

Supplementary Materials: DFT Studies on *cis*-1,4-Polymerization of Dienes Catalyzed by a Cationic Rare-Earth Metal Complex Bearing an Ancillary PNP Ligand

Xingbao Wang, Xiaohui Kang, Guangli Zhou, Jingping Qu, Zhaomin Hou and Yi Luo

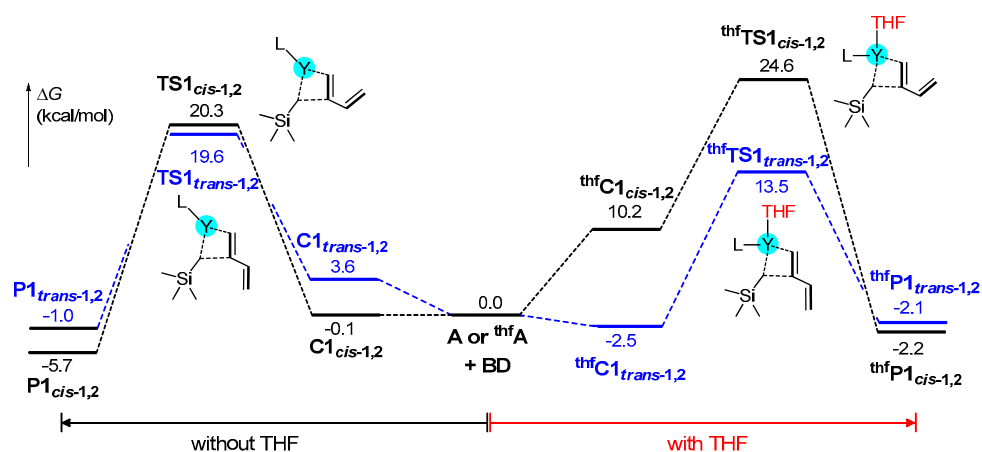


Figure S1. Computed energy profiles (ΔG in kcal/mol) for the first butadiene 1,2-insertion into the Y-alkyl σ -bond of the cationic species ^{thf}A or A .

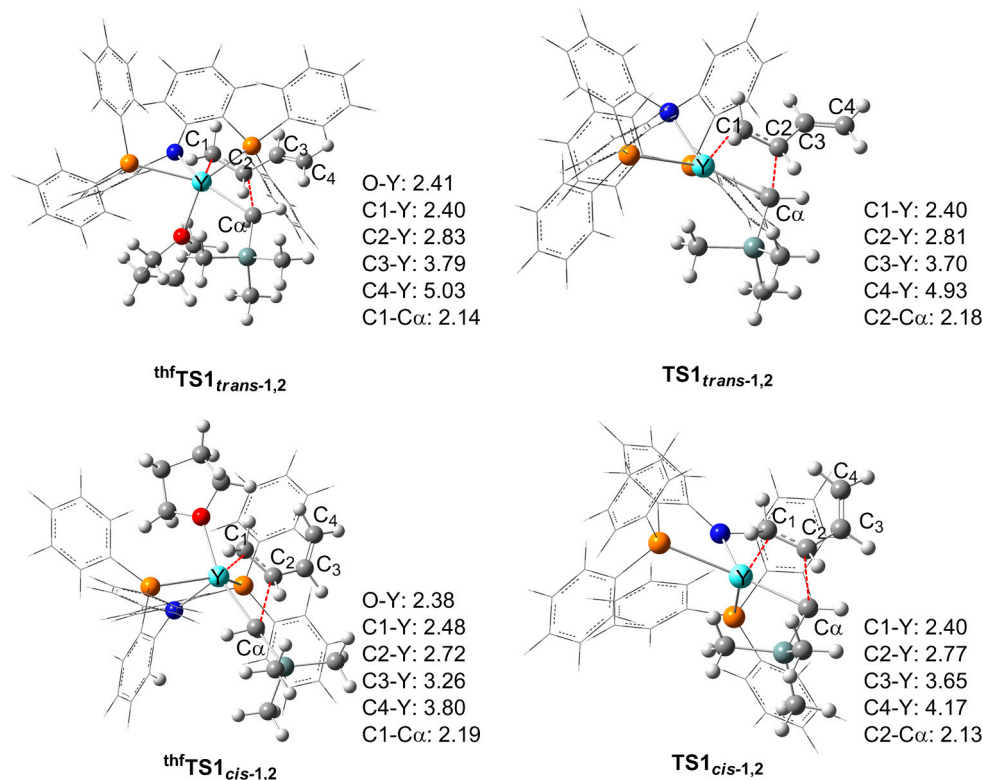


Figure S2. Transition structures (distances in Å) for the 1,2-insertion of butadiene into the Y-alkyl σ -bond of the cationic species ^{thf}A or A .

Optimized coordinates (Å)

10

cis-butadiene E = -155.8596681 a.u.

| | | | |
|---|-------------|--------------|--------------|
| C | 0.000000000 | 1.544955000 | -0.503232000 |
| C | 0.000000000 | 0.734165000 | 0.563084000 |
| C | 0.000000000 | -0.734165000 | 0.563084000 |
| C | 0.000000000 | -1.544955000 | -0.503232000 |
| H | 0.000000000 | 1.168859000 | -1.523654000 |
| H | 0.000000000 | 2.624863000 | -0.386752000 |
| H | 0.000000000 | 1.193935000 | 1.551296000 |
| H | 0.000000000 | -1.193935000 | 1.551296000 |
| H | 0.000000000 | -1.168859000 | -1.523654000 |
| H | 0.000000000 | -2.624863000 | -0.386752000 |

10

trans-butadiene E = -155.8653312 a.u.

| | | | |
|---|--------------|--------------|-------------|
| C | 0.601294000 | 1.749734000 | 0.000000000 |
| C | 0.601294000 | 0.409494000 | 0.000000000 |
| C | -0.601294000 | -0.409494000 | 0.000000000 |
| C | -0.601294000 | -1.749734000 | 0.000000000 |
| H | -0.326353000 | 2.318814000 | 0.000000000 |
| H | 1.524597000 | 2.321846000 | 0.000000000 |
| H | 1.551412000 | -0.126139000 | 0.000000000 |
| H | -1.551412000 | 0.126139000 | 0.000000000 |
| H | -1.524597000 | -2.321846000 | 0.000000000 |
| H | 0.326353000 | -2.318814000 | 0.000000000 |

13

trans-isoprene E = -195.1536413 a.u.

| | | | |
|---|--------------|--------------|--------------|
| C | -1.982355000 | 0.001948000 | 0.000016000 |
| C | -0.829454000 | -0.680686000 | 0.000053000 |
| H | -2.939726000 | -0.511471000 | -0.000007000 |
| H | -2.016350000 | 1.088400000 | -0.000084000 |
| C | 0.515273000 | -0.098486000 | -0.000223000 |
| H | -0.865782000 | -1.770505000 | 0.000108000 |
| C | 1.590370000 | -0.904888000 | -0.000022000 |
| H | 1.488542000 | -1.987825000 | 0.000186000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 2.603084000 | -0.510145000 | 0.000229000 |
| C | 0.653179000 | 1.399983000 | 0.000043000 |
| H | 0.171321000 | 1.841570000 | -0.881562000 |
| H | 0.172235000 | 1.841156000 | 0.882355000 |
| H | 1.704590000 | 1.701593000 | -0.000428000 |

13

THF E = -232.2936148 a.u.

| | | | |
|---|--------------|--------------|--------------|
| C | -1.175930000 | -0.462655000 | 0.000000000 |
| O | -0.000007000 | -1.251995000 | 0.000000000 |
| C | 1.175922000 | -0.462664000 | 0.000000000 |
| C | 0.770963000 | 1.023651000 | 0.000000000 |
| C | -0.770953000 | 1.023657000 | 0.000000000 |
| H | -1.774682000 | -0.718572000 | -0.885504000 |
| H | -1.774682000 | -0.718571000 | 0.885505000 |
| H | 1.774682000 | -0.718595000 | 0.885498000 |
| H | 1.774683000 | -0.718596000 | -0.885497000 |
| H | 1.168052000 | 1.539584000 | 0.879522000 |
| H | 1.168051000 | 1.539583000 | -0.879524000 |
| H | -1.168033000 | 1.539598000 | 0.879522000 |
| H | -1.168033000 | 1.539598000 | -0.879523000 |

97

thf_A E = -1888.854213 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.117318000 | -1.434060000 | -0.424017000 |
| O | 0.184886000 | 0.783646000 | 2.637730000 |
| P | -2.636940000 | -0.337081000 | -0.229392000 |
| P | 2.737061000 | -0.042695000 | -0.363749000 |
| Si | -0.994608000 | 4.168611000 | -0.667955000 |
| C | 0.153675000 | 2.700862000 | -0.913315000 |
| H | 1.174329000 | 3.073828000 | -0.697353000 |
| H | 0.159111000 | 2.455879000 | -1.991771000 |
| C | -2.688384000 | 3.864921000 | -1.454317000 |
| H | -2.601857000 | 3.693512000 | -2.534762000 |
| H | -3.337373000 | 4.739096000 | -1.319192000 |
| H | -3.207788000 | 3.004099000 | -1.015070000 |
| C | -1.268038000 | 4.475294000 | 1.190521000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.785693000 | 3.635524000 | 1.676872000 |
| H | -1.891740000 | 5.363125000 | 1.352298000 |
| H | -0.318975000 | 4.651966000 | 1.714235000 |
| C | -0.273787000 | 5.755357000 | -1.403302000 |
| H | 0.695531000 | 6.003508000 | -0.952943000 |
| H | -0.940241000 | 6.613229000 | -1.248764000 |
| H | -0.115808000 | 5.649257000 | -2.483670000 |
| C | -4.242978000 | 0.064953000 | 0.576116000 |
| C | -5.471972000 | -0.351896000 | 0.050112000 |
| H | -5.504248000 | -0.931610000 | -0.867886000 |
| C | -4.224880000 | 0.830420000 | 1.750886000 |
| H | -3.278832000 | 1.181281000 | 2.160175000 |
| C | -6.660089000 | -0.015973000 | 0.698297000 |
| H | -7.609305000 | -0.340591000 | 0.280876000 |
| C | -5.412520000 | 1.156782000 | 2.400741000 |
| H | -5.387416000 | 1.751579000 | 3.309910000 |
| C | -6.632917000 | 0.733713000 | 1.873249000 |
| H | -7.561145000 | 0.995653000 | 2.373405000 |
| C | -3.028972000 | -0.810846000 | -1.964118000 |
| C | -2.927260000 | 0.166375000 | -2.962228000 |
| H | -2.612695000 | 1.174923000 | -2.707098000 |
| C | -3.426685000 | -2.110748000 | -2.302725000 |
| H | -3.496119000 | -2.877329000 | -1.535357000 |
| C | -3.232148000 | -0.151139000 | -4.284804000 |
| H | -3.152359000 | 0.611235000 | -5.054949000 |
| C | -3.633863000 | -1.444252000 | -4.617466000 |
| H | -3.869378000 | -1.691408000 | -5.649021000 |
| C | -3.730392000 | -2.422150000 | -3.626930000 |
| H | -4.042644000 | -3.430559000 | -3.885180000 |
| C | -0.732156000 | -2.298108000 | 0.282705000 |
| C | -2.068852000 | -1.903810000 | 0.564091000 |
| C | -2.886687000 | -2.691785000 | 1.385145000 |
| H | -3.903305000 | -2.368473000 | 1.593304000 |
| C | -1.123486000 | -4.313918000 | 1.598012000 |
| H | -0.751820000 | -5.257979000 | 1.988908000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.421495000 | -3.894971000 | 1.906183000 |
| H | -3.066646000 | -4.507810000 | 2.528876000 |
| C | -0.291962000 | -3.531889000 | 0.806467000 |
| H | 0.719430000 | -3.862675000 | 0.588190000 |
| C | 1.012679000 | -1.973087000 | -1.359859000 |
| C | 2.304466000 | -1.410822000 | -1.507664000 |
| C | 1.553002000 | -3.519781000 | -3.159580000 |
| H | 1.249137000 | -4.339813000 | -3.805375000 |
| C | 0.662603000 | -3.042397000 | -2.204703000 |
| H | -0.327787000 | -3.479624000 | -2.117535000 |
| C | 2.817948000 | -2.947177000 | -3.310386000 |
| H | 3.506508000 | -3.317381000 | -4.064019000 |
| C | 3.185336000 | -1.890513000 | -2.483147000 |
| H | 4.166146000 | -1.434336000 | -2.588723000 |
| C | 4.066080000 | 0.914513000 | -1.206312000 |
| C | 3.690274000 | 1.904367000 | -2.125474000 |
| H | 2.638920000 | 2.107241000 | -2.310381000 |
| C | 4.662584000 | 2.632419000 | -2.807342000 |
| H | 4.362275000 | 3.396606000 | -3.519102000 |
| C | 5.425858000 | 0.668644000 | -0.975021000 |
| H | 5.731685000 | -0.095684000 | -0.266385000 |
| C | 6.015209000 | 2.386639000 | -2.571101000 |
| H | 6.772523000 | 2.959522000 | -3.099201000 |
| C | 6.394202000 | 1.405911000 | -1.655647000 |
| H | 7.446871000 | 1.209540000 | -1.470623000 |
| C | 4.025555000 | -0.021963000 | 2.124682000 |
| H | 3.921855000 | 1.059540000 | 2.051183000 |
| C | 3.747812000 | -2.228025000 | 1.174237000 |
| H | 3.420581000 | -2.870492000 | 0.361672000 |
| C | 3.577061000 | -0.842738000 | 1.077502000 |
| C | 4.356479000 | -2.783462000 | 2.300973000 |
| H | 4.491914000 | -3.860059000 | 2.362606000 |
| C | 4.806120000 | -1.962964000 | 3.334110000 |
| H | 5.290939000 | -2.397657000 | 4.203983000 |
| C | 4.645084000 | -0.578721000 | 3.241776000 |

