994	0.922200856	0.000000000

2-RC-NMe2: E= -572.127809

C	-2.413873000	-1.543132000	0.000839000
H	-3.198870000	-0.767388000	0.038992000
O	-2.684793000	-2.725277000	0.006489000
C	-3.786673000	2.001570000	0.124056000
N	-4.630175000	2.806791000	0.198058000
C	-1.029209000	-1.024317000	-0.055480000
C	0.069145000	-1.890255000	-0.115149000
C	-0.820244000	0.351524000	-0.056098000
C	1.353070000	-1.387630000	-0.168794000
C	0.476604000	0.859979000	-0.102263000
C	1.581464000	0.003975000	-0.155279000
H	-0.109027000	-2.960523000	-0.133741000
H	-1.683624000	1.019407000	-0.008719000
H	2.192713000	-2.067564000	-0.259025000

H	0.606841000	1.934354000	-0.084380000
N	2.908056000	0.484087000	-0.237256000
C	3.070565000	1.916714000	-0.377086000
H	4.121768000	2.130026000	-0.579955000
H	2.480778000	2.282362000	-1.217418000
H	2.775536000	2.473010000	0.526636000
C	3.842013000	-0.064506000	0.734471000
H	4.862221000	0.184137000	0.434223000
H	3.666336000	0.341975000	1.742905000
H	3.761329000	-1.147246000	0.787654000

2-RC-tBu: E= -595.364292

C	2.917371000	-1.262465000	0.000019000
H	3.645068000	-0.431491000	0.000015000
O	3.272937000	-2.421015000	-0.000123000
C	4.389472000	2.049294000	0.000001000
N	3.530449000	2.844109000	-0.000102000
C	1.486178000	-0.859154000	0.000085000
C	0.471927000	-1.821894000	0.000036000
C	1.155414000	0.491901000	0.000159000
C	-0.854429000	-1.430446000	0.000048000
C	-0.187347000	0.874246000	0.000173000
C	-1.212172000	-0.070251000	0.000134000
H	0.747355000	-2.871451000	-0.000019000
H	1.940543000	1.247766000	0.000170000
H	-1.627964000	-2.192638000	0.000014000
H	-0.409413000	1.934220000	0.000224000
C	-2.693916000	0.313843000	0.000009000
C	-3.371627000	-0.262255000	1.253961000
H	-2.902379000	0.130082000	2.159591000
H	-4.432516000	0.007435000	1.271716000
H	-3.301585000	-1.351534000	1.287371000
C	-3.371321000	-0.262257000	-1.254165000
H	-4.432104000	0.007813000	-1.272337000
H	-2.901542000	0.129788000	-2.159634000
H	-3.301660000	-1.351567000	-1.287347000
C	-2.900750000	1.830930000	-0.000085000
H	-3.971107000	2.055869000	-0.000310000
H	-2.461285000	2.298109000	0.884409000
H	-2.460858000	2.298000000	-0.884413000

2-RC-Me: E= -477.542357

C	-1.615831000	1.485008000	0.003100000
H	-2.497873000	0.820064000	0.003898000
O	-1.728240000	2.691743000	0.005111000
C	-3.742736000	-1.450530000	0.003458000
N	-3.069362000	-2.407703000	-0.000861000
C	-0.297132000	0.797900000	-0.000094000
C	0.890301000	1.536453000	-0.002626000
C	-0.253331000	-0.595084000	-0.003381000

C	2.111120000	0.883431000	-0.007747000
C	0.982416000	-1.240056000	-0.008383000
C	2.172609000	-0.517202000	-0.008005000
H	0.830532000	2.619876000	-0.003627000
H	-1.178188000	-1.171660000	-0.004246000
H	3.034821000	1.456603000	-0.012645000
H	1.010343000	-2.325559000	-0.013468000
C	3.508351000	-1.215333000	0.011895000
H	3.958951000	-1.167219000	1.007857000
H	3.408608000	-2.268387000	-0.255925000
H	4.209661000	-0.751257000	-0.686010000

2-RC-H: E= -438.264978

C	0.662382000	1.643986000	-0.000269000
H	1.718219000	1.319800000	0.000026000
O	0.355681000	2.815925000	-0.000451000
C	3.674840000	-0.336069000	0.002091000
N	3.357720000	-1.462573000	-0.001111000
C	-0.346557000	0.548052000	-0.000191000
C	-1.712171000	0.846916000	0.000271000
C	0.089767000	-0.776887000	-0.000486000
C	-2.644160000	-0.179697000	0.000466000
C	-0.853099000	-1.803951000	-0.000257000
C	-2.211666000	-1.508363000	0.000222000
H	-2.016852000	1.888188000	0.000494000
H	1.156574000	-1.000106000	-0.000943000
H	-3.705769000	0.045621000	0.000802000
H	-0.516065000	-2.834704000	-0.000481000
H	-2.941612000	-2.312115000	0.000406000

