

Electronic Supplementary Information

The origin of the regioselectivity of acrolein dimerization

Ramiro F. Quijano-Quiñones ^{*,1}, Jareth Guadarrama¹, Mariana Quesadas-Rojas^{2,3}, Gonzalo J. Mena-Rejón⁴, Carolina S. Castro¹, David Cáceres-Castillo⁴

¹Laboratorio de Química Teórica, Facultad de Química, Universidad Autónoma de Yucatán, Mérida, Yucatán, México; ²Posgrado en Ciencias del Mar y Limnología, UNAM; ³Escuela Nacional de Educación Superior, Mérida, UNAM; ⁴Laboratorio de Química Farmacéutica, Facultad de Química, Universidad Autónoma de Yucatán, Mérida, Yucatán, México

[*ramiro.quijano@correo.uady.mx](mailto:ramiro.quijano@correo.uady.mx)

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Table S1. MP2 relative activation energy (include ZPE) for acrolein dimerization in the 2CN reaction channel. The energies are in kcal/mol.

	TS1	INT	TS2
2CN	9.8	6.6	7.1

I. B3LYP

Acrolein

Cis

C	1.478700	-0.466700	0.000000
H	2.559000	-0.360400	0.000000
H	1.066000	-1.471800	0.000000
C	0.665600	0.598800	0.000000
H	1.061700	1.612300	0.000000
C	-0.813000	0.464200	-0.000000
H	-1.376600	1.420200	-0.000000
O	-1.412200	-0.597300	-0.000000

Electronic Energy + ZPE = -191.865170

Trans

C	1.766500	0.140700	0.000000
H	1.861300	1.224800	0.000100
H	2.689000	-0.431200	0.000100
C	0.562300	-0.448200	0.000000
H	0.443200	-1.529000	-0.000000
C	-0.676000	0.352100	-0.000000
H	-0.526800	1.454000	0.000000
O	-1.797900	-0.123200	-0.000000

Electronic Energy + ZPE = -191.868560

Transition States

2CN

C	1.353000	0.281100	0.752100
H	1.548800	0.234700	1.818300
C	1.422100	-0.912500	-0.034000
H	1.765500	-1.843200	0.444500
C	0.899600	1.467300	0.120300

H	1.198100	1.546700	-0.923300
H	1.029800	2.386800	0.688400
O	1.001000	-0.917400	-1.207400
C	-1.353000	0.281000	-0.752100
C	-0.899700	1.467300	-0.120300
H	-1.029900	2.386800	-0.688400
H	-1.198200	1.546700	0.923300
H	-1.548900	0.234600	-1.818300
C	-1.422100	-0.912600	0.034000
H	-1.765400	-1.843300	-0.444500
O	-1.000900	-0.917500	1.207400

Electronic Energy + ZPE = -383.697671

2CX

C	0.924900	1.212100	-0.611300
H	1.115700	2.274800	-0.746900
H	0.210900	0.794500	-1.319100
C	2.024900	0.402000	-0.260000
H	2.972900	0.837400	0.045000
C	1.783600	-0.967400	-0.016700
H	2.587600	-1.585600	0.415300
O	0.635400	-1.467100	-0.160900
C	-0.324600	1.222700	0.827800
H	0.246400	1.634600	1.654600
H	-0.987900	1.930300	0.333500
C	-0.848100	-0.070800	0.979500
H	-0.564000	-0.713200	1.804700
C	-1.884700	-0.564300	0.062400
H	-2.250400	-1.590500	0.246500
O	-2.308700	0.093700	-0.879600

Electronic Energy + ZPE = -383.694849

2TN

C	1.928800	0.802700	-0.222400
H	2.593900	1.609500	0.076600
H	1.728600	0.751300	-1.288300
C	2.020300	-0.420300	0.462700
H	2.614400	-0.519100	1.367200
C	1.081600	-1.422000	0.133500
H	1.034800	-2.340700	0.739400
O	0.207300	-1.223200	-0.754100
C	0.161700	1.580700	0.168000
H	0.388500	2.507100	-0.354500
H	0.191100	1.665400	1.252300
C	-0.832500	0.769300	-0.392700
H	-1.078700	0.838100	-1.447500
C	-1.779800	0.015500	0.442800
H	-1.420300	-0.215500	1.469500
O	-2.898800	-0.308300	0.083400

Electronic Energy + ZPE = -383.692219

2TX

C	2.227400	-0.128500	0.019300
H	3.152000	-0.003300	0.576300
C	1.472600	-1.310000	0.174800
H	1.877500	-2.138000	0.778100
C	1.590800	0.959500	-0.607700
H	0.992100	0.719700	-1.481400
H	2.135700	1.898300	-0.679300
O	0.285700	-1.379900	-0.248200
C	-0.829400	0.408600	0.613700
H	-0.859100	-0.171400	1.528800

C	-1.944000	0.193500	-0.320300
H	-1.841800	0.702100	-1.303600
C	0.054100	1.489200	0.449000
H	-0.269300	2.272700	-0.236100
H	0.550000	1.864900	1.339100
O	-2.931500	-0.472600	-0.063600

Electronic Energy + ZPE = -383.691202

3CN

C	-0.572200	-1.117300	1.117600
H	-0.023200	-1.934900	1.577600
H	-1.026100	-0.411900	1.802800
C	-1.133500	-1.273300	-0.146500
H	-0.986900	-2.177500	-0.728700
C	-1.646200	-0.128900	-0.772100
H	-2.023800	-0.182000	-1.801200
O	-1.571900	1.020700	-0.218200
C	0.217600	1.526200	0.334900
H	-0.167200	2.282100	1.008200
H	0.438800	1.852300	-0.674100
C	0.951300	0.442000	0.856900
H	1.180500	0.426500	1.919600
C	1.867400	-0.285400	-0.028900
H	2.631200	-0.910700	0.480100
O	1.805700	-0.261200	-1.251300

Electronic Energy + ZPE = -383.692367

3CX

C	-0.340800	1.355200	-0.278000
H	0.154400	2.287300	-0.017600
H	0.040800	0.851500	-1.158800

C	-1.669600	1.150200	0.089400
H	-2.219100	1.876900	0.680800
C	-2.203600	-0.131800	-0.106500
H	-3.228600	-0.358800	0.218900
O	-1.487500	-1.091400	-0.544300
C	0.217400	-1.342000	0.430700
H	-0.320300	-1.956700	1.140900
H	0.666900	-1.859800	-0.408600
C	0.791500	-0.126700	0.845000
H	0.578000	0.237600	1.846300
C	2.091800	0.286900	0.281300
H	2.672900	0.983600	0.922200
O	2.529300	-0.060200	-0.805100

Electronic Energy + ZPE = -383.690738

3TN

C	-0.262100	-1.111800	0.926000
H	0.539600	-1.800600	1.177500
H	-0.679400	-0.553500	1.756300
C	-1.107500	-1.383500	-0.156800
H	-0.951700	-2.246100	-0.798200
C	-1.981100	-0.366600	-0.557300
H	-2.605800	-0.493000	-1.452600
O	-1.968500	0.775600	0.015100
C	-0.138100	1.580700	0.092700
H	-0.497300	2.318100	0.798900
H	-0.222300	1.861500	-0.951600
C	0.833200	0.643200	0.487300
H	1.239300	0.710200	1.494000
C	1.765400	0.106600	-0.522900
H	1.394700	0.150400	-1.571400