| | | | |
|---|--------------|--------------|-------------|
| H | 5.013061000 | 0.067390000 | 4.034898000 |
| C | 0.543901000 | 1.908048000 | 3.504877000 |
| H | -0.086811000 | 2.754302000 | 3.226621000 |
| H | 1.594522000 | 2.153216000 | 3.315628000 |
| C | 0.135859000 | -0.459186000 | 3.427135000 |
| H | 0.713053000 | -1.216707000 | 2.892497000 |
| H | -0.912112000 | -0.767751000 | 3.481694000 |
| C | 0.325822000 | 1.391860000 | 4.916165000 |
| H | 0.937777000 | 1.930329000 | 5.644842000 |
| H | -0.725295000 | 1.498207000 | 5.207212000 |
| C | 0.709833000 | -0.084625000 | 4.783964000 |
| H | 0.297367000 | -0.707383000 | 5.582284000 |
| H | 1.798451000 | -0.202666000 | 4.781870000 |
| Y | -0.003070000 | 0.709870000 | 0.311540000 |

84

A E = -1656.507424 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.085096000 | -0.748697000 | 1.280981000 |
| P | -2.597217000 | -0.239698000 | -0.248167000 |
| P | 2.499231000 | -0.360547000 | -0.175029000 |
| Si | 0.230174000 | 4.069527000 | -0.736977000 |
| C | -0.088981000 | 3.108263000 | 0.830113000 |
| H | -1.039400000 | 3.390390000 | 1.306283000 |
| H | 0.707265000 | 3.260989000 | 1.573943000 |
| C | 0.364047000 | 2.755672000 | -2.191724000 |
| H | 1.204864000 | 2.033556000 | -2.159865000 |
| H | 0.575288000 | 3.334122000 | -3.099643000 |
| H | -0.572650000 | 2.219894000 | -2.440285000 |
| C | -1.195303000 | 5.184041000 | -1.261081000 |
| H | -2.141653000 | 4.634387000 | -1.334722000 |
| H | -1.006459000 | 5.652384000 | -2.234499000 |
| H | -1.336795000 | 5.986480000 | -0.527366000 |
| C | 1.874280000 | 4.985072000 | -0.745840000 |
| H | 1.831169000 | 5.831532000 | -0.049897000 |
| H | 2.123505000 | 5.380341000 | -1.737707000 |
| H | 2.696839000 | 4.338430000 | -0.418226000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.220022000 | 0.547465000 | -0.604686000 |
| C | -4.336865000 | 1.935746000 | -0.438989000 |
| H | -3.489784000 | 2.519486000 | -0.082692000 |
| C | -5.543240000 | 2.575551000 | -0.709360000 |
| H | -5.628084000 | 3.650029000 | -0.571565000 |
| C | -6.637936000 | 1.837317000 | -1.162212000 |
| H | -7.577203000 | 2.337706000 | -1.380577000 |
| C | -6.524606000 | 0.459203000 | -1.335363000 |
| H | -7.375378000 | -0.118140000 | -1.686588000 |
| C | -5.321212000 | -0.188682000 | -1.056027000 |
| H | -5.242671000 | -1.263465000 | -1.190705000 |
| C | -2.709040000 | -1.972635000 | -0.843669000 |
| C | -2.425907000 | -2.227867000 | -2.193005000 |
| H | -2.154444000 | -1.411265000 | -2.859944000 |
| C | -2.509713000 | -3.525927000 | -2.691841000 |
| H | -2.295131000 | -3.717924000 | -3.739560000 |
| C | -2.867450000 | -4.575532000 | -1.845122000 |
| H | -2.928662000 | -5.588573000 | -2.232913000 |
| C | -3.147808000 | -4.325308000 | -0.502083000 |
| H | -3.429852000 | -5.142056000 | 0.156684000 |
| C | -3.070948000 | -3.027637000 | 0.001614000 |
| H | -3.292541000 | -2.836062000 | 1.047769000 |
| C | -2.465033000 | -0.297276000 | 1.593924000 |
| C | -1.184678000 | -0.574642000 | 2.144762000 |
| C | -1.053922000 | -0.580910000 | 3.546863000 |
| H | -0.077750000 | -0.782820000 | 3.978857000 |
| C | -2.143698000 | -0.321454000 | 4.366521000 |
| H | -2.014482000 | -0.329528000 | 5.445621000 |
| C | -3.396987000 | -0.032525000 | 3.816315000 |
| H | -4.246101000 | 0.172647000 | 4.461572000 |
| C | -3.550628000 | -0.011081000 | 2.435758000 |
| H | -4.521132000 | 0.212751000 | 2.002018000 |
| C | 0.764853000 | -1.846394000 | 1.427315000 |
| C | 0.412057000 | -2.999784000 | 2.156284000 |
| H | -0.554094000 | -3.041057000 | 2.649092000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.269531000 | -4.090308000 | 2.237258000 |
| H | 0.958137000 | -4.964228000 | 2.804039000 |
| C | 2.508259000 | -4.084789000 | 1.592990000 |
| H | 3.171563000 | -4.941908000 | 1.655223000 |
| C | 2.874815000 | -2.961299000 | 0.860889000 |
| H | 3.829083000 | -2.943208000 | 0.340395000 |
| C | 2.028807000 | -1.849739000 | 0.780107000 |
| C | 3.424280000 | -0.946854000 | -1.653471000 |
| C | 2.689600000 | -1.317888000 | -2.788579000 |
| H | 1.602755000 | -1.251320000 | -2.784597000 |
| C | 3.341303000 | -1.793099000 | -3.923729000 |
| H | 2.764266000 | -2.081690000 | -4.798058000 |
| C | 4.732903000 | -1.892671000 | -3.937895000 |
| H | 5.242235000 | -2.257843000 | -4.825323000 |
| C | 5.469136000 | -1.521756000 | -2.813718000 |
| H | 6.552867000 | -1.599651000 | -2.821631000 |
| C | 4.820653000 | -1.050674000 | -1.672518000 |
| H | 5.402060000 | -0.760816000 | -0.801855000 |
| C | 3.714538000 | 0.571193000 | 0.852186000 |
| C | 4.357869000 | 1.687913000 | 0.294945000 |
| H | 4.198730000 | 1.947957000 | -0.749731000 |
| C | 5.229180000 | 2.451710000 | 1.067425000 |
| H | 5.735810000 | 3.305183000 | 0.625004000 |
| C | 5.452353000 | 2.119394000 | 2.404975000 |
| H | 6.130215000 | 2.717723000 | 3.007344000 |
| C | 4.809567000 | 1.016440000 | 2.963936000 |
| H | 4.986798000 | 0.750570000 | 4.002501000 |
| C | 3.943326000 | 0.240988000 | 2.192607000 |
| H | 3.454370000 | -0.625125000 | 2.629065000 |
| Y | -0.039097000 | 0.987073000 | -0.118819000 |

107

thf_C1_cis E = -2044.723648 a.u.

| | | | |
|---|--------------|--------------|--------------|
| N | -0.023386000 | -0.260968000 | 1.311519000 |
| P | 2.733469000 | -0.256557000 | -0.013425000 |
| P | -2.748692000 | -0.344738000 | -0.098278000 |

| | | | |
|----|--------------|--------------|--------------|
| Si | -0.072884000 | 4.578438000 | -0.438365000 |
| C | -0.032921000 | 2.636722000 | -0.680060000 |
| H | -0.780358000 | 2.191001000 | 0.006465000 |
| H | 1.001987000 | 2.280529000 | -0.496995000 |
| C | -1.867530000 | 5.215091000 | -0.785778000 |
| H | -2.108199000 | 5.195452000 | -1.862021000 |
| H | -1.957541000 | 6.259487000 | -0.440605000 |
| H | -2.611496000 | 4.609690000 | -0.240311000 |
| C | 0.407976000 | 4.931111000 | 1.399879000 |
| H | -0.288946000 | 4.420758000 | 2.085465000 |
| H | 0.368822000 | 6.015514000 | 1.600895000 |
| H | 1.429433000 | 4.571747000 | 1.608794000 |
| C | 1.201714000 | 5.388795000 | -1.644993000 |
| H | 2.217646000 | 5.013000000 | -1.436896000 |
| H | 1.202871000 | 6.483563000 | -1.506189000 |
| H | 0.953319000 | 5.177295000 | -2.698852000 |
| C | 4.159036000 | -1.305943000 | -0.699362000 |
| C | 3.855190000 | -2.352279000 | -1.593364000 |
| H | 2.820446000 | -2.523094000 | -1.895886000 |
| C | 4.884347000 | -3.165964000 | -2.095575000 |
| H | 4.650868000 | -3.973479000 | -2.793029000 |
| C | 6.216302000 | -2.934457000 | -1.710491000 |
| H | 7.015630000 | -3.563702000 | -2.105696000 |
| C | 6.518941000 | -1.887903000 | -0.823338000 |
| H | 7.553357000 | -1.703987000 | -0.526887000 |
| C | 5.494021000 | -1.070379000 | -0.314737000 |
| H | 5.733786000 | -0.248969000 | 0.363022000 |
| C | 3.623773000 | 1.344033000 | 0.497989000 |
| C | 4.220393000 | 2.124436000 | -0.516351000 |
| H | 4.199075000 | 1.787918000 | -1.556415000 |
| C | 4.873150000 | 3.321591000 | -0.178684000 |
| H | 5.350145000 | 3.917918000 | -0.959187000 |
| C | 4.923503000 | 3.743690000 | 1.162718000 |
| H | 5.434489000 | 4.672397000 | 1.422654000 |
| C | 4.325517000 | 2.965212000 | 2.167943000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.374580000 | 3.286199000 | 3.210437000 |
| C | 3.674078000 | 1.761493000 | 1.840273000 |
| H | 3.222626000 | 1.145035000 | 2.620225000 |
| C | 2.304331000 | -1.094669000 | 1.627366000 |
| C | 0.960479000 | -0.952189000 | 2.086616000 |
| C | 0.632296000 | -1.604280000 | 3.309558000 |
| H | -0.387141000 | -1.523241000 | 3.689646000 |
| C | 1.582969000 | -2.338871000 | 4.025695000 |
| H | 1.289372000 | -2.828077000 | 4.957289000 |
| C | 2.903400000 | -2.466197000 | 3.553209000 |
| H | 3.642253000 | -3.041743000 | 4.112604000 |
| C | 3.255019000 | -1.840998000 | 2.347771000 |
| H | 4.271091000 | -1.934208000 | 1.957259000 |
| C | -1.040175000 | 0.429049000 | 2.046608000 |
| C | -0.753439000 | 1.121925000 | 3.256594000 |
| H | 0.262214000 | 1.083066000 | 3.653059000 |
| C | -1.739868000 | 1.844672000 | 3.935245000 |
| H | -1.481564000 | 2.363543000 | 4.861095000 |
| C | -3.052214000 | 1.921877000 | 3.429927000 |
| H | -3.820463000 | 2.485465000 | 3.961308000 |
| C | -3.360188000 | 1.265904000 | 2.229423000 |
| H | -4.370103000 | 1.320903000 | 1.817488000 |
| C | -2.374180000 | 0.528258000 | 1.546910000 |
| C | -4.361873000 | 0.489643000 | -0.654171000 |
| C | -5.622311000 | -0.034280000 | -0.304472000 |
| H | -5.693393000 | -0.955872000 | 0.275382000 |
| C | -6.790583000 | 0.634900000 | -0.710590000 |
| H | -7.766662000 | 0.227763000 | -0.439940000 |
| C | -6.704842000 | 1.822808000 | -1.455866000 |
| H | -7.614569000 | 2.338521000 | -1.768171000 |
| C | -5.446664000 | 2.346250000 | -1.800055000 |
| H | -5.376897000 | 3.269340000 | -2.379065000 |
| C | -4.275071000 | 1.680540000 | -1.403243000 |
| H | -3.299777000 | 2.089934000 | -1.669886000 |
| C | -3.345567000 | -2.072181000 | 0.433575000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.287267000 | -2.483293000 | 1.777632000 |
| H | -2.922547000 | -1.791893000 | 2.539804000 |
| C | -3.721459000 | -3.774369000 | 2.130728000 |
| H | -3.683952000 | -4.090673000 | 3.175109000 |
| C | -4.220495000 | -4.646669000 | 1.148724000 |
| H | -4.569350000 | -5.642383000 | 1.428167000 |
| C | -4.285567000 | -4.230802000 | -0.194195000 |
| H | -4.694530000 | -4.899137000 | -0.955135000 |
| C | -3.843326000 | -2.946536000 | -0.556860000 |
| H | -3.914479000 | -2.615318000 | -1.596615000 |
| C | 1.434165000 | 0.239065000 | -3.227608000 |
| C | 0.089748000 | 0.153715000 | -3.628053000 |
| H | 2.178913000 | -0.459270000 | -3.616003000 |
| H | 1.837739000 | 1.196941000 | -2.870664000 |
| H | -0.227336000 | -0.714597000 | -4.219998000 |
| C | -0.935806000 | 0.990794000 | -3.114402000 |
| C | -0.597817000 | 2.352433000 | -2.598516000 |
| H | -1.458771000 | 3.029230000 | -2.588383000 |
| H | 0.273519000 | 2.816889000 | -3.082677000 |
| Y | 0.024475000 | -0.072966000 | -0.999133000 |
| H | -1.970143000 | 0.813023000 | -3.419697000 |
| O | 0.069829000 | -2.355564000 | -1.301465000 |
| C | -0.084498000 | -3.150024000 | -2.598721000 |
| C | 0.127727000 | -3.365139000 | -0.134714000 |
| C | 0.273554000 | -4.593302000 | -2.216082000 |
| H | -1.134173000 | -3.057478000 | -2.915035000 |
| H | 0.594889000 | -2.698230000 | -3.331655000 |
| C | -0.268795000 | -4.707452000 | -0.765203000 |
| H | 1.162541000 | -3.353253000 | 0.233364000 |
| H | -0.571416000 | -3.002169000 | 0.626318000 |
| H | 1.366113000 | -4.736421000 | -2.229691000 |
| H | -0.198423000 | -5.316410000 | -2.898231000 |
| H | 0.182784000 | -5.549479000 | -0.219089000 |
| H | -1.364050000 | -4.815736000 | -0.770404000 |