2-RC-Br: E= -3011.853759

C	2.946372000	-1.201193000	-0.000699000
H	3.661113000	-0.359636000	0.001639000
O	3.314065000	-2.354644000	0.001227000
C	4.380031000	2.063802000	-0.000839000
N	3.495455000	2.829969000	-0.000715000
C	1.503857000	-0.823309000	-0.000404000
C	0.518917000	-1.813494000	-0.000478000
C	1.149726000	0.524753000	-0.000112000
C	-0.823153000	-1.466278000	-0.000271000
C	-0.197465000	0.885374000	0.000086000
C	-1.159057000	-0.113422000	0.000011000
H	0.824224000	-2.854417000	-0.000718000
H	1.922130000	1.294636000	-0.000069000
H	-1.598566000	-2.222156000	-0.000328000
H	-0.481820000	1.930064000	0.000299000
Br	-3.006376000	0.368613000	0.000303000

2-RC-CF3: E= -775.319997

C	-2.873454000	-1.224591000	0.007446000
H	-3.605078000	-0.397877000	0.011832000
O	-3.214087000	-2.385586000	0.010207000
C	-4.383924000	1.954392000	0.011719000
N	-3.527345000	2.751396000	-0.006042000
C	-1.434549000	-0.819914000	-0.002063000
C	-0.434566000	-1.797600000	-0.008293000
C	-1.106087000	0.533641000	-0.008685000
C	0.896946000	-1.423656000	-0.019831000
C	0.236895000	0.910822000	-0.018661000
C	1.224529000	-0.064332000	-0.026766000
H	-0.725985000	-2.842067000	-0.005773000
H	-1.893038000	1.288310000	-0.006580000
H	1.683931000	-2.169843000	-0.029986000
H	0.501361000	1.961443000	-0.026916000
C	2.673855000	0.314736000	0.000218000
F	3.409772000	-0.436170000	-0.843152000
F	2.886522000	1.595081000	-0.332828000
F	3.219823000	0.139306000	1.221264000

2-RC-CN: E= -530.514783

C	-2.049696000	1.289189000	-0.000654000
H	-2.840473000	0.518802000	-0.001562000
O	-2.300845000	2.472295000	-0.000015000
C	-3.758319000	-1.776097000	0.001429000
N	-2.972630000	-2.643150000	0.000309000
C	-0.643558000	0.778758000	-0.000410000
C	0.424202000	1.681161000	0.000525000
C	-0.416024000	-0.597204000	-0.001115000
C	1.725450000	1.213960000	0.000725000
C	0.892002000	-1.071749000	-0.000957000
C	1.956824000	-0.169498000	-0.000033000
H	0.209381000	2.743986000	0.001065000
H	-1.256813000	-1.291974000	-0.001849000
H	2.566731000	1.897443000	0.001440000
H	1.084266000	-2.138209000	-0.001542000
C	3.311212000	-0.651899000	0.000164000
N	4.399932000	-1.026583000	0.000337000

2-RC-NO2: E= -642.762702

C	2.401315000	-1.221577000	-0.000845000
H	3.156811000	-0.418517000	-0.001734000
O	2.691272000	-2.395363000	0.000475000
C	4.700746000	2.124810000	0.004838000
N	3.552781000	1.894148000	-0.002412000
C	0.973942000	-0.764665000	-0.000939000
C	-0.056745000	-1.708643000	-0.000031000
C	0.696304000	0.602874000	-0.001605000
C	-1.377544000	-1.295471000	0.000356000
C	-0.629853000	1.028755000	-0.001235000

C	-1.634310000	0.072997000	-0.000200000
H	0.198865000	-2.762220000	0.000479000
H	1.530425000	1.307603000	-0.001998000
H	-2.200528000	-1.997236000	0.001066000
H	-0.884315000	2.080165000	-0.001553000
N	-3.042112000	0.519372000	0.000399000
O	-3.261244000	1.712118000	-0.000246000
O	-3.907411000	-0.334119000	0.001744000

2-TS-NMe2: E= -572.113393 (i = -175 cm-1)