O 2.859000 -0.370300 -0.273400

Electronic Energy + ZPE = -383.691412

3TX

C -0.224000 1.267500 -0.393600

H 0.482700 2.072200 -0.211600

H -0.138000 0.772300 -1.354600

C -1.488600 1.294700 0.202700

H -1.770900 2.077700 0.900700

C -2.273500 0.139800 0.097200

H -3.243000 0.079400 0.611200

O -1.824500 -0.910400 -0.473000

C -0.040000 -1.473400 0.255600

H -0.560800 -1.972600 1.062000

H 0.147700 -2.083500 -0.622200

C 0.787400 -0.367000 0.514900

H 0.833600 0.038400 1.521500

C 2.031300 -0.229200 -0.269400

H 2.023200 -0.751300 -1.252400

O 3.008200 0.406900 0.085700

Electronic Energy + ZPE = -383.691423

Products

2CN

C -2.20037100 0.00509400 0.07127100

H -3.28498200 -0.01008600 0.11010400

C -1.55755700 -1.16442300 -0.03983900

H -2.05373700 -2.12541400 -0.12070300

C -1.46904800 1.32437500 0.09571400

H -1.50506100 1.77141300 1.09944600

H -1.96419700 2.04041200 -0.57183500

O	-0.19403400	-1.31281500	-0.07438300
C	0.55348200	-0.14680900	0.29615600
C	-0.01219800	1.12551100	-0.35121600
H	0.62243100	1.97281900	-0.07710800
H	0.03342800	1.01253200	-1.44105900
H	0.51552300	-0.04302100	1.39243000
C	1.99516000	-0.41744100	-0.09845000
H	2.17009800	-1.38706900	-0.60922700
O	2.89524500	0.36413700	0.12140100

Electronic Energy + ZPE = -383.757018

2CX

C	0.85126700	1.45924800	-0.18640100
H	1.47850600	2.29723000	0.14174400
H	0.22388600	1.85313200	-0.99798000
C	1.71773300	0.32914400	-0.68062200
H	2.55524200	0.54224000	-1.33768900
C	1.51886700	-0.94393500	-0.31306500
H	2.16041000	-1.76673400	-0.60927200
O	0.49636800	-1.38722100	0.49012600
C	-0.02319100	0.97869000	0.98321400
H	0.56506600	0.94554800	1.90636800
H	-0.87459000	1.64465400	1.14869400
C	-0.55255200	-0.43539600	0.71149400
H	-1.09624400	-0.81257900	1.58665000
C	-1.52884000	-0.49200000	-0.46547200
H	-1.36554600	-1.33498400	-1.16963500
O	-2.43967200	0.29434500	-0.61059800

Electronic Energy + ZPE = -383.756095

3TN

C	0.59514800	1.43914700	0.44633500
H	0.22752200	2.35695600	-0.03334200
H	1.01251300	1.75533500	1.41170600
C	1.64481300	0.78742000	-0.41809900
H	2.39749400	1.40011300	-0.90359400
C	1.66268500	-0.53464900	-0.64590100
H	2.37161300	-1.01907000	-1.30908300
O	0.79858900	-1.44256500	-0.10601200
C	-0.03040900	-0.94856600	0.95539000
H	0.56237900	-0.93114100	1.87916200
H	-0.84364600	-1.66848400	1.05696100
C	-0.57165100	0.46286200	0.66859100
H	-1.17185600	0.75929700	1.53968500
C	-1.53856800	0.43852700	-0.51312200
H	-1.30056700	1.12200800	-1.35725600
O	-2.52703300	-0.26286700	-0.54941400

Electronic Energy + ZPE = -383.753914

3TX

C	0.18602600	1.35149700	0.13442400
H	-0.13898500	2.17329700	-0.51541400
H	-0.06143600	1.65966600	1.16189900
C	1.66867400	1.12605000	-0.01520800
H	2.33505200	1.98171000	-0.05049000
C	2.19428500	-0.09661800	-0.16390600
H	3.24743700	-0.28515100	-0.34183400
O	1.48378500	-1.26451100	-0.13220000
C	0.14729900	-1.15130300	0.36436600
H	-0.34562500	-2.08766900	0.09518700
H	0.18745900	-1.06937900	1.46042500
C	-0.58813100	0.06622200	-0.23470100

H	-0.63231200	-0.05684400	-1.32178200
C	-2.00705300	0.10844000	0.28654100
H	-2.10802700	0.37149900	1.36481500
O	-2.99505500	-0.12459700	-0.37803700

Electronic Energy + ZPE = -383.753987

II. M062X

Acrolein

Cis

C	1.457000	-0.470300	0.000000
H	2.538500	-0.386700	0.000000
H	1.016300	-1.463600	0.000000
C	0.668400	0.606100	0.000000
H	1.073300	1.614700	0.000000
C	-0.812700	0.466200	-0.000000
H	-1.389800	1.411300	0.000000
O	-1.389300	-0.598400	-0.000000

Electronic Energy + ZPE = -191.768233

Trans

C	1.756200	0.144300	0.000000
H	1.833500	1.229700	0.000100
H	2.684600	-0.416500	0.000100
C	0.563700	-0.454500	0.000000
H	0.445300	-1.534600	-0.000000
C	-0.675300	0.351200	-0.000000
H	-0.523300	1.451300	0.000000
O	-1.788500	-0.122000	-0.000000

Electronic Energy + ZPE = -191.771122

Transition States

2CN

C	-1.475000	-0.402800	-0.721400
H	-1.684300	-0.595500	-1.768000
C	-0.828500	-1.378600	0.067500
H	-0.617000	-2.371100	-0.352300
C	-1.593500	0.877500	-0.153700
H	-1.813400	0.890800	0.910500
H	-2.099000	1.644000	-0.735700
O	-0.367700	-1.059300	1.189500
C	0.941000	0.770400	0.756400
C	0.113100	1.639400	0.032800
H	-0.192500	2.554500	0.533100
H	0.364000	1.744100	-1.019200
H	1.072800	0.851500	1.829000
C	1.720700	-0.212900	0.012200
H	2.439000	-0.830700	0.575600
O	1.525600	-0.396400	-1.181400

Electronic Energy + ZPE = -383.509886

2CX

C	0.915100	1.194700	-0.614700
H	1.096300	2.258900	-0.743700
H	0.162900	0.774700	-1.281500
C	2.003000	0.379800	-0.273500
H	2.963600	0.794900	0.013600
C	1.716800	-0.974500	-0.026800
H	2.487700	-1.626800	0.408900
O	0.549000	-1.418700	-0.168500
C	-0.307500	1.190900	0.880900
H	0.287100	1.589500	1.695800

H	-0.966000	1.900500	0.384100
C	-0.803100	-0.106400	0.989000
H	-0.549700	-0.764300	1.811500
C	-1.836200	-0.554100	0.031600
H	-2.206500	-1.586300	0.149700
O	-2.224600	0.153200	-0.876300