thf_TS1_cis E = -2044.728872 a.u. Imaginary frequency=157i

| | | | |
|----|--------------|--------------|--------------|
| N | 0.004950000 | -0.421676000 | 1.398949000 |
| P | 2.745144000 | -0.270267000 | 0.142463000 |
| P | -2.737660000 | -0.198690000 | 0.123585000 |
| Si | 0.022196000 | 4.381754000 | -0.808745000 |
| C | -0.086468000 | 2.509667000 | -0.580142000 |
| H | -0.842486000 | 2.316131000 | 0.206550000 |
| H | 0.898228000 | 2.248876000 | -0.121286000 |
| C | -1.619619000 | 5.115022000 | -1.394830000 |
| H | -1.951091000 | 4.721972000 | -2.362886000 |
| H | -1.516252000 | 6.201484000 | -1.506534000 |
| H | -2.417995000 | 4.944073000 | -0.662376000 |
| C | 0.473443000 | 5.176308000 | 0.844058000 |
| H | -0.279929000 | 4.959253000 | 1.611005000 |
| H | 0.548321000 | 6.267256000 | 0.751514000 |
| H | 1.437522000 | 4.806521000 | 1.213004000 |
| C | 1.380632000 | 4.806089000 | -2.057894000 |
| H | 2.349015000 | 4.398961000 | -1.741711000 |
| H | 1.495436000 | 5.895227000 | -2.123412000 |
| H | 1.179746000 | 4.448566000 | -3.075317000 |
| C | 4.109930000 | -1.142914000 | -0.739629000 |
| C | 3.784757000 | -1.992383000 | -1.806484000 |
| H | 2.747190000 | -2.100083000 | -2.116001000 |
| C | 4.782239000 | -2.693709000 | -2.480898000 |
| H | 4.520501000 | -3.349604000 | -3.307221000 |
| C | 6.116775000 | -2.543556000 | -2.103621000 |
| H | 6.896121000 | -3.084003000 | -2.633702000 |
| C | 6.449346000 | -1.692741000 | -1.050350000 |
| H | 7.488150000 | -1.570202000 | -0.756041000 |
| C | 5.452847000 | -0.994419000 | -0.369055000 |
| H | 5.722220000 | -0.330087000 | 0.447362000 |
| C | 3.563432000 | 1.197485000 | 0.907138000 |
| C | 4.070924000 | 2.196136000 | 0.061983000 |
| H | 4.008897000 | 2.082510000 | -1.018375000 |
| C | 4.679678000 | 3.327452000 | 0.599652000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 5.081431000 | 4.090511000 | -0.061632000 |
| C | 4.774889000 | 3.478541000 | 1.984544000 |
| H | 5.247714000 | 4.362550000 | 2.403417000 |
| C | 4.268023000 | 2.491280000 | 2.827333000 |
| H | 4.346821000 | 2.601862000 | 3.905525000 |
| C | 3.665699000 | 1.351354000 | 2.293378000 |
| H | 3.286563000 | 0.577418000 | 2.954328000 |
| C | 2.271941000 | -1.368977000 | 1.531781000 |
| C | 0.940686000 | -1.263174000 | 2.016108000 |
| C | 0.593043000 | -2.099055000 | 3.101957000 |
| H | -0.414435000 | -2.043163000 | 3.502724000 |
| C | 1.501186000 | -2.988918000 | 3.658739000 |
| H | 1.185870000 | -3.617999000 | 4.487745000 |
| C | 2.802198000 | -3.094065000 | 3.158684000 |
| H | 3.510264000 | -3.794169000 | 3.591695000 |
| C | 3.174821000 | -2.280998000 | 2.095578000 |
| H | 4.182628000 | -2.347732000 | 1.694165000 |
| C | -0.944484000 | 0.191692000 | 2.233970000 |
| C | -0.594596000 | 0.698660000 | 3.504044000 |
| H | 0.430537000 | 0.587623000 | 3.844257000 |
| C | -1.523313000 | 1.337676000 | 4.313538000 |
| H | -1.210309000 | 1.719096000 | 5.282351000 |
| C | -2.843838000 | 1.506944000 | 3.889132000 |
| H | -3.571094000 | 2.006677000 | 4.522005000 |
| C | -3.211493000 | 1.033373000 | 2.635894000 |
| H | -4.231493000 | 1.169481000 | 2.287338000 |
| C | -2.285471000 | 0.380283000 | 1.810049000 |
| C | -4.241856000 | 0.787347000 | -0.306894000 |
| C | -5.541882000 | 0.273280000 | -0.226067000 |
| H | -5.709088000 | -0.748565000 | 0.099793000 |
| C | -6.635969000 | 1.073425000 | -0.557487000 |
| H | -7.639407000 | 0.661616000 | -0.490316000 |
| C | -6.447247000 | 2.392628000 | -0.963684000 |
| H | -7.301823000 | 3.012351000 | -1.220727000 |
| C | -5.156053000 | 2.916479000 | -1.032866000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.999331000 | 3.947067000 | -1.339834000 |
| C | -4.061444000 | 2.118492000 | -0.710302000 |
| H | -3.061957000 | 2.542488000 | -0.751446000 |
| C | -3.373754000 | -1.922883000 | 0.331938000 |
| C | -3.257126000 | -2.609395000 | 1.544731000 |
| H | -2.827672000 | -2.108822000 | 2.407442000 |
| C | -3.713388000 | -3.923850000 | 1.656365000 |
| H | -3.623793000 | -4.444560000 | 2.606107000 |
| C | -4.300101000 | -4.560376000 | 0.563678000 |
| H | -4.667500000 | -5.578647000 | 0.657758000 |
| C | -4.428612000 | -3.878880000 | -0.648299000 |
| H | -4.902181000 | -4.362037000 | -1.499117000 |
| C | -3.959586000 | -2.571806000 | -0.766614000 |
| H | -4.085274000 | -2.041676000 | -1.708953000 |
| C | 1.783270000 | 0.794760000 | -3.182251000 |
| C | 0.645081000 | 0.185391000 | -3.614387000 |
| H | 2.757936000 | 0.367114000 | -3.392613000 |
| H | 1.771967000 | 1.779120000 | -2.717602000 |
| H | 0.750218000 | -0.766915000 | -4.131178000 |
| C | -0.696865000 | 0.647766000 | -3.327659000 |
| C | -0.931041000 | 1.932297000 | -2.873991000 |
| H | -1.942324000 | 2.252928000 | -2.651625000 |
| H | -0.217473000 | 2.717801000 | -3.081549000 |
| Y | 0.052655000 | 0.117161000 | -0.875339000 |
| H | -1.535688000 | -0.029621000 | -3.477335000 |
| O | -0.164840000 | -2.239741000 | -1.566573000 |
| C | -0.831090000 | -2.846373000 | -2.707621000 |
| C | 0.160477000 | -3.292826000 | -0.592337000 |
| C | -0.452161000 | -4.315037000 | -2.657688000 |
| H | -1.910633000 | -2.707811000 | -2.589147000 |
| H | -0.494570000 | -2.333559000 | -3.609296000 |
| C | -0.433979000 | -4.578075000 | -1.151577000 |
| H | 1.250637000 | -3.337171000 | -0.516119000 |
| H | -0.258552000 | -3.002127000 | 0.371289000 |
| H | 0.539897000 | -4.472803000 | -3.096731000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.168362000 | -4.941494000 | -3.196821000 |
| H | 0.162936000 | -5.451522000 | -0.874622000 |
| H | -1.451820000 | -4.724496000 | -0.775837000 |