C	-2.690967000	-0.658170000	0.585222000
H	-3.013310000	-0.200270000	1.538036000
O	-3.208012000	-1.709374000	0.194550000
C	-3.430268000	1.026949000	-0.368903000
N	-3.946984000	1.967670000	-0.817711000
C	-1.221549000	-0.388785000	0.300558000
C	-0.485795000	-1.315470000	-0.432955000
C	-0.566075000	0.724919000	0.806902000
C	0.869626000	-1.125154000	-0.663542000
C	0.797691000	0.915712000	0.600762000
C	1.536591000	-0.011150000	-0.142024000
H	-1.011178000	-2.178514000	-0.827893000
H	-1.141630000	1.470000000	1.350037000
H	1.422541000	-1.832248000	-1.274766000
H	1.274368000	1.796677000	1.014577000
N	2.932467000	0.141154000	-0.404611000
C	3.493240000	1.439354000	-0.100534000
H	4.509592000	1.486355000	-0.498928000
H	2.901557000	2.222409000	-0.575616000
H	3.545283000	1.647952000	0.982007000
C	3.755158000	-0.922742000	0.150077000
H	4.767491000	-0.850166000	-0.256284000
H	3.815660000	-0.864668000	1.250106000
H	3.349430000	-1.897083000	-0.114797000

2-TS-tBu: E= -595.350849 (i = -165 cm-1)

C	-3.025801000	-0.652964000	0.542432000
H	-3.389896000	-0.189143000	1.477012000
O	-3.548967000	-1.684384000	0.114252000
C	-3.661775000	1.070722000	-0.443326000
N	-4.131862000	2.021954000	-0.920435000
C	-1.538633000	-0.413397000	0.335178000
C	-0.782343000	-1.353642000	-0.345861000
C	-0.889844000	0.693134000	0.881822000
C	0.596573000	-1.190716000	-0.493808000
C	0.479350000	0.851075000	0.742467000
C	1.256946000	-0.088584000	0.047216000
H	-1.296101000	-2.216011000	-0.757369000
H	-1.481937000	1.449217000	1.390750000
H	1.149649000	-1.946892000	-1.039748000

H	0.950725000	1.730221000	1.173006000
C	2.765280000	0.133728000	-0.092045000
C	3.024247000	1.454459000	-0.835070000
H	2.573455000	1.430001000	-1.830208000
H	2.597923000	2.305872000	-0.300793000
H	4.099908000	1.628983000	-0.946219000
C	3.449314000	-0.991996000	-0.873121000
H	3.055329000	-1.073000000	-1.889277000
H	4.522469000	-0.792121000	-0.945903000
H	3.322085000	-1.959081000	-0.379778000
C	3.408594000	0.203979000	1.302448000
H	4.489023000	0.364216000	1.220370000
H	2.991858000	1.020333000	1.895935000
H	3.238824000	-0.725989000	1.851251000

2-TS-Me: E= -477.528568 (i = -169 cm-1)

C	1.909857000	0.694523000	0.578608000
H	2.273488000	0.234349000	1.515290000
O	2.373080000	1.771483000	0.194121000
C	2.700157000	-0.948331000	-0.422919000
N	3.255153000	-1.849220000	-0.906437000
C	0.449350000	0.359384000	0.316306000
C	-0.346376000	1.268476000	-0.366276000
C	-0.135407000	-0.803608000	0.816143000
C	-1.704007000	1.014467000	-0.560602000
C	-1.486978000	-1.051885000	0.630093000
C	-2.294671000	-0.145669000	-0.066927000
H	0.122635000	2.174050000	-0.736101000
H	0.494288000	-1.527764000	1.326390000
H	-2.314447000	1.733259000	-1.102115000
H	-1.927748000	-1.967064000	1.018767000
C	-3.757426000	-0.439788000	-0.288696000
H	-4.255439000	-0.717593000	0.644423000
H	-4.277343000	0.427939000	-0.700321000
H	-3.893141000	-1.269909000	-0.988617000

2-TS-H: E= -438.251946 (i = -163 cm-1)

C	1.347130000	0.761737000	0.638689000
H	1.716411000	0.299243000	1.571547000
O	1.716071000	1.892401000	0.314957000
C	2.347247000	-0.762605000	-0.387361000
N	3.015202000	-1.582994000	-0.871545000
C	-0.057137000	0.290649000	0.290844000
C	-0.900456000	1.137813000	-0.418585000
C	-0.542199000	-0.937463000	0.736861000
C	-2.213090000	0.758409000	-0.692336000
C	-1.851850000	-1.317210000	0.474128000
C	-2.694159000	-0.468201000	-0.245135000
H	-0.500159000	2.091944000	-0.744201000
H	0.134133000	-1.605743000	1.263232000