Electronic Energy + ZPE = -383.506007

2TN

C	-1.962300	0.731300	0.187500
H	-2.641000	1.516100	-0.135300
H	-1.756100	0.699500	1.252600
C	-1.959700	-0.485500	-0.495200
H	-2.511700	-0.628000	-1.418300
C	-0.973300	-1.412700	-0.107500
H	-0.820100	-2.331000	-0.692200
O	-0.167400	-1.130000	0.815500
C	-0.187300	1.582100	-0.169300
H	-0.461700	2.493900	0.353100
H	-0.221000	1.648000	-1.253900
C	0.783900	0.773700	0.410100
H	1.051800	0.872100	1.457100
C	1.722700	0.009800	-0.438500
H	1.311900	-0.281600	-1.430900
O	2.855400	-0.267600	-0.122400

Electronic Energy + ZPE = -383.502768

2TX

C	2.212000	-0.173400	0.009600
H	3.146700	-0.079000	0.552200
C	1.399800	-1.308900	0.182900

H	1.749500	-2.148700	0.799900
C	1.611900	0.912600	-0.631900
H	0.959300	0.680100	-1.467800
H	2.161700	1.846200	-0.716800
O	0.214800	-1.310300	-0.239100
C	-0.787300	0.396100	0.630100
H	-0.846200	-0.170800	1.552400
C	-1.893700	0.193100	-0.328800
H	-1.741900	0.666900	-1.322400
C	0.069600	1.483900	0.477700
H	-0.233700	2.255000	-0.228900
H	0.598000	1.850900	1.350600
O	-2.898200	-0.429900	-0.080600

Electronic Energy + ZPE = -383.501508

3CN

C	-0.645000	-1.033900	1.198500
H	-0.159700	-1.827000	1.761100
H	-1.081800	-0.228600	1.777000
C	-1.101800	-1.254100	-0.083900
H	-0.932300	-2.188100	-0.607500
C	-1.512500	-0.116800	-0.803700
H	-1.772900	-0.197100	-1.865800
O	-1.468600	1.033100	-0.276600
C	0.294700	1.542400	0.326600
H	-0.093200	2.313200	0.981900
H	0.531300	1.842500	-0.687800
C	0.987600	0.455900	0.865900
H	1.226100	0.423400	1.924400
C	1.774700	-0.358400	-0.060000
H	2.530200	-1.035600	0.384900

O 1.589400 -0.347300 -1.264400

Electronic Energy + ZPE = -383.506378

3CX

C -0.324400 1.335100 -0.274500

H 0.198400 2.256300 -0.027200

H 0.048000 0.790200 -1.136600

C -1.641200 1.154000 0.108300

H -2.176200 1.874800 0.717000

C -2.176200 -0.130100 -0.104400

H -3.189400 -0.372000 0.245600

O -1.464500 -1.056900 -0.579700

C 0.224900 -1.348100 0.445800

H -0.346400 -1.963000 1.129500

H 0.679700 -1.851600 -0.400900

C 0.787300 -0.147500 0.873300

H 0.570300 0.223700 1.870300

C 2.069600 0.281400 0.277800

H 2.683500 0.955000 0.909000

O 2.451000 -0.040900 -0.828200

Electronic Energy + ZPE = -383.503214

3TN

C -0.238500 -1.069700 0.966300

H 0.590700 -1.703300 1.269200

H -0.705300 -0.476400 1.744700

C -1.013600 -1.397100 -0.139500

H -0.790100 -2.250800 -0.770300

C -1.919100 -0.414100 -0.567700

H -2.497400 -0.555500 -1.490700

O -1.971600 0.706100 0.017500

C	-0.173200	1.598300	0.055800
H	-0.568300	2.345100	0.732700
H	-0.276300	1.823700	-1.001000
C	0.816000	0.714600	0.480200
H	1.221100	0.801800	1.484900
C	1.716400	0.114000	-0.522400
H	1.322400	0.122900	-1.562800
O	2.793600	-0.379000	-0.272800

Electronic Energy + ZPE = -383.504135

3TX

C	-0.205300	1.259300	-0.377300
H	0.526500	2.040400	-0.190700
H	-0.120200	0.733300	-1.323000
C	-1.458100	1.299400	0.217600
H	-1.732800	2.067600	0.932400
C	-2.245700	0.145100	0.079700
H	-3.210100	0.065900	0.599400
O	-1.792700	-0.871600	-0.519300
C	-0.054000	-1.482300	0.283900
H	-0.619100	-1.959100	1.074200
H	0.138100	-2.096900	-0.590600
C	0.780300	-0.400100	0.552400
H	0.826100	0.026400	1.549500
C	2.000000	-0.245000	-0.264600
H	1.983300	-0.793500	-1.232300
O	2.955800	0.428900	0.048100

Electronic Energy + ZPE = -383.503550

Products

2CN

C	-2.18286500	0.02230700	0.06715300
H	-3.26663100	0.01562100	0.10330500
C	-1.55544500	-1.14988500	-0.05636800
H	-2.06546100	-2.10206100	-0.14948700
C	-1.43850200	1.33186300	0.10180200
H	-1.46431800	1.76606900	1.10940000
H	-1.92731800	2.05513000	-0.55934300
O	-0.19934800	-1.31117700	-0.08579700
C	0.53923800	-0.16386700	0.30825700
C	0.00687600	1.10876000	-0.34705300
H	0.66068200	1.94288100	-0.08137400
H	0.04814600	0.97785500	-1.43455600
H	0.47390200	-0.06272200	1.40436500
C	1.98462200	-0.43975900	-0.05268900
H	2.19120000	-1.45523100	-0.44517000
O	2.85262900	0.38692000	0.07657800

Electronic Energy + ZPE = -383.584125

2CX

C	0.70074600	1.48892100	-0.12614400
H	1.30261700	2.34471300	0.19684300
H	-0.00134400	1.86909100	-0.87845500
C	1.59403600	0.43145400	-0.71839300
H	2.36473700	0.71445300	-1.42718600
C	1.51105700	-0.85757200	-0.37512100
H	2.18680900	-1.62330300	-0.73925000
O	0.57846000	-1.38392200	0.47594400
C	-0.06439400	0.90685900	1.06558300
H	0.57997100	0.85822700	1.94874100
H	-0.94218900	1.50959600	1.30980800
C	-0.51423000	-0.51393900	0.73376800

H	-1.05369800	-0.96352300	1.57537100
C	-1.44902600	-0.54315000	-0.47269000
H	-1.30160800	-1.40059300	-1.16108600
O	-2.30401400	0.28590900	-0.65929500

Electronic Energy + ZPE = -383.584684

3TN

C	-0.09457800	1.11127900	0.95504100
H	-0.92999100	1.79443700	0.77274800
H	0.26838800	1.30282600	1.97153800
C	0.98981600	1.35431000	-0.06231800
H	1.29493900	2.37090400	-0.28287100
C	1.54904900	0.36592700	-0.76389600
H	2.27177300	0.52166200	-1.55677400
O	1.27468600	-0.96271500	-0.59641700
C	0.60287500	-1.26826000	0.61668000
H	1.30840100	-1.17187600	1.45256300
H	0.29239500	-2.31285400	0.53071200
C	-0.58518300	-0.33126200	0.83455900
H	-1.10956600	-0.65230100	1.74642800
C	-1.57571700	-0.51335600	-0.30310500
H	-1.77134700	-1.56874300	-0.59163100
O	-2.14250800	0.38823000	-0.86664200

Electronic Energy + ZPE = -383.582622

3TX

C	0.19958200	1.35509900	0.12402400
H	-0.10635500	2.17927900	-0.52930100
H	-0.04717300	1.66332400	1.15046100
C	1.67671200	1.10434400	-0.01696800
H	2.36068200	1.94464000	-0.04997400