107

thf_P1_cis E = -2044.787 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.016242000 | -0.228756000 | 1.314775000 |
| P | 2.713763000 | -0.260977000 | 0.048580000 |
| P | -2.740822000 | -0.296544000 | 0.002149000 |
| Si | 0.002766000 | 4.540410000 | -0.487600000 |
| C | -0.119064000 | 2.696893000 | -1.043850000 |
| H | -0.839085000 | 2.250295000 | -0.332314000 |
| H | 0.887089000 | 2.279720000 | -0.843515000 |
| C | -1.719766000 | 5.296687000 | -0.622479000 |
| H | -2.094712000 | 5.307139000 | -1.652705000 |
| H | -1.702227000 | 6.337627000 | -0.276850000 |
| H | -2.445573000 | 4.759061000 | -0.000406000 |
| C | 0.597075000 | 4.579525000 | 1.294963000 |
| H | -0.073956000 | 4.016527000 | 1.954065000 |
| H | 0.636436000 | 5.611898000 | 1.663809000 |
| H | 1.602124000 | 4.153724000 | 1.394207000 |
| C | 1.211198000 | 5.438283000 | -1.620044000 |
| H | 2.213781000 | 4.998440000 | -1.562034000 |
| H | 1.297627000 | 6.491050000 | -1.324300000 |
| H | 0.892079000 | 5.420512000 | -2.668558000 |
| C | 4.096645000 | -1.246167000 | -0.672680000 |
| C | 3.786996000 | -2.256703000 | -1.592397000 |
| H | 2.750958000 | -2.421859000 | -1.877468000 |
| C | 4.795377000 | -3.040511000 | -2.149151000 |
| H | 4.545785000 | -3.819406000 | -2.865196000 |
| C | 6.126622000 | -2.814836000 | -1.799426000 |
| H | 6.915002000 | -3.419718000 | -2.238838000 |
| C | 6.444239000 | -1.805586000 | -0.891456000 |
| H | 7.480520000 | -1.623590000 | -0.619727000 |
| C | 5.436506000 | -1.022909000 | -0.329084000 |
| H | 5.695795000 | -0.234049000 | 0.371367000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.531573000 | 1.315617000 | 0.558819000 |
| C | 4.012646000 | 2.171939000 | -0.443944000 |
| H | 3.915284000 | 1.896940000 | -1.492370000 |
| C | 4.649605000 | 3.363320000 | -0.103931000 |
| H | 5.034405000 | 4.012027000 | -0.886402000 |
| C | 4.800769000 | 3.717580000 | 1.238220000 |
| H | 5.298579000 | 4.646456000 | 1.502651000 |
| C | 4.317398000 | 2.874387000 | 2.237218000 |
| H | 4.438570000 | 3.143103000 | 3.283239000 |
| C | 3.685346000 | 1.675867000 | 1.901622000 |
| H | 3.324468000 | 1.014890000 | 2.684514000 |
| C | 2.261216000 | -1.115992000 | 1.609140000 |
| C | 0.924271000 | -0.958315000 | 2.061119000 |
| C | 0.569015000 | -1.634333000 | 3.249373000 |
| H | -0.447075000 | -1.541398000 | 3.620912000 |
| C | 1.481169000 | -2.419123000 | 3.942502000 |
| H | 1.161088000 | -2.927700000 | 4.848759000 |
| C | 2.791355000 | -2.572148000 | 3.481877000 |
| H | 3.502836000 | -3.189741000 | 4.021756000 |
| C | 3.168067000 | -1.918651000 | 2.314259000 |
| H | 4.181526000 | -2.030781000 | 1.937668000 |
| C | -0.993390000 | 0.475538000 | 2.039960000 |
| C | -0.680489000 | 1.166695000 | 3.230463000 |
| H | 0.337119000 | 1.123090000 | 3.607199000 |
| C | -1.636917000 | 1.901708000 | 3.918362000 |
| H | -1.351742000 | 2.423284000 | 4.828743000 |
| C | -2.949193000 | 1.987518000 | 3.445595000 |
| H | -3.696832000 | 2.563401000 | 3.982797000 |
| C | -3.283317000 | 1.323514000 | 2.271469000 |
| H | -4.298733000 | 1.381905000 | 1.888893000 |
| C | -2.330515000 | 0.569649000 | 1.571800000 |
| C | -4.289028000 | 0.515154000 | -0.593193000 |
| C | -5.560108000 | -0.021460000 | -0.351031000 |
| H | -5.666599000 | -0.953363000 | 0.195800000 |
| C | -6.699685000 | 0.639037000 | -0.810256000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -7.680381000 | 0.212468000 | -0.617423000 |
| C | -6.584104000 | 1.840031000 | -1.507591000 |
| H | -7.473950000 | 2.351345000 | -1.864271000 |
| C | -5.321909000 | 2.384142000 | -1.745760000 |
| H | -5.224544000 | 3.321424000 | -2.287029000 |
| C | -4.181551000 | 1.723221000 | -1.295972000 |
| H | -3.203045000 | 2.154028000 | -1.487092000 |
| C | -3.297288000 | -1.991515000 | 0.490438000 |
| C | -3.338290000 | -2.411995000 | 1.823997000 |
| H | -3.055752000 | -1.723626000 | 2.615472000 |
| C | -3.760172000 | -3.704560000 | 2.139939000 |
| H | -3.794235000 | -4.019823000 | 3.179444000 |
| C | -4.153898000 | -4.581709000 | 1.130628000 |
| H | -4.494415000 | -5.582864000 | 1.380463000 |
| C | -4.121068000 | -4.166536000 | -0.202477000 |
| H | -4.443606000 | -4.840808000 | -0.991894000 |
| C | -3.684921000 | -2.882357000 | -0.522583000 |
| H | -3.676289000 | -2.561219000 | -1.562728000 |
| C | 1.310804000 | 0.211865000 | -3.242623000 |
| C | -0.046221000 | 0.266065000 | -3.580042000 |
| H | 1.964084000 | -0.517972000 | -3.712782000 |
| H | 1.817964000 | 1.121702000 | -2.913412000 |
| H | -0.457572000 | -0.578721000 | -4.139598000 |
| C | -0.975978000 | 1.147256000 | -3.019175000 |
| C | -0.569312000 | 2.532087000 | -2.517777000 |
| H | -1.423856000 | 3.199445000 | -2.680326000 |
| H | 0.236928000 | 2.919601000 | -3.156977000 |
| Y | 0.007237000 | -0.170297000 | -1.013563000 |
| H | -2.011044000 | 1.035543000 | -3.332680000 |
| O | 0.044287000 | -2.513703000 | -1.299901000 |
| C | -0.119166000 | -3.232199000 | -2.559566000 |
| C | 0.154206000 | -3.476105000 | -0.191965000 |
| C | 0.282092000 | -4.665130000 | -2.253514000 |
| H | -1.171028000 | -3.157253000 | -2.857089000 |
| H | 0.509027000 | -2.741329000 | -3.305947000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.179685000 | -4.827297000 | -0.803512000 |
| H | 1.181157000 | -3.424059000 | 0.179930000 |
| H | -0.535295000 | -3.158561000 | 0.590654000 |
| H | 1.368412000 | -4.785763000 | -2.330901000 |
| H | -0.189544000 | -5.375200000 | -2.938540000 |
| H | 0.329840000 | -5.642093000 | -0.281791000 |
| H | -1.257980000 | -5.010838000 | -0.758657000 |

107

thf_C1_trans E = -2044.73424 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.035742000 | -1.077911000 | -1.292865000 |
| P | -2.733015000 | -0.313176000 | -0.492128000 |
| P | 2.735172000 | -0.392140000 | -0.148769000 |
| Si | 0.811575000 | 4.364849000 | -0.246860000 |
| C | 0.460530000 | 2.562304000 | -0.663667000 |
| H | 1.274163000 | 2.232651000 | -1.340729000 |
| H | -0.433783000 | 2.574337000 | -1.327620000 |
| C | 1.543999000 | 4.591920000 | 1.492439000 |
| H | 0.833359000 | 4.288065000 | 2.271313000 |
| H | 1.785179000 | 5.647060000 | 1.672738000 |
| H | 2.466075000 | 4.017847000 | 1.646093000 |
| C | 2.033495000 | 5.106926000 | -1.487538000 |
| H | 2.984153000 | 4.559252000 | -1.501788000 |
| H | 2.258277000 | 6.155720000 | -1.256671000 |
| H | 1.623619000 | 5.070657000 | -2.504434000 |
| C | -0.784671000 | 5.384364000 | -0.323498000 |
| H | -1.245984000 | 5.316383000 | -1.316598000 |
| H | -0.569341000 | 6.443687000 | -0.136145000 |
| H | -1.533822000 | 5.075973000 | 0.416250000 |
| C | -4.244691000 | -0.546694000 | 0.539287000 |
| C | -4.087518000 | -0.862102000 | 1.897287000 |
| H | -3.089649000 | -0.951948000 | 2.322508000 |
| C | -5.200566000 | -1.061495000 | 2.710598000 |
| H | -5.067751000 | -1.314456000 | 3.759407000 |
| C | -6.484650000 | -0.931432000 | 2.179668000 |
| H | -7.353662000 | -1.080123000 | 2.814535000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.648929000 | -0.607055000 | 0.834350000 |
| H | -7.646653000 | -0.503274000 | 0.416683000 |
| C | -5.536231000 | -0.416739000 | 0.014478000 |
| H | -5.675889000 | -0.166784000 | -1.033243000 |
| C | -3.333517000 | 0.488481000 | -2.041368000 |
| C | -3.558957000 | 1.872550000 | -2.028339000 |
| H | -3.387733000 | 2.448049000 | -1.121148000 |
| C | -4.014717000 | 2.520327000 | -3.174162000 |
| H | -4.191178000 | 3.592296000 | -3.154316000 |
| C | -4.237554000 | 1.793549000 | -4.344198000 |
| H | -4.587481000 | 2.299784000 | -5.239639000 |
| C | -4.011466000 | 0.417864000 | -4.363206000 |
| H | -4.188501000 | -0.150929000 | -5.272121000 |
| C | -3.562049000 | -0.236711000 | -3.216372000 |
| H | -3.392989000 | -1.309676000 | -3.234613000 |
| C | -2.212288000 | -2.002914000 | -0.979740000 |
| C | -0.861683000 | -2.152300000 | -1.388976000 |
| C | -0.463994000 | -3.427347000 | -1.840835000 |
| H | 0.558163000 | -3.570181000 | -2.176721000 |
| C | -1.349205000 | -4.498170000 | -1.854463000 |
| H | -1.002226000 | -5.467950000 | -2.202709000 |
| C | -2.667332000 | -4.345900000 | -1.417505000 |
| H | -3.355308000 | -5.185991000 | -1.425431000 |
| C | -3.090303000 | -3.093683000 | -0.984321000 |
| H | -4.117888000 | -2.951874000 | -0.659436000 |
| C | 1.030765000 | -0.961972000 | -2.286252000 |
| C | 0.727709000 | -1.127687000 | -3.651002000 |
| H | -0.289625000 | -1.383181000 | -3.932849000 |
| C | 1.697142000 | -0.949566000 | -4.629435000 |
| H | 1.428768000 | -1.076383000 | -5.675171000 |
| C | 3.000920000 | -0.589134000 | -4.281341000 |
| H | 3.756271000 | -0.439225000 | -5.047072000 |
| C | 3.322702000 | -0.419528000 | -2.939379000 |
| H | 4.333193000 | -0.135105000 | -2.660169000 |
| C | 2.361222000 | -0.617436000 | -1.940075000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.299250000 | 0.580690000 | -0.084770000 |
| C | 5.558978000 | -0.018768000 | -0.226238000 |
| H | 5.641148000 | -1.092965000 | -0.367125000 |
| C | 6.713043000 | 0.761326000 | -0.179365000 |
| H | 7.685570000 | 0.289262000 | -0.290339000 |
| C | 6.621998000 | 2.140448000 | 0.009985000 |
| H | 7.524353000 | 2.744544000 | 0.048335000 |
| C | 5.372388000 | 2.741646000 | 0.154540000 |
| H | 5.295918000 | 3.814775000 | 0.307085000 |
| C | 4.216156000 | 1.964445000 | 0.111417000 |
| H | 3.243833000 | 2.433788000 | 0.228723000 |
| C | 3.263390000 | -2.059661000 | 0.456929000 |
| C | 3.190516000 | -3.208032000 | -0.337715000 |
| H | 2.846499000 | -3.132330000 | -1.364811000 |
| C | 3.585796000 | -4.445093000 | 0.174569000 |
| H | 3.530628000 | -5.329439000 | -0.454735000 |
| C | 4.066823000 | -4.544764000 | 1.478375000 |
| H | 4.384718000 | -5.506750000 | 1.870949000 |
| C | 4.154715000 | -3.400415000 | 2.273964000 |
| H | 4.550555000 | -3.467541000 | 3.284236000 |
| C | 3.748057000 | -2.166918000 | 1.769820000 |
| H | 3.842355000 | -1.277395000 | 2.389907000 |
| C | -1.823567000 | 2.195678000 | 5.663027000 |
| C | -2.261947000 | 1.974102000 | 4.414110000 |
| H | -2.341545000 | 1.795319000 | 6.529447000 |
| H | -0.945408000 | 2.808015000 | 5.859269000 |
| H | -3.159641000 | 1.377852000 | 4.250882000 |
| C | -1.619948000 | 2.526866000 | 3.232020000 |
| C | -2.079117000 | 2.374366000 | 1.973159000 |
| H | -1.612305000 | 2.901611000 | 1.142757000 |
| H | -2.997843000 | 1.826862000 | 1.774999000 |
| Y | -0.047153000 | 0.506975000 | 0.323330000 |
| H | -0.731752000 | 3.136512000 | 3.404123000 |
| O | 0.087849000 | -0.720415000 | 2.368135000 |
| C | 0.634492000 | -0.341060000 | 3.662264000 |

| | | | |
|---|--------------|--------------|-------------|
| C | -0.113396000 | -2.175274000 | 2.324488000 |
| C | 0.255454000 | -1.483338000 | 4.586554000 |
| H | 1.721326000 | -0.238448000 | 3.560726000 |
| H | 0.193214000 | 0.618549000 | 3.935614000 |
| C | 0.391271000 | -2.698188000 | 3.664483000 |
| H | -1.183894000 | -2.347218000 | 2.181080000 |
| H | 0.435548000 | -2.570020000 | 1.466488000 |
| H | -0.776919000 | -1.362040000 | 4.933149000 |
| H | 0.906781000 | -1.537244000 | 5.463337000 |
| H | -0.187871000 | -3.561065000 | 4.004591000 |
| H | 1.439428000 | -3.001630000 | 3.580706000 |