H	-2.863894000	1.422712000	-1.253207000
H	-2.217788000	-2.279798000	0.818019000
H	-3.716613000	-0.765390000	-0.456867000

2-TS-Br: E= -3011.842388 (i = -143 cm-1)

C	3.031735000	0.672344000	0.537531000
H	3.420883000	0.195832000	1.453149000
O	3.540689000	1.700741000	0.098894000
C	3.668947000	-1.101502000	-0.470722000
N	4.124315000	-2.071622000	-0.924224000
C	1.549021000	0.411578000	0.333362000
C	0.786256000	1.350334000	-0.349833000
C	0.922217000	-0.703961000	0.884220000
C	-0.589344000	1.182643000	-0.496643000
C	-0.448104000	-0.887915000	0.758320000
C	-1.186903000	0.064981000	0.064740000
H	1.294402000	2.214880000	-0.762887000
H	1.528686000	-1.452676000	1.385713000
H	-1.186671000	1.910301000	-1.033180000
H	-0.936490000	-1.759014000	1.178101000
Br	-3.077700000	-0.175569000	-0.117381000

2-TS-CF3: E= -775.310599 (i = -124 cm-1)

C	-2.973397000	-0.698324000	0.546513000
H	-3.373290000	-0.207296000	1.448640000
O	-3.486336000	-1.717928000	0.101514000
C	-3.587890000	1.122866000	-0.477982000
N	-4.027375000	2.107178000	-0.916965000
C	-1.493491000	-0.432527000	0.337868000
C	-0.733934000	-1.360776000	-0.363992000
C	-0.867359000	0.673083000	0.913971000
C	0.639383000	-1.187073000	-0.504676000
C	0.500060000	0.850955000	0.790366000
C	1.254575000	-0.086044000	0.080290000
H	-1.244315000	-2.216884000	-0.790501000
H	-1.475946000	1.408643000	1.431085000
H	1.232322000	-1.910428000	-1.052940000
H	0.987504000	1.711153000	1.236442000
C	2.720385000	0.140159000	-0.090484000
F	3.001479000	1.021991000	-1.073464000
F	3.297845000	0.638592000	1.021594000
F	3.390237000	-0.985687000	-0.398943000

2-TS-CN: E= -530.506392 (i = -115 cm-1)

C	2.190176000	0.725881000	0.565862000
H	2.598473000	0.232084000	1.462028000
O	2.675193000	1.763319000	0.135962000
C	2.869165000	-1.088043000	-0.478316000
N	3.329361000	-2.062090000	-0.919218000

C	0.727327000	0.406398000	0.325109000
C	-0.045643000	1.299078000	-0.410916000
C	0.127794000	-0.715012000	0.899124000
C	-1.404309000	1.075042000	-0.585911000
C	-1.226874000	-0.946964000	0.742704000
C	-2.000367000	-0.047212000	-0.004255000
H	0.446474000	2.165801000	-0.837386000
H	0.750091000	-1.422462000	1.438459000
H	-2.011894000	1.763256000	-1.162958000
H	-1.696668000	-1.820367000	1.180407000
C	-3.407560000	-0.275877000	-0.166971000
N	-4.538829000	-0.455712000	-0.293184000

2-TS-NO2: E= -642.754895 (i = -101 cm-1)

C	-2.594877000	-0.668664000	0.635415000
H	-3.014482000	-0.070663000	1.459183000
O	-3.094413000	-1.731353000	0.300630000
C	-3.211336000	1.074885000	-0.614864000
N	-3.637513000	2.014149000	-1.154768000
C	-1.127701000	-0.392984000	0.378199000
C	-0.366495000	-1.353548000	-0.282654000
C	-0.513566000	0.760067000	0.870304000
C	0.996489000	-1.167849000	-0.467824000
C	0.845521000	0.959641000	0.708292000
C	1.582429000	-0.014622000	0.037854000
H	-0.870210000	-2.242315000	-0.644508000
H	-1.127135000	1.516866000	1.348464000
H	1.607097000	-1.897013000	-0.983704000
H	1.340534000	1.848404000	1.075864000
N	3.025287000	0.182409000	-0.135287000
O	3.528118000	1.183398000	0.339329000
O	3.652169000	-0.666138000	-0.741615000