C	2.17767600	-0.12449700	-0.16494700
H	3.22773100	-0.32912700	-0.34139200
O	1.44820800	-1.27314900	-0.12879900
C	0.13300900	-1.12519300	0.38018600
H	-0.38564400	-2.05701100	0.14826300
H	0.18880300	-1.00322300	1.47252400
C	-0.58020600	0.08442100	-0.24242000
H	-0.61821900	-0.05477300	-1.32760900
C	-1.99561700	0.13828300	0.27641400
H	-2.10107400	0.45907500	1.33726700
O	-2.97141900	-0.15146700	-0.37094900

Electronic Energy + ZPE = -383.580853

III. MP2

Acrolein

Cis

C	1.46725100	-0.47452600	0.00000200
H	2.54384000	-0.38106900	0.00000600
H	1.03748000	-1.46751300	-0.00000400
C	0.66787500	0.60580200	0.00000400
H	1.07682700	1.60944100	0.00001000
C	-0.80847700	0.47466800	-0.00000200
H	-1.37760300	1.41864300	-0.00000700
O	-1.40505500	-0.60189500	-0.00000300

Electronic Energy + ZPE = -191.291947

Trans

C	1.76693400	0.14200000	0.00004400
H	1.85264500	1.22209000	0.00006500
H	2.68601600	-0.42648500	0.00005900

C	0.56114400	-0.45325900	0.00000000
H	0.44633600	-1.53021700	-0.00002200
C	-0.66848400	0.35445100	-0.00001700
H	-0.51708200	1.44940100	-0.00001500
O	-1.80318500	-0.12174300	-0.00003100

Electronic Energy + ZPE = -191.321499

Intermediary

2CN

C	-1.30886900	0.20386500	-0.71013700
H	-1.64404300	0.12661800	-1.73662300
C	-1.32655000	-0.91487000	0.15209300
H	-1.67555500	-1.88812100	-0.20707200
C	-0.80439400	1.44159400	-0.13311600
H	-1.21945200	1.56858200	0.86622100
H	-1.00804100	2.31087600	-0.75505500
O	-0.76754200	-0.80805700	1.29195000
C	1.30968400	0.20092900	0.71000900
C	0.80792200	1.43979400	0.13305600
H	1.01354900	2.30861800	0.75498400
H	1.22321000	1.56585900	-0.86630100
H	1.64494300	0.12295200	1.73641100
C	1.32457900	-0.91786700	-0.15219500
H	1.67143000	-1.89189800	0.20694400
O	0.76500800	-0.80996300	-1.29167100

Electronic Energy + ZPE = -382.573362

Transition States

2CN (1)

C	-1.37235000	0.27828200	-0.74899600
H	-1.53279900	0.21403900	-1.81768900

C	-1.39193600	-0.91888600	0.04882500
H	-1.69603800	-1.86180500	-0.42294200
C	-1.00074700	1.46611400	-0.12349500
H	-1.18599600	1.52329700	0.94142600
H	-1.08054500	2.39178100	-0.68050800
O	-0.97661900	-0.90312700	1.23145000
C	1.37221900	0.27866000	0.74900000
C	1.00029100	1.46637600	0.12346700
H	1.07983000	2.39207600	0.68046200
H	1.18553800	1.52358800	-0.94145300
H	1.53267000	0.21448700	1.81769600
C	1.39221500	-0.91851500	-0.04880500
H	1.69661100	-1.86132700	0.42299000
O	0.97694200	-0.90291300	-1.23144300

Electronic Energy + ZPE = -382.568297

2CN (2)

C	0.91339500	0.77637000	0.72272600
H	1.23899600	0.96369800	1.73759200
C	1.65268300	-0.08871700	-0.13354800
H	2.49051100	-0.67011200	0.26872500
C	-0.11661300	1.58924500	0.07346100
H	0.22736200	1.88489800	-0.91655000
H	-0.38240100	2.46435800	0.66342300
O	1.19825200	-0.31881500	-1.29242600
C	-1.29689700	-0.57276300	-0.67135200
C	-1.50011200	0.79183600	-0.19589800
H	-2.10137700	1.39354000	-0.87452500
H	-1.96034200	0.75706800	0.79220700
H	-1.57839900	-0.90132400	-1.66338800
C	-0.62924300	-1.42633300	0.20718800

H -0.35260500 -2.44261300 -0.07559100

O -0.16338000 -0.91460100 1.29900600

Electronic Energy + ZPE = -382.572588

2CX

C 0.896200 1.198600 -0.634300

H 1.058500 2.258200 -0.799800

H 0.142300 0.738100 -1.266300

C 1.995200 0.424000 -0.264000

H 2.931600 0.875900 0.042900

C 1.766000 -0.956300 -0.003600

H 2.561600 -1.559200 0.452000

O 0.620000 -1.462400 -0.176200

C -0.342300 1.199000 0.886200

H 0.256000 1.593500 1.697700

H -0.973800 1.917800 0.376400

C -0.871200 -0.089500 1.018800

H -0.584900 -0.746600 1.829800

C -1.856800 -0.560400 0.051400

H -2.262000 -1.570900 0.203900

O -2.201500 0.112500 -0.931700

Electronic Energy + ZPE = -382.560886

2TN

C -1.960700 0.739300 0.228700

H -2.666300 1.513800 -0.051500

H -1.721100 0.682800 1.283200

C -1.981700 -0.463900 -0.476200

H -2.541100 -0.571700 -1.398400

C -0.991700 -1.423800 -0.140100

H -0.855500 -2.312500 -0.767000

O	-0.169000	-1.184300	0.795900
C	-0.209600	1.567400	-0.187600
H	-0.490600	2.490000	0.305800
H	-0.251200	1.607500	-1.270500
C	0.812900	0.811700	0.396100
H	1.065800	0.929700	1.442900
C	1.738900	0.045600	-0.435300
H	1.354000	-0.207500	-1.444300
O	2.876200	-0.289400	-0.097600

Electronic Energy + ZPE = -382.556566

2TX

C	2.212000	-0.134500	-0.014400
H	3.139500	0.001200	0.529900
C	1.442700	-1.308500	0.190400
H	1.828500	-2.113200	0.826600
C	1.572000	0.931000	-0.652700
H	0.912800	0.668200	-1.471100
H	2.120600	1.858300	-0.778300
O	0.249100	-1.366500	-0.236800
C	-0.819800	0.407900	0.648700
H	-0.858500	-0.183600	1.554500
C	-1.914400	0.239200	-0.302200
H	-1.809000	0.808600	-1.246600
C	0.088500	1.466600	0.494400
H	-0.213000	2.269200	-0.171800
H	0.629400	1.799500	1.370700
O	-2.903600	-0.473300	-0.113100

Electronic Energy + ZPE = -382.555360

3CN

C	-0.535700	-0.969900	1.247900
H	-0.016800	-1.720200	1.835100
H	-1.045700	-0.197400	1.807100
C	-1.017400	-1.289300	-0.013500
H	-0.796700	-2.236400	-0.488600
C	-1.534700	-0.232200	-0.783200
H	-1.799200	-0.382700	-1.832600
O	-1.564100	0.959100	-0.304400
C	0.231100	1.574800	0.247700
H	-0.167000	2.362800	0.871600
H	0.430800	1.821900	-0.785300
C	0.941600	0.522400	0.830400
H	1.209200	0.572000	1.879500
C	1.796000	-0.284800	-0.052100
H	2.606700	-0.859200	0.427300
O	1.600800	-0.370000	-1.267700