107

thf_TS1_trans E = -2044.717075 a.u. Imaginary frequency=233i

| | | | |
|----|--------------|--------------|--------------|
| N | 0.027999000 | -0.348544000 | 1.438145000 |
| P | 2.755412000 | -0.209906000 | 0.164373000 |
| P | -2.705030000 | -0.282116000 | 0.138886000 |
| Si | -0.360486000 | 4.381253000 | -0.811266000 |
| C | -0.172951000 | 2.493427000 | -0.725301000 |
| H | -0.931277000 | 2.183419000 | 0.028285000 |
| H | 0.824593000 | 2.345729000 | -0.250679000 |
| C | -2.037738000 | 4.863347000 | -1.533248000 |
| H | -2.152633000 | 4.569059000 | -2.583308000 |
| H | -2.154595000 | 5.953508000 | -1.494306000 |
| H | -2.866257000 | 4.427797000 | -0.962482000 |
| C | -0.234218000 | 5.055333000 | 0.946393000 |
| H | -1.007960000 | 4.630459000 | 1.596825000 |
| H | -0.352207000 | 6.146222000 | 0.957173000 |
| H | 0.739705000 | 4.821999000 | 1.392960000 |
| C | 1.021852000 | 5.139444000 | -1.854006000 |
| H | 2.008762000 | 4.787289000 | -1.530196000 |
| H | 1.012941000 | 6.230158000 | -1.736850000 |
| H | 0.920791000 | 4.934830000 | -2.926162000 |
| C | 4.210994000 | -1.025527000 | -0.617997000 |
| C | 4.003094000 | -1.894505000 | -1.697280000 |
| H | 3.001864000 | -2.040525000 | -2.095099000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.080695000 | -2.553114000 | -2.287199000 |
| H | 4.910889000 | -3.223518000 | -3.125682000 |
| C | 6.374408000 | -2.341554000 | -1.811879000 |
| H | 7.214859000 | -2.850074000 | -2.276227000 |
| C | 6.589451000 | -1.468294000 | -0.745873000 |
| H | 7.596831000 | -1.295658000 | -0.376908000 |
| C | 5.514736000 | -0.811222000 | -0.149225000 |
| H | 5.692883000 | -0.128215000 | 0.676741000 |
| C | 3.444262000 | 1.347795000 | 0.880850000 |
| C | 3.879897000 | 2.346404000 | -0.003643000 |
| H | 3.834350000 | 2.183840000 | -1.079018000 |
| C | 4.397263000 | 3.542294000 | 0.487849000 |
| H | 4.745570000 | 4.304986000 | -0.203496000 |
| C | 4.471154000 | 3.757741000 | 1.865478000 |
| H | 4.872290000 | 4.692043000 | 2.248490000 |
| C | 4.036663000 | 2.770054000 | 2.747279000 |
| H | 4.100955000 | 2.930908000 | 3.820122000 |
| C | 3.526768000 | 1.565806000 | 2.259710000 |
| H | 3.205251000 | 0.792368000 | 2.951174000 |
| C | 2.301481000 | -1.258350000 | 1.603234000 |
| C | 0.974241000 | -1.144365000 | 2.097410000 |
| C | 0.649033000 | -1.916258000 | 3.234363000 |
| H | -0.351287000 | -1.842208000 | 3.650043000 |
| C | 1.573179000 | -2.767765000 | 3.825988000 |
| H | 1.276714000 | -3.349957000 | 4.695148000 |
| C | 2.865413000 | -2.891652000 | 3.310664000 |
| H | 3.585512000 | -3.562292000 | 3.769660000 |
| C | 3.218209000 | -2.132628000 | 2.200540000 |
| H | 4.222049000 | -2.211449000 | 1.792019000 |
| C | -0.933788000 | 0.306189000 | 2.225612000 |
| C | -0.600432000 | 0.904624000 | 3.459298000 |
| H | 0.420118000 | 0.818053000 | 3.819999000 |
| C | -1.537335000 | 1.608972000 | 4.201998000 |
| H | -1.237775000 | 2.062575000 | 5.143486000 |
| C | -2.848816000 | 1.754903000 | 3.741852000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.580994000 | 2.310916000 | 4.319729000 |
| C | -3.203699000 | 1.180970000 | 2.527522000 |
| H | -4.218181000 | 1.296161000 | 2.156837000 |
| C | -2.273050000 | 0.452564000 | 1.773386000 |
| C | -4.236922000 | 0.576822000 | -0.419836000 |
| C | -5.505094000 | 0.229718000 | 0.069282000 |
| H | -5.609750000 | -0.575339000 | 0.791380000 |
| C | -6.637670000 | 0.908417000 | -0.376125000 |
| H | -7.615761000 | 0.632485000 | 0.008557000 |
| C | -6.517959000 | 1.935993000 | -1.312140000 |
| H | -7.403580000 | 2.460601000 | -1.659943000 |
| C | -5.261436000 | 2.285635000 | -1.804321000 |
| H | -5.163423000 | 3.083293000 | -2.535517000 |
| C | -4.126923000 | 1.606086000 | -1.363073000 |
| H | -3.150544000 | 1.882943000 | -1.751881000 |
| C | -3.285102000 | -2.003939000 | 0.483766000 |
| C | -3.001656000 | -2.647463000 | 1.692555000 |
| H | -2.476783000 | -2.113725000 | 2.478798000 |
| C | -3.415607000 | -3.963727000 | 1.902313000 |
| H | -3.198185000 | -4.450537000 | 2.849354000 |
| C | -4.120762000 | -4.645317000 | 0.911592000 |
| H | -4.452826000 | -5.665770000 | 1.082095000 |
| C | -4.413815000 | -4.005975000 | -0.294739000 |
| H | -4.979633000 | -4.524822000 | -1.064182000 |
| C | -3.993899000 | -2.695201000 | -0.511109000 |
| H | -4.251401000 | -2.198516000 | -1.444288000 |
| C | 1.668787000 | -0.897364000 | -4.442918000 |
| C | 1.330884000 | 0.189415000 | -3.718790000 |
| H | 2.707530000 | -1.116541000 | -4.667726000 |
| H | 0.924820000 | -1.552007000 | -4.890929000 |
| H | 2.148180000 | 0.831844000 | -3.376831000 |
| C | -0.005138000 | 0.653486000 | -3.372748000 |
| C | -0.217589000 | 1.960941000 | -2.915888000 |
| H | -1.206036000 | 2.396668000 | -3.007385000 |
| H | 0.596005000 | 2.674247000 | -2.995284000 |

| | | | |
|---|--------------|--------------|--------------|
| Y | 0.036591000 | 0.100164000 | -0.850366000 |
| H | -0.866784000 | 0.083254000 | -3.724362000 |
| O | -0.168129000 | -2.209004000 | -1.474399000 |
| C | -0.901445000 | -2.766189000 | -2.602445000 |
| C | 0.301142000 | -3.298191000 | -0.611416000 |
| C | -0.560606000 | -4.246673000 | -2.612461000 |
| H | -1.968453000 | -2.596825000 | -2.424716000 |
| H | -0.584155000 | -2.233742000 | -3.498669000 |
| C | -0.399920000 | -4.546721000 | -1.121146000 |
| H | 1.388270000 | -3.361655000 | -0.723780000 |
| H | 0.055695000 | -3.040910000 | 0.419492000 |
| H | 0.379595000 | -4.420313000 | -3.148351000 |
| H | -1.342878000 | -4.843003000 | -3.090302000 |
| H | 0.187259000 | -5.448232000 | -0.924684000 |
| H | -1.378107000 | -4.659876000 | -0.642599000 |

107

thf_P1_trans E = -2044.778141 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.285605000 | -0.290903000 | 1.268977000 |
| P | 2.868314000 | 0.392322000 | 0.018124000 |
| P | -2.209206000 | -1.438555000 | -0.019849000 |
| Si | -2.906767000 | 4.883738000 | -0.345985000 |
| C | -1.649157000 | 3.536176000 | -0.838212000 |
| H | -1.334112000 | 3.009241000 | 0.076289000 |
| H | -0.757705000 | 4.064305000 | -1.206773000 |
| C | -4.539694000 | 4.087480000 | 0.168992000 |
| H | -5.025092000 | 3.573960000 | -0.669868000 |
| H | -5.243476000 | 4.842275000 | 0.540273000 |
| H | -4.387915000 | 3.352261000 | 0.968302000 |
| C | -2.177543000 | 5.851575000 | 1.101800000 |
| H | -2.009905000 | 5.204370000 | 1.971209000 |
| H | -2.848942000 | 6.659920000 | 1.415584000 |
| H | -1.215987000 | 6.307732000 | 0.836389000 |
| C | -3.190662000 | 6.041956000 | -1.810363000 |
| H | -2.254606000 | 6.509007000 | -2.140207000 |
| H | -3.882446000 | 6.849160000 | -1.540533000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.622276000 | 5.518752000 | -2.672097000 |
| C | 4.521468000 | -0.048785000 | -0.660763000 |
| C | 4.596904000 | -1.003654000 | -1.682940000 |
| H | 3.683698000 | -1.445022000 | -2.075015000 |
| C | 5.831577000 | -1.375125000 | -2.212652000 |
| H | 5.881389000 | -2.113323000 | -3.008900000 |
| C | 7.000833000 | -0.787517000 | -1.731430000 |
| H | 7.963357000 | -1.071549000 | -2.147837000 |
| C | 6.932953000 | 0.175438000 | -0.724268000 |
| H | 7.841996000 | 0.642385000 | -0.355030000 |
| C | 5.700229000 | 0.547331000 | -0.191185000 |
| H | 5.654129000 | 1.309964000 | 0.581625000 |
| C | 3.025215000 | 2.184769000 | 0.447597000 |
| C | 3.225868000 | 3.103577000 | -0.594220000 |
| H | 3.329610000 | 2.752559000 | -1.618435000 |
| C | 3.324204000 | 4.465645000 | -0.320969000 |
| H | 3.492205000 | 5.168083000 | -1.133094000 |
| C | 3.211955000 | 4.925154000 | 0.992319000 |
| H | 3.288387000 | 5.987925000 | 1.205086000 |
| C | 3.011380000 | 4.017136000 | 2.030349000 |
| H | 2.935436000 | 4.369776000 | 3.055544000 |
| C | 2.918672000 | 2.650817000 | 1.762462000 |
| H | 2.780758000 | 1.946957000 | 2.578149000 |
| C | 2.700569000 | -0.466537000 | 1.630134000 |
| C | 1.369676000 | -0.644761000 | 2.088918000 |
| C | 1.199088000 | -1.237659000 | 3.355635000 |
| H | 0.195069000 | -1.372744000 | 3.745213000 |
| C | 2.288929000 | -1.661568000 | 4.107586000 |
| H | 2.115441000 | -2.124932000 | 5.075760000 |
| C | 3.591989000 | -1.512892000 | 3.629900000 |
| H | 4.440527000 | -1.855030000 | 4.214677000 |
| C | 3.787181000 | -0.908951000 | 2.391390000 |
| H | 4.796057000 | -0.775270000 | 2.009776000 |
| C | -0.900888000 | 0.155049000 | 1.883224000 |
| C | -0.875635000 | 1.068755000 | 2.957485000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.087424000 | 1.394864000 | 3.338994000 |
| C | -2.046196000 | 1.558420000 | 3.519365000 |
| H | -1.987564000 | 2.262622000 | 4.345477000 |
| C | -3.291708000 | 1.166347000 | 3.021084000 |
| H | -4.208604000 | 1.551399000 | 3.457446000 |
| C | -3.345124000 | 0.272053000 | 1.958430000 |
| H | -4.309662000 | -0.035547000 | 1.565384000 |
| C | -2.172760000 | -0.251729000 | 1.395137000 |
| C | -3.942432000 | -1.442153000 | -0.649906000 |
| C | -4.966974000 | -2.114661000 | 0.033131000 |
| H | -4.748145000 | -2.652113000 | 0.951890000 |
| C | -6.266356000 | -2.106160000 | -0.468784000 |
| H | -7.053818000 | -2.628478000 | 0.067755000 |
| C | -6.555485000 | -1.434529000 | -1.657340000 |
| H | -7.569418000 | -1.432883000 | -2.047835000 |
| C | -5.541087000 | -0.772884000 | -2.347032000 |
| H | -5.759707000 | -0.255857000 | -3.277458000 |
| C | -4.239374000 | -0.779590000 | -1.847300000 |
| H | -3.452833000 | -0.268377000 | -2.394418000 |
| C | -2.057880000 | -3.119935000 | 0.739800000 |
| C | -1.835940000 | -3.313600000 | 2.106191000 |
| H | -1.772831000 | -2.456542000 | 2.769577000 |
| C | -1.718056000 | -4.605243000 | 2.622463000 |
| H | -1.551014000 | -4.745061000 | 3.687137000 |
| C | -1.829107000 | -5.710695000 | 1.781746000 |
| H | -1.746611000 | -6.715131000 | 2.187768000 |
| C | -2.061333000 | -5.524583000 | 0.417381000 |
| H | -2.169748000 | -6.383866000 | -0.239526000 |
| C | -2.167816000 | -4.236821000 | -0.103082000 |
| H | -2.367535000 | -4.101219000 | -1.164444000 |
| C | 1.155847000 | 0.933031000 | -3.156625000 |
| C | 0.210203000 | 1.833669000 | -2.655105000 |
| H | 2.181996000 | 1.245410000 | -3.321178000 |
| H | 0.813645000 | 0.124404000 | -3.811989000 |
| H | 0.599534000 | 2.759048000 | -2.222761000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.125003000 | 1.514307000 | -2.373454000 |
| C | -2.148611000 | 2.524377000 | -1.877921000 |
| H | -3.004093000 | 1.980535000 | -1.457735000 |
| H | -2.549202000 | 3.066444000 | -2.750046000 |
| Y | 0.244650000 | -0.182372000 | -1.007887000 |
| H | -1.546582000 | 0.709228000 | -2.995892000 |
| O | 0.966830000 | -2.309592000 | -1.737879000 |
| C | 0.876596000 | -2.915317000 | -3.061047000 |
| C | 1.467513000 | -3.294954000 | -0.768699000 |
| C | 1.685513000 | -4.198689000 | -2.963780000 |
| H | -0.181033000 | -3.110702000 | -3.273125000 |
| H | 1.267291000 | -2.195119000 | -3.783558000 |
| C | 1.453073000 | -4.621642000 | -1.511187000 |
| H | 2.477322000 | -2.986176000 | -0.481840000 |
| H | 0.811825000 | -3.268466000 | 0.104401000 |
| H | 2.747303000 | -3.997973000 | -3.144903000 |
| H | 1.352323000 | -4.946762000 | -3.688352000 |
| H | 2.221866000 | -5.302734000 | -1.136215000 |
| H | 0.479482000 | -5.109543000 | -1.398753000 |

107

thf_TS1_anti_syn_isomerism E = -2044.741835 a.u. Imaginary frequency=162i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.034984000 | -0.233809000 | 1.360483000 |
| P | 2.688116000 | -0.612902000 | 0.161498000 |
| P | -2.729164000 | -0.509566000 | 0.094076000 |
| Si | 0.038684000 | 5.149805000 | -0.383759000 |
| C | 0.210658000 | 3.311241000 | -0.864242000 |
| H | -0.077693000 | 2.720452000 | 0.023107000 |
| H | 1.280013000 | 3.112103000 | -1.034866000 |
| C | -1.786641000 | 5.572493000 | -0.143053000 |
| H | -2.357312000 | 5.466843000 | -1.073596000 |
| H | -1.906022000 | 6.608512000 | 0.196755000 |
| H | -2.249732000 | 4.922450000 | 0.609496000 |
| C | 0.972411000 | 5.433000000 | 1.232280000 |
| H | 0.535571000 | 4.844752000 | 2.048369000 |
| H | 0.938538000 | 6.488172000 | 1.529558000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.026779000 | 5.145429000 | 1.143745000 |
| C | 0.773163000 | 6.231736000 | -1.747493000 |
| H | 1.833558000 | 6.004856000 | -1.912660000 |
| H | 0.701647000 | 7.294268000 | -1.484786000 |
| H | 0.251405000 | 6.096552000 | -2.702443000 |
| C | 4.067521000 | -1.668987000 | -0.455168000 |
| C | 3.819560000 | -2.576667000 | -1.492897000 |
| H | 2.827062000 | -2.635214000 | -1.934292000 |
| C | 4.839494000 | -3.393549000 | -1.978049000 |
| H | 4.638433000 | -4.092170000 | -2.786056000 |
| C | 6.120783000 | -3.303122000 | -1.435730000 |
| H | 6.918480000 | -3.934855000 | -1.816537000 |
| C | 6.380400000 | -2.390865000 | -0.413027000 |
| H | 7.380539000 | -2.310092000 | 0.003972000 |
| C | 5.361875000 | -1.574062000 | 0.074458000 |
| H | 5.576532000 | -0.853785000 | 0.859233000 |
| C | 3.531360000 | 0.957388000 | 0.648070000 |
| C | 3.958528000 | 1.819263000 | -0.372329000 |
| H | 3.774475000 | 1.568201000 | -1.414824000 |
| C | 4.628850000 | 2.998894000 | -0.057665000 |
| H | 4.964733000 | 3.657718000 | -0.853918000 |
| C | 4.866075000 | 3.333213000 | 1.276711000 |
| H | 5.388788000 | 4.253797000 | 1.521594000 |
| C | 4.432674000 | 2.484599000 | 2.294208000 |
| H | 4.617259000 | 2.741688000 | 3.333859000 |
| C | 3.767481000 | 1.297801000 | 1.984422000 |
| H | 3.441126000 | 0.634497000 | 2.780594000 |
| C | 2.109488000 | -1.364746000 | 1.735446000 |
| C | 0.803450000 | -1.010859000 | 2.171669000 |
| C | 0.381005000 | -1.520527000 | 3.416634000 |
| H | -0.607524000 | -1.260548000 | 3.781633000 |
| C | 1.193405000 | -2.357721000 | 4.170674000 |
| H | 0.825890000 | -2.736555000 | 5.121235000 |
| C | 2.460136000 | -2.728304000 | 3.715297000 |
| H | 3.089778000 | -3.391311000 | 4.300940000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.908104000 | -2.225336000 | 2.498293000 |
| H | 3.896521000 | -2.495642000 | 2.136359000 |
| C | -0.993712000 | 0.593823000 | 1.975959000 |
| C | -0.663080000 | 1.446792000 | 3.046228000 |
| H | 0.351593000 | 1.428902000 | 3.433781000 |
| C | -1.605081000 | 2.309705000 | 3.592624000 |
| H | -1.318910000 | 2.959641000 | 4.415706000 |
| C | -2.905481000 | 2.361081000 | 3.082867000 |
| H | -3.637515000 | 3.042710000 | 3.505914000 |
| C | -3.255727000 | 1.526009000 | 2.027175000 |
| H | -4.265105000 | 1.555942000 | 1.626269000 |
| C | -2.322929000 | 0.634196000 | 1.482154000 |
| C | -4.299174000 | 0.122439000 | -0.634418000 |
| C | -5.553201000 | -0.249762000 | -0.131171000 |
| H | -5.623011000 | -0.939524000 | 0.705403000 |
| C | -6.715923000 | 0.259526000 | -0.707177000 |
| H | -7.684730000 | -0.033805000 | -0.311880000 |
| C | -6.637529000 | 1.140929000 | -1.785247000 |
| H | -7.546108000 | 1.534895000 | -2.232392000 |
| C | -5.392350000 | 1.512596000 | -2.291695000 |
| H | -5.327191000 | 2.195892000 | -3.134236000 |
| C | -4.227233000 | 1.001581000 | -1.723153000 |
| H | -3.258865000 | 1.288197000 | -2.124112000 |
| C | -3.224370000 | -2.101162000 | 0.893266000 |
| C | -3.312951000 | -2.256540000 | 2.280071000 |
| H | -3.104845000 | -1.413999000 | 2.933141000 |
| C | -3.683451000 | -3.486457000 | 2.825721000 |
| H | -3.753066000 | -3.596450000 | 3.904638000 |
| C | -3.974171000 | -4.566031000 | 1.993869000 |
| H | -4.267660000 | -5.520536000 | 2.421983000 |
| C | -3.898195000 | -4.415270000 | 0.608107000 |
| H | -4.141468000 | -5.249518000 | -0.044903000 |
| C | -3.519818000 | -3.191480000 | 0.060513000 |
| H | -3.482389000 | -3.075044000 | -1.021559000 |
| C | 1.490027000 | 1.643098000 | -4.186887000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.909158000 | 1.089478000 | -3.115289000 |
| H | 2.472605000 | 1.334721000 | -4.537878000 |
| H | 0.998185000 | 2.436625000 | -4.746180000 |
| H | 1.558965000 | 0.300501000 | -2.649654000 |
| C | -0.416351000 | 1.395480000 | -2.478019000 |
| C | -0.612162000 | 2.868649000 | -2.083657000 |
| H | -1.676923000 | 3.027734000 | -1.866647000 |
| H | -0.381445000 | 3.531265000 | -2.934113000 |
| Y | 0.002721000 | -0.297173000 | -0.903478000 |
| H | -1.214208000 | 1.090052000 | -3.177717000 |
| O | -0.065181000 | -2.344787000 | -2.032900000 |
| C | -0.351150000 | -2.493621000 | -3.460988000 |
| C | -0.034530000 | -3.663835000 | -1.387930000 |
| C | -0.053845000 | -3.952226000 | -3.759066000 |
| H | -1.406287000 | -2.246402000 | -3.622040000 |
| H | 0.276838000 | -1.779477000 | -3.998937000 |
| C | -0.488279000 | -4.641962000 | -2.462614000 |
| H | 0.994962000 | -3.843555000 | -1.064727000 |
| H | -0.693163000 | -3.629025000 | -0.516509000 |
| H | 1.017075000 | -4.097789000 | -3.939757000 |
| H | -0.599244000 | -4.308555000 | -4.637090000 |
| H | -0.035398000 | -5.628044000 | -2.329098000 |
| H | -1.576805000 | -4.762520000 | -2.437886000 |

107

thf_C1_trans_1,2 E = -2044.747494 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.035620000 | -0.518874000 | -1.583506000 |
| P | -2.725373000 | -0.103461000 | -0.448461000 |
| P | 2.723681000 | -0.472519000 | -0.273234000 |
| Si | 0.415798000 | 4.171186000 | 0.349969000 |
| C | -0.449019000 | 2.567427000 | 0.809667000 |
| H | -1.386161000 | 2.596117000 | 0.215843000 |
| H | -0.789773000 | 2.669317000 | 1.859392000 |
| C | 1.742628000 | 4.638653000 | 1.624231000 |
| H | 1.289088000 | 4.883806000 | 2.593383000 |
| H | 2.285793000 | 5.533129000 | 1.294424000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.485663000 | 3.850710000 | 1.796685000 |
| C | 1.215840000 | 4.034552000 | -1.361484000 |
| H | 1.989993000 | 3.259357000 | -1.414072000 |
| H | 1.682161000 | 4.984757000 | -1.650941000 |
| H | 0.468054000 | 3.795480000 | -2.128313000 |
| C | -0.816024000 | 5.608784000 | 0.289332000 |
| H | -1.603901000 | 5.425324000 | -0.451778000 |
| H | -0.324185000 | 6.552884000 | 0.022868000 |
| H | -1.307113000 | 5.753887000 | 1.259798000 |
| C | -3.939581000 | -0.865539000 | 0.715066000 |
| C | -4.276131000 | -2.224863000 | 0.731971000 |
| H | -3.866615000 | -2.898673000 | -0.014091000 |
| C | -5.156762000 | -2.722602000 | 1.695408000 |
| H | -5.422595000 | -3.776610000 | 1.683875000 |
| C | -5.704145000 | -1.874307000 | 2.655808000 |
| H | -6.396232000 | -2.262898000 | 3.397807000 |
| C | -5.365281000 | -0.519746000 | 2.654634000 |
| H | -5.790602000 | 0.150641000 | 3.396804000 |
| C | -4.486156000 | -0.020007000 | 1.696861000 |
| H | -4.236727000 | 1.039374000 | 1.701202000 |
| C | -3.683832000 | 1.191434000 | -1.354896000 |
| C | -2.957567000 | 2.087704000 | -2.152597000 |
| H | -1.873146000 | 2.021769000 | -2.202359000 |
| C | -3.620743000 | 3.059100000 | -2.898680000 |
| H | -3.049640000 | 3.747637000 | -3.515683000 |
| C | -5.011767000 | 3.151224000 | -2.848072000 |
| H | -5.528223000 | 3.913254000 | -3.425192000 |
| C | -5.737339000 | 2.262514000 | -2.056972000 |
| H | -6.821553000 | 2.326095000 | -2.019050000 |
| C | -5.079376000 | 1.282574000 | -1.313882000 |
| H | -5.658498000 | 0.592450000 | -0.707578000 |
| C | -2.289858000 | -1.333814000 | -1.734311000 |
| C | -0.929589000 | -1.376510000 | -2.139341000 |
| C | -0.584545000 | -2.328626000 | -3.124234000 |
| H | 0.452985000 | -2.405561000 | -3.434075000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.538509000 | -3.145918000 | -3.713055000 |
| H | -1.229106000 | -3.862244000 | -4.470152000 |
| C | -2.886061000 | -3.047301000 | -3.354475000 |
| H | -3.637374000 | -3.663429000 | -3.839198000 |
| C | -3.247984000 | -2.138007000 | -2.369257000 |
| H | -4.295086000 | -2.030733000 | -2.097281000 |
| C | 1.048288000 | -0.059874000 | -2.449455000 |
| C | 0.766939000 | 0.365584000 | -3.763716000 |
| H | -0.254727000 | 0.301662000 | -4.127278000 |
| C | 1.766594000 | 0.864242000 | -4.588558000 |
| H | 1.512473000 | 1.189943000 | -5.594113000 |
| C | 3.084859000 | 0.965380000 | -4.135131000 |
| H | 3.863731000 | 1.358655000 | -4.781530000 |
| C | 3.387201000 | 0.558347000 | -2.841185000 |
| H | 4.406670000 | 0.635160000 | -2.473322000 |
| C | 2.390046000 | 0.040569000 | -2.003311000 |
| C | 4.322375000 | 0.330811000 | 0.169805000 |
| C | 5.532422000 | -0.369658000 | 0.237703000 |
| H | 5.564624000 | -1.431785000 | 0.013929000 |
| C | 6.706159000 | 0.297249000 | 0.590075000 |
| H | 7.641212000 | -0.254187000 | 0.639493000 |
| C | 6.683786000 | 1.662146000 | 0.871190000 |
| H | 7.600631000 | 2.176898000 | 1.144715000 |
| C | 5.481698000 | 2.366973000 | 0.798683000 |
| H | 5.457003000 | 3.431940000 | 1.012664000 |
| C | 4.306245000 | 1.703947000 | 0.455582000 |
| H | 3.375452000 | 2.263430000 | 0.394327000 |
| C | 3.102238000 | -2.277968000 | -0.322576000 |
| C | 3.218297000 | -2.983815000 | -1.524676000 |
| H | 3.102379000 | -2.463220000 | -2.471034000 |
| C | 3.496610000 | -4.350937000 | -1.509212000 |
| H | 3.588233000 | -4.891163000 | -2.447661000 |
| C | 3.668662000 | -5.020140000 | -0.298390000 |
| H | 3.892302000 | -6.083390000 | -0.290816000 |
| C | 3.563084000 | -4.319924000 | 0.904588000 |