Electronic Energy + ZPE = -382.554884

3CX

C	-0.288200	1.318800	-0.274200
H	0.230400	2.244600	-0.046400
H	0.061300	0.781000	-1.146400
C	-1.614400	1.166600	0.104500
H	-2.126000	1.899000	0.716800
C	-2.188900	-0.103200	-0.096300
H	-3.191300	-0.326800	0.282500
O	-1.493300	-1.055200	-0.595800
C	0.209200	-1.356400	0.454500
H	-0.372800	-1.944500	1.148500
H	0.666500	-1.882700	-0.372500
C	0.757200	-0.136900	0.851200

H	0.542300	0.235900	1.846200
C	2.073500	0.259600	0.295000
H	2.701000	0.873300	0.964600
O	2.468200	-0.041100	-0.829400

Electronic Energy + ZPE = -382.550709

3TN

C	-0.240100	-1.048700	0.982800
H	0.558700	-1.704100	1.311900
H	-0.727800	-0.465200	1.752700
C	-1.006500	-1.392800	-0.127900
H	-0.766600	-2.248600	-0.747000
C	-1.913100	-0.423000	-0.589900
H	-2.455500	-0.566100	-1.529300
O	-1.990500	0.713000	0.003000
C	-0.163800	1.599300	0.066700
H	-0.536700	2.348000	0.750200
H	-0.259600	1.831000	-0.986500
C	0.796000	0.677200	0.489000
H	1.216200	0.769300	1.484400
C	1.700900	0.095200	-0.525200
H	1.289400	0.071500	-1.552400
O	2.820600	-0.347800	-0.285100

Electronic Energy + ZPE = -382.552639

3TX

C	-0.199700	1.236800	-0.414500
H	0.514900	2.041000	-0.279000
H	-0.150900	0.705500	-1.357000
C	-1.441900	1.302100	0.207700
H	-1.683300	2.083400	0.918000

C	-2.254800	0.157400	0.121600
H	-3.186600	0.090200	0.691300
O	-1.832900	-0.882200	-0.499200
C	-0.042000	-1.481700	0.264900
H	-0.580800	-1.970500	1.063000
H	0.155800	-2.084800	-0.612700
C	0.755800	-0.364800	0.518500
H	0.802000	0.051000	1.517800
C	1.997500	-0.226700	-0.275100
H	1.975800	-0.730200	-1.260100
O	2.990800	0.391600	0.096600

Electronic Energy + ZPE = -382.552202

Products

2CN

C	-2.18723200	0.02901400	0.09046400
H	-3.26778900	0.01842200	0.14483000
C	-1.56123000	-1.15461200	-0.03381900
H	-2.07300300	-2.10388100	-0.11154300
C	-1.44108800	1.33408200	0.09997200
H	-1.43595300	1.77638800	1.10110600
H	-1.93969200	2.05258000	-0.55485300
O	-0.19634300	-1.32321500	-0.08835700
C	0.54301600	-0.15212500	0.29103000
C	-0.01020100	1.09979700	-0.38117700
H	0.64509900	1.94111100	-0.15286300
H	0.00236600	0.94160300	-1.46288600
H	0.48402300	-0.03834000	1.38206800
C	1.98040700	-0.42478600	-0.09040600
H	2.16680400	-1.38697300	-0.59530400
O	2.88085800	0.37457300	0.13749000

Electronic Energy + ZPE = -382.623496

2CX

C	0.69702900	1.49333600	-0.12428100
H	1.29273500	2.34992600	0.19972900
H	-0.01205700	1.87238300	-0.86592300
C	1.59335000	0.44625400	-0.72200700
H	2.36115700	0.72970600	-1.43022200
C	1.51832600	-0.85437400	-0.38355500
H	2.19892600	-1.61154500	-0.74802500
O	0.58770200	-1.39691700	0.47581200
C	-0.05169000	0.90010900	1.06889600
H	0.60535400	0.83520400	1.93810400
H	-0.91897600	1.50357900	1.33734000
C	-0.51477300	-0.51144800	0.72919600
H	-1.04917400	-0.96349000	1.56899300
C	-1.44219000	-0.54000400	-0.47812500
H	-1.27330800	-1.37145900	-1.18405800
O	-2.33832300	0.27847500	-0.64539700

Electronic Energy + ZPE = -382.623864

3TN

C	-0.09425300	1.10551500	0.97272700
H	-0.93085600	1.78763800	0.81036300
H	0.27935700	1.28357300	1.98509400
C	0.97365800	1.35965300	-0.05463000
H	1.27845600	2.37429000	-0.27344500
C	1.53200400	0.37281900	-0.77715300
H	2.23933700	0.53591500	-1.57834400
O	1.25879200	-0.96823700	-0.61847200
C	0.60969100	-1.26326400	0.62688100

H	1.33100400	-1.14378900	1.44174200
H	0.31479500	-2.30973900	0.55651300
C	-0.58156100	-0.33522100	0.84578700
H	-1.10098000	-0.65959300	1.75712900
C	-1.56582300	-0.52156200	-0.29174300
H	-1.78366500	-1.57336400	-0.55506100
O	-2.11751000	0.39291500	-0.89092800

Electronic Energy + ZPE = -382.622403

3TX

C	0.16885800	1.34429700	0.15065200
H	-0.16937100	2.16137800	-0.49157600
H	-0.07334400	1.63384300	1.17997100
C	1.64663500	1.13378000	-0.01792500
H	2.31097900	1.98655600	-0.05749700
C	2.18256600	-0.08796600	-0.18660500
H	3.23044400	-0.26255900	-0.38786100
O	1.48135300	-1.26659700	-0.14932200
C	0.16323200	-1.13285500	0.39809700
H	-0.33443200	-2.07630900	0.18196100
H	0.24697900	-1.00299900	1.48376000
C	-0.57831100	0.05647600	-0.21918600
H	-0.60667000	-0.07621800	-1.30290000
C	-1.99423900	0.08993600	0.28686600
H	-2.10953000	0.32183200	1.36352600
O	-2.98479000	-0.12184500	-0.40577500

Electronic Energy + ZPE = -382.620638

IV. ω B97XD

Acrolein

Cis

C	1.466600	-0.467900	0.000000
H	2.547100	-0.370300	0.000000
H	1.042300	-1.468100	-0.000000
C	0.666400	0.600900	0.000000
H	1.068000	1.611300	0.000000
C	-0.812000	0.464400	-0.000000
H	-1.380900	1.415200	0.000000
O	-1.400300	-0.596600	-0.000000

Electronic Energy + ZPE = -191.793126

Trans

C	-1.759400	0.142600	-0.000000
H	-1.848100	1.227100	-0.000100
H	-2.683300	-0.426200	-0.000000
C	-0.563200	-0.450200	0.000000
H	-0.447000	-1.530600	0.000100
C	0.676000	0.351600	0.000000
H	0.527600	1.452700	0.000100
O	1.791300	-0.123400	-0.000000