| | | | |
|---|--------------|--------------|-------------|
| H | 3.710992000 | -4.834610000 | 1.850424000 |
| C | 3.274127000 | -2.956747000 | 0.893881000 |
| H | 3.205821000 | -2.413993000 | 1.835172000 |
| C | -0.555621000 | 2.260571000 | 5.617145000 |
| C | 0.267722000 | 1.325023000 | 5.120909000 |
| H | -1.143527000 | 2.086139000 | 6.513376000 |
| H | -0.653753000 | 3.238217000 | 5.149969000 |
| H | 0.359033000 | 0.365166000 | 5.630650000 |
| C | 1.100914000 | 1.532178000 | 3.946123000 |
| C | 1.923354000 | 0.608910000 | 3.409167000 |
| H | 2.604838000 | 0.860054000 | 2.600265000 |
| H | 2.024986000 | -0.385572000 | 3.841478000 |
| Y | 0.002797000 | 0.285667000 | 0.553499000 |
| H | 1.067187000 | 2.525610000 | 3.501439000 |
| O | -0.604951000 | -1.516773000 | 1.953968000 |
| C | -1.236187000 | -1.530485000 | 3.273600000 |
| C | -0.489631000 | -2.885568000 | 1.445754000 |
| C | -1.629525000 | -2.980958000 | 3.523248000 |
| H | -0.491774000 | -1.168759000 | 3.986518000 |
| H | -2.086511000 | -0.845009000 | 3.250155000 |
| C | -0.616354000 | -3.759327000 | 2.679836000 |
| H | -1.304516000 | -3.052596000 | 0.734104000 |
| H | 0.470093000 | -2.969831000 | 0.931440000 |
| H | -2.647342000 | -3.164420000 | 3.166646000 |
| H | -1.586624000 | -3.234425000 | 4.586195000 |
| H | -0.953404000 | -4.769278000 | 2.430621000 |
| H | 0.347687000 | -3.837657000 | 3.195263000 |

107

thf_TS1_trans_1,2 E = -2044.724758 a.u. Imaginary frequency=332i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.190856000 | -0.383494000 | 1.528087000 |
| P | 2.666807000 | -0.198863000 | 0.383600000 |
| P | -2.778755000 | -0.266210000 | 0.050753000 |
| Si | -0.197449000 | 4.119249000 | -0.370758000 |
| C | 0.748467000 | 2.645547000 | -1.143012000 |
| H | 1.338307000 | 2.154289000 | -0.329990000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.555603000 | 3.126322000 | -1.703822000 |
| C | -1.223826000 | 5.014179000 | -1.681247000 |
| H | -0.609798000 | 5.367533000 | -2.518563000 |
| H | -1.687472000 | 5.899965000 | -1.229004000 |
| H | -2.035556000 | 4.403335000 | -2.094242000 |
| C | -1.322978000 | 3.606275000 | 1.052943000 |
| H | -2.173862000 | 2.986953000 | 0.747521000 |
| H | -1.746185000 | 4.507707000 | 1.514968000 |
| H | -0.786997000 | 3.066738000 | 1.842931000 |
| C | 1.111830000 | 5.310482000 | 0.284379000 |
| H | 1.773492000 | 4.826779000 | 1.012378000 |
| H | 0.644413000 | 6.172063000 | 0.777407000 |
| H | 1.740543000 | 5.694970000 | -0.527911000 |
| C | 3.777239000 | -1.187212000 | -0.713171000 |
| C | 4.085623000 | -2.540434000 | -0.527503000 |
| H | 3.706321000 | -3.074312000 | 0.337928000 |
| C | 4.891724000 | -3.213104000 | -1.448338000 |
| H | 5.133142000 | -4.260020000 | -1.283113000 |
| C | 5.395789000 | -2.548479000 | -2.564697000 |
| H | 6.029261000 | -3.073976000 | -3.273900000 |
| C | 5.085988000 | -1.202440000 | -2.764629000 |
| H | 5.476508000 | -0.674240000 | -3.630474000 |
| C | 4.276579000 | -0.529649000 | -1.851576000 |
| H | 4.045606000 | 0.521097000 | -2.018185000 |
| C | 3.749789000 | 1.083946000 | 1.159614000 |
| C | 3.141146000 | 1.938878000 | 2.091257000 |
| H | 2.089185000 | 1.813928000 | 2.341153000 |
| C | 3.884945000 | 2.930418000 | 2.725661000 |
| H | 3.407215000 | 3.579985000 | 3.454363000 |
| C | 5.240163000 | 3.085126000 | 2.429991000 |
| H | 5.820340000 | 3.859681000 | 2.923783000 |
| C | 5.847970000 | 2.238372000 | 1.505872000 |
| H | 6.905485000 | 2.346786000 | 1.280227000 |
| C | 5.108940000 | 1.238982000 | 0.870982000 |
| H | 5.601101000 | 0.578254000 | 0.163636000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.123555000 | -1.236667000 | 1.788529000 |
| C | 0.750368000 | -1.205551000 | 2.164448000 |
| C | 0.372408000 | -2.078889000 | 3.214654000 |
| H | -0.672634000 | -2.118184000 | 3.505312000 |
| C | 1.293293000 | -2.860069000 | 3.894565000 |
| H | 0.947951000 | -3.507839000 | 4.696744000 |
| C | 2.653232000 | -2.811040000 | 3.571676000 |
| H | 3.381957000 | -3.391669000 | 4.129005000 |
| C | 3.050573000 | -1.998061000 | 2.520341000 |
| H | 4.105350000 | -1.930705000 | 2.264739000 |
| C | -1.247738000 | 0.090874000 | 2.329327000 |
| C | -1.039777000 | 0.542700000 | 3.650338000 |
| H | -0.041223000 | 0.481928000 | 4.074065000 |
| C | -2.079041000 | 1.060689000 | 4.412314000 |
| H | -1.874965000 | 1.403760000 | 5.423657000 |
| C | -3.371144000 | 1.158025000 | 3.889619000 |
| H | -4.181905000 | 1.566332000 | 4.485458000 |
| C | -3.600514000 | 0.734573000 | 2.586089000 |
| H | -4.595402000 | 0.822075000 | 2.157939000 |
| C | -2.562676000 | 0.203014000 | 1.809706000 |
| C | -4.317229000 | 0.578418000 | -0.515318000 |
| C | -5.585728000 | 0.017097000 | -0.312079000 |
| H | -5.682499000 | -0.949764000 | 0.173716000 |
| C | -6.728119000 | 0.692634000 | -0.737594000 |
| H | -7.706619000 | 0.248788000 | -0.575097000 |
| C | -6.617827000 | 1.930994000 | -1.369629000 |
| H | -7.510370000 | 2.453495000 | -1.702562000 |
| C | -5.359897000 | 2.494588000 | -1.578718000 |
| H | -5.268138000 | 3.456496000 | -2.075850000 |
| C | -4.215664000 | 1.819234000 | -1.157971000 |
| H | -3.239152000 | 2.262973000 | -1.333252000 |
| C | -3.255986000 | -2.051652000 | 0.040998000 |
| C | -3.362853000 | -2.802984000 | 1.216098000 |
| H | -3.182251000 | -2.330504000 | 2.177641000 |
| C | -3.718458000 | -4.151700000 | 1.155148000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.805861000 | -4.726486000 | 2.073372000 |
| C | -3.976143000 | -4.755256000 | -0.074589000 |
| H | -4.262962000 | -5.802434000 | -0.117999000 |
| C | -3.875485000 | -4.008414000 | -1.250606000 |
| H | -4.090017000 | -4.470922000 | -2.210664000 |
| C | -3.509218000 | -2.665483000 | -1.195619000 |
| H | -3.442309000 | -2.087288000 | -2.115008000 |
| C | 1.794594000 | 2.823575000 | -4.503268000 |
| C | 1.275843000 | 1.843077000 | -3.757409000 |
| H | 2.676992000 | 2.666624000 | -5.117002000 |
| H | 1.341719000 | 3.812144000 | -4.544774000 |
| H | 1.753525000 | 0.860978000 | -3.765900000 |
| C | 0.028998000 | 1.957648000 | -2.966170000 |
| C | -0.832489000 | 0.801306000 | -2.958840000 |
| H | -1.904786000 | 0.999530000 | -2.970653000 |
| H | -0.545161000 | 0.009056000 | -3.652609000 |
| Y | -0.011701000 | 0.273988000 | -0.734425000 |
| H | -0.445738000 | 2.931435000 | -3.050144000 |
| O | 0.354065000 | -1.942162000 | -1.490662000 |
| C | 0.773536000 | -2.342562000 | -2.830641000 |
| C | 0.197224000 | -3.133830000 | -0.648075000 |
| C | 1.108612000 | -3.822518000 | -2.728702000 |
| H | -0.065298000 | -2.156956000 | -3.508130000 |
| H | 1.625984000 | -1.721940000 | -3.118131000 |
| C | 0.163808000 | -4.296525000 | -1.623387000 |
| H | 1.057352000 | -3.177950000 | 0.025360000 |
| H | -0.716793000 | -3.007356000 | -0.067838000 |
| H | 2.152857000 | -3.957067000 | -2.430001000 |
| H | 0.952640000 | -4.338092000 | -3.680572000 |
| H | 0.488565000 | -5.228822000 | -1.152865000 |
| H | -0.850837000 | -4.441460000 | -2.009029000 |

107

thf_P1_trans_1,2 E = -2044.74619 a.u.

| | | | |
|---|--------------|--------------|-------------|
| N | -0.054404000 | 0.058225000 | 1.502059000 |
| P | 2.315472000 | -1.288630000 | 0.188329000 |