Electronic Energy + ZPE = -191.796008

Transition States

2CN

C	-1.461500	-0.224500	-0.735500
H	-1.660600	-0.365000	-1.792300
C	-0.992500	-1.309000	0.047100
H	-0.930600	-2.310300	-0.401500
C	-1.446600	1.048500	-0.141800
H	-1.692600	1.063100	0.917200

H	-1.867200	1.869500	-0.718000
O	-0.533000	-1.100800	1.189700
C	1.069600	0.695600	0.758600
C	0.307100	1.648200	0.069500
H	0.094800	2.575300	0.596400
H	0.558600	1.762100	-0.982000
H	1.212700	0.737400	1.832000
C	1.674500	-0.379700	0.002500
H	2.317000	-1.092300	0.544000
O	1.416100	-0.538400	-1.189600

Electronic Energy + ZPE = -383.558199

2CX

C	0.918800	1.196200	-0.624600
H	1.105800	2.258600	-0.763100
H	0.183900	0.773400	-1.308200
C	2.006400	0.389300	-0.265200
H	2.957700	0.819300	0.033100
C	1.747300	-0.970600	-0.014000
H	2.538600	-1.598800	0.422700
O	0.595300	-1.449600	-0.154600
C	-0.324700	1.223500	0.842600
H	0.259600	1.641300	1.656100
H	-0.979300	1.924500	0.328200
C	-0.827400	-0.066300	0.989200
H	-0.549900	-0.705100	1.818800
C	-1.851400	-0.561700	0.053300
H	-2.210400	-1.591400	0.219900
O	-2.260300	0.101700	-0.882300

Electronic Energy + ZPE = -383.554121

2TN

C	-1.938600	0.762100	0.196300
H	-2.607300	1.557000	-0.123900
H	-1.747100	0.721700	1.264100
C	-1.970400	-0.453200	-0.490100
H	-2.528900	-0.570300	-1.413500
C	-1.017500	-1.420600	-0.117800
H	-0.914200	-2.340200	-0.712700
O	-0.190300	-1.185000	0.797700
C	-0.171300	1.592400	-0.158800
H	-0.431600	2.504300	0.371900
H	-0.205100	1.673300	-1.242700
C	0.807800	0.784900	0.407000
H	1.066800	0.867100	1.456900
C	1.733700	0.009900	-0.438900
H	1.331000	-0.260800	-1.439500
O	2.862100	-0.290600	-0.116100

Electronic Energy + ZPE = -382.551255

2TX

C	2.211500	-0.141600	0.010600
H	3.141500	-0.019700	0.556900
C	1.440600	-1.305800	0.182500
H	1.831500	-2.133600	0.792300
C	1.586900	0.933900	-0.627600
H	0.953900	0.691500	-1.476000
H	2.128200	1.872900	-0.712700
O	0.255800	-1.357300	-0.232200
C	-0.809600	0.411800	0.628200
H	-0.849900	-0.157500	1.549200
C	-1.906300	0.180700	-0.329400

H	-1.761100	0.645000	-1.328000
C	0.052800	1.493200	0.464600
H	-0.256500	2.265900	-0.238500
H	0.571700	1.866300	1.341400
O	-2.907700	-0.450800	-0.075000

Electronic Energy + ZPE = -383.550034

3CN

C	-0.564700	-1.053000	1.169500
H	-0.015600	-1.838400	1.682100
H	-1.035300	-0.312200	1.804800
C	-1.090600	-1.277800	-0.091500
H	-0.906400	-2.198600	-0.633600
C	-1.600100	-0.163800	-0.772700
H	-1.937500	-0.259800	-1.811700
O	-1.565000	0.992900	-0.255300
C	0.232200	1.542900	0.299300
H	-0.166400	2.310900	0.950200
H	0.436400	1.833600	-0.724200
C	0.955700	0.477600	0.845800
H	1.198000	0.487600	1.905100
C	1.833100	-0.291000	-0.041700
H	2.608700	-0.907500	0.455800
O	1.718000	-0.308500	-1.254800

Electronic Energy + ZPE = -383.552974

3CX

C	-0.325300	1.331200	-0.279700
H	0.185100	2.257700	-0.027900
H	0.042700	0.813800	-1.159800
C	-1.649300	1.150300	0.094700

H	-2.182000	1.878900	0.697000
C	-2.193200	-0.126100	-0.106800
H	-3.214300	-0.348900	0.231800
O	-1.490100	-1.073800	-0.560800
C	0.223700	-1.337600	0.453600
H	-0.342200	-1.935300	1.155600
H	0.669800	-1.862000	-0.383700
C	0.784900	-0.122700	0.851500
H	0.572800	0.252500	1.848700
C	2.081100	0.285400	0.273700
H	2.674200	0.979500	0.903200
O	2.497800	-0.066100	-0.812600

Electronic Energy + ZPE = -383.550373

3TN

C	-0.243800	-1.056600	0.967100
H	0.572500	-1.709200	1.264400
H	-0.704500	-0.480600	1.762100
C	-1.039000	-1.387700	-0.128500
H	-0.825700	-2.251400	-0.749500
C	-1.938600	-0.409700	-0.567200
H	-2.526700	-0.571100	-1.480900
O	-1.987100	0.725700	-0.008000
C	-0.147200	1.597100	0.075100
H	-0.535800	2.329300	0.770500
H	-0.253200	1.845800	-0.975300
C	0.821500	0.681000	0.484900
H	1.237500	0.769600	1.485600
C	1.728000	0.103500	-0.526700
H	1.332600	0.116500	-1.566100
O	2.814400	-0.377500	-0.284400

Electronic Energy + ZPE = -383.551763

3TX

C	-0.209500	1.248100	-0.381300
H	0.508400	2.042300	-0.196600
H	-0.127900	0.747000	-1.340700
C	-1.468500	1.291900	0.209800
H	-1.739200	2.068200	0.918100
C	-2.263200	0.146200	0.085300
H	-3.231600	0.087700	0.600800
O	-1.824500	-0.887500	-0.499000
C	-0.036100	-1.474500	0.281500
H	-0.589800	-1.948200	1.081000
H	0.146200	-2.091900	-0.592200
C	0.782700	-0.373400	0.531400
H	0.832500	0.042600	1.533100
C	2.015300	-0.235100	-0.270700
H	1.998000	-0.769300	-1.246100
O	2.984500	0.412800	0.062300

Electronic Energy + ZPE = -383.551070

Products

2CN

C	-2.18839500	0.01094600	0.06792600
H	-3.27221100	-0.00162400	0.10284000
C	-1.55084900	-1.15655000	-0.04567200
H	-2.05238600	-2.11348800	-0.13178200
C	-1.45383000	1.32486900	0.09908600
H	-1.48320100	1.76078300	1.10611500
H	-1.94749400	2.04476900	-0.56248700
O	-0.19576300	-1.30820000	-0.07552900

C	0.54519500	-0.15426200	0.29883200
C	-0.00560600	1.11660900	-0.35060800
H	0.63603200	1.95796500	-0.07814700
H	0.03718300	0.99904000	-1.43938900
H	0.50010600	-0.04793900	1.39442300
C	1.98604600	-0.42546300	-0.08321100
H	2.17338100	-1.41182400	-0.55250000
O	2.87241500	0.37262900	0.10588000

Electronic Energy + ZPE = -383.630901

2CX

C	0.79729900	1.46705300	-0.16959100
H	1.41568600	2.31195100	0.15158000
H	0.14140500	1.85026700	-0.96147900
C	1.67239000	0.36087200	-0.69354300
H	2.48824700	0.59567600	-1.36857600
C	1.51113700	-0.91461700	-0.33051500
H	2.16475200	-1.71863500	-0.64856700
O	0.52185700	-1.38136600	0.48735800
C	-0.03477200	0.95354400	1.00925700
H	0.57509000	0.91367100	1.91701000
H	-0.89495900	1.59841800	1.20405700
C	-0.53643800	-0.46076200	0.71739000
H	-1.08316300	-0.85904500	1.57954600
C	-1.49391600	-0.50443200	-0.47048200
H	-1.32166900	-1.33823500	-1.18147500
O	-2.39430500	0.28586500	-0.62075600

Electronic Energy + ZPE = -383.630968

3TN

C	0.57289300	1.43550600	0.45520400
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H	0.19813800	2.35073000	-0.02066000
H	0.98592300	1.74501200	1.42269700
C	1.62867000	0.80034400	-0.40943000
H	2.37496700	1.42237200	-0.89074500
C	1.65828300	-0.51559900	-0.64543400
H	2.37220200	-0.98664100	-1.31161600
O	0.80608700	-1.42881100	-0.11384700
C	-0.00611400	-0.95098800	0.95198900
H	0.59983700	-0.91380800	1.86634200
H	-0.80472900	-1.68353000	1.07381800
C	-0.57620000	0.44485900	0.66673500
H	-1.19494800	0.72529100	1.52699700
C	-1.50883400	0.38791400	-0.53340500
H	-1.18451000	0.94699400	-1.43658500
O	-2.55097100	-0.22351900	-0.52917800

Electronic Energy + ZPE = -383.628672

3TX

C	0.18373200	1.34790200	0.13404400
H	-0.13779200	2.17135200	-0.51279900
H	-0.06019100	1.64874900	1.16336200
C	1.66287100	1.11962500	-0.01507100
H	2.33201100	1.97186600	-0.04909000
C	2.18211100	-0.10126400	-0.16422800
H	3.23457400	-0.28978600	-0.34201500
O	1.47241800	-1.26012100	-0.13174900
C	0.14884600	-1.14166400	0.36499300
H	-0.34977600	-2.07753300	0.10734500
H	0.19051700	-1.04713900	1.46024500
C	-0.58299000	0.06800900	-0.23869900
H	-0.62450000	-0.05550100	-1.32517300

C	-1.99715200	0.10687900	0.28496800
H	-2.09516300	0.36557000	1.36348300
O	-2.98169100	-0.12544100	-0.37592500

Electronic Energy + ZPE = -383.627929

V. ω B97X

Acrolein

Cis

C	1.45949300	-0.47008100	0.00000600
H	2.54178900	-0.38255900	0.00001800
H	1.02299500	-1.46608700	-0.00001100
C	0.66844300	0.60372500	0.00001500
H	1.07416300	1.61342800	0.00003400
C	-0.81128300	0.46661500	-0.00000200
H	-1.38546600	1.41444400	0.00001000
O	-1.39417500	-0.59759800	-0.00002000

Electronic Energy + ZPE = -191.805607

Trans

C	1.75763700	0.14327400	0.00004300
H	1.84139600	1.22910800	0.00006200
H	2.68511800	-0.42128700	0.00006400
C	0.56446900	-0.45218500	0.00000300
H	0.44590800	-1.53325100	-0.00001300
C	-0.67559500	0.35168200	-0.00001900
H	-0.52607800	1.45279100	0.00000500
O	-1.79067600	-0.12299800	-0.00003500

Electronic Energy + ZPE = -191.808272

Transition States

2CN

C	-1.47201200	-0.33024900	-0.72537400
H	-1.68196600	-0.50105700	-1.77693500
C	-0.89709000	-1.35526200	0.05833000
H	-0.75200000	-2.35552200	-0.37439900
C	-1.53887600	0.94607900	-0.14690600
H	-1.76404100	0.95998400	0.91705900
H	-2.01302000	1.73701900	-0.72507800
O	-0.42989100	-1.08581400	1.18972900
C	0.99369300	0.74935800	0.75401200
C	0.19301900	1.65083900	0.04647400
H	-0.07776100	2.57231800	0.55776600
H	0.43844600	1.75851000	-1.00761900
H	1.13252900	0.81619400	1.82780700
C	1.70386400	-0.27746100	0.00908300
H	2.39715300	-0.92966700	0.56591900
O	1.48302500	-0.45888600	-1.18450900

Electronic Energy + ZPE = -383.577796

2CX

C	0.92156500	1.19349100	-0.62087200
H	1.10885500	2.25725000	-0.75577900
H	0.17725600	0.77557300	-1.29851900
C	2.00635400	0.38045500	-0.26911400
H	2.96510500	0.80195000	0.02071300
C	1.73234500	-0.97404200	-0.01989400
H	2.51459200	-1.61917300	0.40911800
O	0.56867400	-1.43487500	-0.15390800
C	-0.31957400	1.21442100	0.85678700
H	0.26456300	1.63033700	1.67249700
H	-0.97556400	1.91429900	0.34151500
C	-0.81286200	-0.07809800	0.98847400

H	-0.54840400	-0.72276800	1.81925800
C	-1.84229100	-0.55914900	0.04400000
H	-2.20675700	-1.59004100	0.19358500
O	-2.24528300	0.12113900	-0.88092500

Electronic Energy + ZPE = -383.574237

2TN

C	-1.94379600	0.75299400	0.18536700
H	-2.61428000	1.54583400	-0.13963900
H	-1.75595700	0.71461700	1.25450900
C	-1.96339500	-0.46430100	-0.49717900
H	-2.51775200	-0.59367000	-1.42267600
C	-1.00431200	-1.41646300	-0.11042800
H	-0.88402500	-2.34332400	-0.69164000
O	-0.18447400	-1.15965500	0.81001100
C	-0.17361100	1.59039900	-0.15654700
H	-0.43475000	2.50081500	0.37774300
H	-0.20250000	1.67625000	-1.24120400
C	0.79568700	0.77392100	0.41018300
H	1.06325700	0.85878700	1.45891700
C	1.72583900	0.00196400	-0.43979400
H	1.31734500	-0.28506400	-1.43394400
O	2.86074800	-0.27851200	-0.12397200

Electronic Energy + ZPE = -383.571027

2TX

C	2.21317400	-0.15459100	0.01444900
H	3.14769700	-0.04577800	0.55769600
C	1.42640000	-1.30620000	0.18172500
H	1.79960600	-2.14504000	0.78823800
C	1.59905800	0.92522600	-0.62459900

H	0.96171700	0.68632100	-1.47160400
H	2.14320100	1.86375000	-0.70870800
O	0.23865400	-1.33509900	-0.23550600
C	-0.79744000	0.40440400	0.62469400
H	-0.84843100	-0.16101000	1.54903500
C	-1.89972700	0.17744800	-0.33361300
H	-1.74993600	0.62978700	-1.33742000
C	0.05575200	1.49115800	0.46547800
H	-0.25278600	2.25902800	-0.24422200
H	0.57217200	1.86930600	1.34263400
O	-2.90822200	-0.43753000	-0.07005100

Electronic Energy + ZPE = -383.569841

3CN

C	-0.56196400	-1.03108100	1.18041500
H	-0.01725400	-1.80899900	1.71150700
H	-1.04168700	-0.28174300	1.80031500
C	-1.08252700	-1.27831700	-0.07861900
H	-0.89714100	-2.20778100	-0.60758000
C	-1.59129000	-0.17199600	-0.77182200
H	-1.92726800	-0.27520900	-1.81168000
O	-1.55995300	0.98842300	-0.26061300
C	0.23701600	1.54155000	0.28634000
H	-0.15975300	2.32128400	0.92631500
H	0.44294000	1.81713700	-0.74194200
C	0.95392900	0.47940100	0.84513300
H	1.20367800	0.50294900	1.90350400
C	1.82831400	-0.29245300	-0.04417500
H	2.61682000	-0.89978300	0.44521700
O	1.69480300	-0.31973300	-1.25554900

Electronic Energy + ZPE = -383.573667

3CX

C	-0.32050900	1.32321500	-0.27316600
H	0.19251000	2.25067300	-0.02496600
H	0.04885200	0.80135100	-1.15116800
C	-1.64700000	1.14929200	0.09459800
H	-2.18357600	1.88048900	0.69209000
C	-2.18793800	-0.12724600	-0.11099400
H	-3.21166100	-0.35463600	0.21957300
O	-1.47784800	-1.07155400	-0.56318100
C	0.22453800	-1.33148600	0.46353900
H	-0.34520300	-1.93046600	1.16301500
H	0.67608900	-1.85710200	-0.37167400
C	0.78344200	-0.11588700	0.85887100
H	0.58057300	0.25817600	1.85954800
C	2.07965200	0.28095700	0.27188900
H	2.69724300	0.95424900	0.90108400
O	2.47185600	-0.06292100	-0.82630800

Electronic Energy + ZPE = -383.570920

3TN

C	-0.24137800	-1.04871000	0.96609000
H	0.57919000	-1.69522000	1.26932600
H	-0.71088900	-0.47381400	1.75771400
C	-1.03099000	-1.38847300	-0.13053300
H	-0.81327700	-2.25339100	-0.75038900
C	-1.93587300	-0.41465900	-0.56642000
H	-2.52576700	-0.57460200	-1.48023400
O	-1.98722100	0.71896800	-0.00212000
C	-0.15233600	1.59466200	0.06848600
H	-0.54435300	2.33174900	0.75864000
H	-0.25989500	1.83677100	-0.98447200

C	0.81635900	0.68291500	0.48252300
H	1.23465300	0.77603500	1.48293800
C	1.72880100	0.10848600	-0.52713000
H	1.34483400	0.13188600	-1.57113300
O	2.81072200	-0.37956100	-0.27794000

Electronic Energy + ZPE = -383.572241

3TX

C	-0.20530500	1.24181400	-0.37396800
H	0.51876300	2.03202600	-0.18897100
H	-0.12479900	0.73855600	-1.33316400
C	-1.46674900	1.29259200	0.21081900
H	-1.74128400	2.06981800	0.91798400
C	-2.26000700	0.14736400	0.07745800
H	-3.23340900	0.08345200	0.58432700
O	-1.81353800	-0.88356800	-0.50812800
C	-0.04119000	-1.47157900	0.29318500
H	-0.60224800	-1.93903200	1.09259500
H	0.14507400	-2.09797600	-0.57473200
C	0.77987500	-0.37255300	0.53771600
H	0.83784200	0.04773100	1.53834400
C	2.01068100	-0.24160500	-0.26931600
H	1.99678900	-0.79189300	-1.23634400
O	2.97596800	0.41870800	0.05120300

Electronic Energy + ZPE = -383.571415

Products

2CN

C	-2.18629900	0.01684000	0.07020900
H	-3.27121700	0.00831200	0.11136200
C	-1.55586400	-1.15315200	-0.04677600

H	-2.06159500	-2.10949000	-0.13142800
C	-1.44610600	1.32865200	0.09758300
H	-1.47610600	1.76866200	1.10333000
H	-1.93792300	2.04797300	-0.56699700
O	-0.19834700	-1.31023100	-0.08320800
C	0.54328600	-0.15813400	0.30040800
C	0.00048400	1.11267700	-0.34934300
H	0.64857800	1.95107700	-0.07881900
H	0.04480100	0.99148400	-1.43859800
H	0.49059000	-0.05617700	1.39686100
C	1.98492500	-0.43168500	-0.07270200
H	2.17929700	-1.42809900	-0.51801600
O	2.86597400	0.37711400	0.09896200

Electronic Energy + ZPE = -383.657884

2CX

C	0.77096000	1.47267200	-0.15707500
H	1.38020000	2.32447400	0.16546800
H	0.10452300	1.85187000	-0.94289400
C	1.65892400	0.38223200	-0.69431500
H	2.46825000	0.63349300	-1.37322000
C	1.51733200	-0.89743700	-0.34145300
H	2.18091700	-1.69130900	-0.66881500
O	0.53656000	-1.38432500	0.47974800
C	-0.04639900	0.93914400	1.02169800
H	0.56926400	0.89900900	1.92651600
H	-0.91411800	1.57207800	1.22715900
C	-0.53257100	-0.47615300	0.71920900
H	-1.07578900	-0.89050900	1.57703200
C	-1.48577200	-0.51661800	-0.47002800
H	-1.32683900	-1.35942000	-1.17418200

O -2.37171600 0.28898500 -0.63040800

Electronic Energy + ZPE = -383.657828

3TN

C 0.63127400 1.43728800 0.42568800

H 0.28746100 2.35886800 -0.06264800

H 1.07696500 1.74740700 1.37885800

C 1.64030700 0.73612600 -0.44494400

H 2.40576500 1.31219900 -0.95527500

C 1.60695400 -0.58455600 -0.64758700

H 2.28616400 -1.10399000 -1.31644800

O 0.72578300 -1.44774000 -0.07679800

C -0.05117600 -0.90733600 0.98851500

H 0.56685300 -0.88256900 1.89610800

H -0.88433800 -1.59775600 1.13010400

C -0.55396000 0.50286900 0.67299800

H -1.15184700 0.84073800 1.52983400

C -1.50538800 0.46409200 -0.51376800

H -1.28555000 1.16716400 -1.34563800

O -2.46447600 -0.26888100 -0.56574000

Electronic Energy + ZPE = -383.655441

3TX

C 0.23847400 1.37059900 0.10202300

H -0.03689600 2.19526300 -0.56585600

H -0.00373300 1.70489600 1.12203100

C 1.70864000 1.07471300 -0.02367500

H 2.41795900 1.89544600 -0.05784800

C 2.17496100 -0.16913600 -0.15048900

H 3.22138000 -0.40685100 -0.31259800

O 1.41159000 -1.29646300 -0.11163600

C	0.09373900	-1.10698000	0.38308700
H	-0.45050000	-2.02352400	0.14557900
H	0.14307300	-0.98949600	1.47658100
C	-0.57802500	0.12093700	-0.24829100
H	-0.61662700	-0.03268400	-1.33241600
C	-1.99792800	0.21106700	0.25621100
H	-2.12423600	0.68056600	1.25780500
O	-2.96028800	-0.20738900	-0.34417300

Electronic Energy + ZPE = -383.654216