| | | | |
|----|--------------|--------------|--------------|
| P | -2.747080000 | 0.019641000 | 0.228136000 |
| Si | 1.930406000 | 5.268149000 | -0.341967000 |
| C | 2.002720000 | 3.457047000 | -0.953939000 |
| H | 1.912838000 | 2.796821000 | -0.073658000 |
| H | 3.029493000 | 3.328551000 | -1.329511000 |
| C | 2.407846000 | 6.399765000 | -1.775702000 |
| H | 3.401439000 | 6.154940000 | -2.170313000 |
| H | 2.432629000 | 7.447041000 | -1.450830000 |
| H | 1.695073000 | 6.335509000 | -2.606760000 |
| C | 0.222588000 | 5.746168000 | 0.301097000 |
| H | -0.536144000 | 5.704841000 | -0.489062000 |
| H | 0.239398000 | 6.773373000 | 0.686570000 |
| H | -0.107169000 | 5.092276000 | 1.116952000 |
| C | 3.199858000 | 5.424892000 | 1.047896000 |
| H | 2.953216000 | 4.774826000 | 1.896653000 |
| H | 3.242556000 | 6.453402000 | 1.426072000 |
| H | 4.208217000 | 5.161216000 | 0.705913000 |
| C | 2.228075000 | -2.996244000 | -0.516139000 |
| C | 1.609787000 | -4.051896000 | 0.165545000 |
| H | 1.233211000 | -3.899838000 | 1.172794000 |
| C | 1.487734000 | -5.304865000 | -0.438591000 |
| H | 1.013642000 | -6.117586000 | 0.105406000 |
| C | 1.984075000 | -5.518730000 | -1.723366000 |
| H | 1.899836000 | -6.498502000 | -2.185739000 |
| C | 2.602266000 | -4.471113000 | -2.410259000 |
| H | 3.003704000 | -4.633858000 | -3.407285000 |
| C | 2.714785000 | -3.216155000 | -1.815682000 |
| H | 3.205388000 | -2.409988000 | -2.356936000 |
| C | 4.118227000 | -0.883963000 | 0.228147000 |
| C | 4.474346000 | 0.439653000 | 0.525701000 |
| H | 3.703209000 | 1.186541000 | 0.703004000 |
| C | 5.815013000 | 0.806182000 | 0.614480000 |
| H | 6.078928000 | 1.833381000 | 0.851056000 |
| C | 6.814146000 | -0.143223000 | 0.398176000 |
| H | 7.860271000 | 0.142849000 | 0.462961000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 6.466800000 | -1.459821000 | 0.101750000 |
| H | 7.241336000 | -2.204613000 | -0.060760000 |
| C | 5.125191000 | -1.833059000 | 0.018423000 |
| H | 4.869226000 | -2.864410000 | -0.205686000 |
| C | 1.832390000 | -1.440504000 | 1.943229000 |
| C | 0.693021000 | -0.720076000 | 2.388568000 |
| C | 0.350172000 | -0.862589000 | 3.753462000 |
| H | -0.518827000 | -0.339142000 | 4.138547000 |
| C | 1.103454000 | -1.644513000 | 4.617128000 |
| H | 0.800268000 | -1.720119000 | 5.658643000 |
| C | 2.238133000 | -2.327108000 | 4.170392000 |
| H | 2.833499000 | -2.927148000 | 4.851638000 |
| C | 2.589995000 | -2.215936000 | 2.832471000 |
| H | 3.474829000 | -2.729669000 | 2.463646000 |
| C | -0.900024000 | 1.057269000 | 2.034373000 |
| C | -0.444629000 | 1.999656000 | 2.977655000 |
| H | 0.575898000 | 1.921879000 | 3.342638000 |
| C | -1.276498000 | 3.010770000 | 3.441131000 |
| H | -0.897809000 | 3.721470000 | 4.171391000 |
| C | -2.585583000 | 3.128866000 | 2.965013000 |
| H | -3.233122000 | 3.923296000 | 3.324267000 |
| C | -3.051705000 | 2.221601000 | 2.020928000 |
| H | -4.063599000 | 2.313735000 | 1.637255000 |
| C | -2.231345000 | 1.181621000 | 1.563525000 |
| C | -4.287922000 | 0.739511000 | -0.482637000 |
| C | -5.544464000 | 0.529125000 | 0.103056000 |
| H | -5.634739000 | -0.086640000 | 0.993592000 |
| C | -6.683452000 | 1.104646000 | -0.457273000 |
| H | -7.653021000 | 0.936561000 | 0.003747000 |
| C | -6.580587000 | 1.893849000 | -1.602862000 |
| H | -7.470781000 | 2.340622000 | -2.037110000 |
| C | -5.334426000 | 2.107331000 | -2.190948000 |
| H | -5.249719000 | 2.722062000 | -3.083148000 |
| C | -4.193909000 | 1.529216000 | -1.636194000 |
| H | -3.224572000 | 1.703332000 | -2.096323000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.322401000 | -1.529366000 | 1.053807000 |
| C | -3.093572000 | -1.779951000 | 2.409734000 |
| H | -2.609016000 | -1.028830000 | 3.024962000 |
| C | -3.498632000 | -2.988052000 | 2.978099000 |
| H | -3.319622000 | -3.170227000 | 4.034318000 |
| C | -4.137839000 | -3.951696000 | 2.200570000 |
| H | -4.458067000 | -4.888800000 | 2.647635000 |
| C | -4.376182000 | -3.705029000 | 0.847519000 |
| H | -4.888782000 | -4.445906000 | 0.239499000 |
| C | -3.966641000 | -2.503278000 | 0.274849000 |
| H | -4.178942000 | -2.310970000 | -0.775116000 |
| C | 2.360545000 | 0.958832000 | -2.602232000 |
| C | 1.398778000 | 1.863445000 | -2.868003000 |
| H | 2.524952000 | 0.102874000 | -3.253774000 |
| H | 3.083212000 | 1.099478000 | -1.802245000 |
| H | 0.760813000 | 1.694107000 | -3.740360000 |
| C | 0.984690000 | 3.048808000 | -2.028856000 |
| C | -0.345315000 | 2.549594000 | -1.410127000 |
| H | -0.642361000 | 3.183604000 | -0.563356000 |
| H | -1.151664000 | 2.636271000 | -2.158044000 |
| Y | -0.005399000 | 0.272192000 | -0.765361000 |
| H | 0.826136000 | 3.897048000 | -2.714597000 |
| O | -0.558012000 | -1.299663000 | -2.460316000 |
| C | -0.756040000 | -0.998507000 | -3.875356000 |
| C | -1.015611000 | -2.659841000 | -2.177521000 |
| C | -1.217929000 | -2.304094000 | -4.510250000 |
| H | -1.516978000 | -0.213628000 | -3.946019000 |
| H | 0.189272000 | -0.626543000 | -4.276989000 |
| C | -1.916766000 | -3.011740000 | -3.347148000 |
| H | -0.135298000 | -3.306190000 | -2.122800000 |
| H | -1.522388000 | -2.643620000 | -1.209215000 |
| H | -0.358399000 | -2.889913000 | -4.853513000 |
| H | -1.874959000 | -2.129290000 | -5.366486000 |
| H | -1.997065000 | -4.092693000 | -3.490332000 |
| H | -2.924516000 | -2.607767000 | -3.197264000 |

107

thf_C1_cis_1,2 E = -2044.729627 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.085959000 | -0.270591000 | 1.454786000 |
| P | 2.827506000 | 0.102090000 | 0.170829000 |
| P | -2.636157000 | -0.492237000 | 0.172773000 |
| Si | -1.099077000 | 4.246240000 | -0.670136000 |
| C | -0.210545000 | 2.591566000 | -0.548434000 |
| H | -0.071305000 | 2.464050000 | 0.549291000 |
| H | 0.814613000 | 2.774005000 | -0.941600000 |
| C | -1.787078000 | 4.610291000 | -2.403140000 |
| H | -1.017441000 | 4.563159000 | -3.184343000 |
| H | -2.193505000 | 5.629402000 | -2.424228000 |
| H | -2.606068000 | 3.939378000 | -2.691095000 |
| C | -2.519889000 | 4.321210000 | 0.571040000 |
| H | -3.287580000 | 3.564442000 | 0.377122000 |
| H | -3.006921000 | 5.303881000 | 0.541528000 |
| H | -2.155407000 | 4.163517000 | 1.593246000 |
| C | 0.103373000 | 5.656253000 | -0.269010000 |
| H | 0.512751000 | 5.551369000 | 0.743622000 |
| H | -0.393105000 | 6.633400000 | -0.321963000 |
| H | 0.949481000 | 5.679729000 | -0.967772000 |
| C | 4.011511000 | -0.866761000 | -0.869232000 |
| C | 4.122005000 | -2.261396000 | -0.799073000 |
| H | 3.575111000 | -2.812890000 | -0.040551000 |
| C | 4.964815000 | -2.950360000 | -1.673075000 |
| H | 5.055276000 | -4.030596000 | -1.591041000 |
| C | 5.704575000 | -2.258301000 | -2.629850000 |
| H | 6.366842000 | -2.795407000 | -3.303139000 |
| C | 5.603554000 | -0.868596000 | -2.706230000 |
| H | 6.188980000 | -0.318283000 | -3.438061000 |
| C | 4.763219000 | -0.178327000 | -1.835790000 |
| H | 4.715188000 | 0.906975000 | -1.889689000 |
| C | 3.855317000 | 1.504968000 | 0.803179000 |
| C | 3.232318000 | 2.721614000 | 1.106294000 |
| H | 2.171470000 | 2.857007000 | 0.916138000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.970353000 | 3.771328000 | 1.652774000 |
| H | 3.477445000 | 4.712197000 | 1.881874000 |
| C | 5.333573000 | 3.616266000 | 1.895692000 |
| H | 5.908516000 | 4.435865000 | 2.318009000 |
| C | 5.960472000 | 2.407394000 | 1.591757000 |
| H | 7.023811000 | 2.282148000 | 1.777761000 |
| C | 5.227615000 | 1.354983000 | 1.048887000 |
| H | 5.729789000 | 0.422231000 | 0.808410000 |
| C | 2.456651000 | -0.922825000 | 1.650665000 |
| C | 1.117062000 | -0.946502000 | 2.122264000 |
| C | 0.858127000 | -1.724986000 | 3.273357000 |
| H | -0.160149000 | -1.779506000 | 3.645868000 |
| C | 1.866947000 | -2.408685000 | 3.935302000 |
| H | 1.620692000 | -2.994560000 | 4.817484000 |
| C | 3.187846000 | -2.351756000 | 3.480368000 |
| H | 3.981082000 | -2.874598000 | 4.006145000 |
| C | 3.467375000 | -1.608459000 | 2.341882000 |
| H | 4.491220000 | -1.550244000 | 1.981377000 |
| C | -0.938674000 | 0.288312000 | 2.245162000 |
| C | -0.660610000 | 0.934015000 | 3.467844000 |
| H | 0.366572000 | 0.969259000 | 3.819486000 |
| C | -1.668126000 | 1.525231000 | 4.219037000 |
| H | -1.413754000 | 2.015589000 | 5.155411000 |
| C | -2.992828000 | 1.510782000 | 3.775384000 |
| H | -3.778795000 | 1.978757000 | 4.360533000 |
| C | -3.290196000 | 0.898352000 | 2.563830000 |
| H | -4.313518000 | 0.895004000 | 2.198321000 |
| C | -2.287386000 | 0.282712000 | 1.803440000 |
| C | -4.231352000 | 0.224931000 | -0.408178000 |
| C | -5.471967000 | -0.334741000 | -0.074534000 |
| H | -5.521536000 | -1.222917000 | 0.548835000 |
| C | -6.649741000 | 0.243477000 | -0.546429000 |
| H | -7.607413000 | -0.197039000 | -0.282456000 |
| C | -6.601258000 | 1.380761000 | -1.351871000 |
| H | -7.521313000 | 1.827441000 | -1.718660000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -5.369761000 | 1.943261000 | -1.686904000 |
| H | -5.327332000 | 2.831910000 | -2.311024000 |
| C | -4.190170000 | 1.365100000 | -1.221719000 |
| H | -3.230551000 | 1.808019000 | -1.476042000 |
| C | -3.073445000 | -2.251416000 | 0.535943000 |
| C | -3.100027000 | -2.761727000 | 1.838261000 |
| H | -2.872686000 | -2.111451000 | 2.678243000 |
| C | -3.434353000 | -4.098736000 | 2.061013000 |
| H | -3.457816000 | -4.484494000 | 3.076750000 |
| C | -3.750989000 | -4.931888000 | 0.989758000 |
| H | -4.019993000 | -5.969575000 | 1.167187000 |
| C | -3.731078000 | -4.427480000 | -0.312426000 |
| H | -3.991610000 | -5.069467000 | -1.150077000 |
| C | -3.386550000 | -3.097043000 | -0.539500000 |
| H | -3.384152000 | -2.708714000 | -1.556164000 |
| C | 1.570423000 | 0.684234000 | -3.426306000 |
| C | 0.540083000 | 1.551442000 | -3.461780000 |
| H | 2.597240000 | 1.033014000 | -3.418549000 |
| H | 1.437161000 | -0.394340000 | -3.474664000 |
| H | 0.763999000 | 2.615198000 | -3.434303000 |
| C | -0.891141000 | 1.219383000 | -3.477815000 |
| C | -1.430058000 | 0.015938000 | -3.751381000 |
| H | -2.506305000 | -0.127123000 | -3.726436000 |
| H | -0.831205000 | -0.832633000 | -4.069140000 |
| Y | 0.032522000 | 0.267494000 | -0.760530000 |
| H | -1.553033000 | 2.047730000 | -3.246660000 |
| O | 0.295983000 | -2.148992000 | -1.500401000 |
| C | 0.338462000 | -2.887636000 | -2.747475000 |
| C | 0.349240000 | -3.108083000 | -0.385343000 |
| C | 0.912805000 | -4.248251000 | -2.398759000 |
| H | -0.683062000 | -2.971746000 | -3.138282000 |
| H | 0.954613000 | -2.332019000 | -3.458045000 |
| C | 0.303070000 | -4.491688000 | -1.018752000 |
| H | 1.282222000 | -2.927903000 | 0.152643000 |
| H | -0.491902000 | -2.903052000 | 0.276651000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.005229000 | -4.193393000 | -2.341388000 |
| H | 0.641365000 | -5.010145000 | -3.134983000 |
| H | 0.856391000 | -5.225350000 | -0.425770000 |
| H | -0.732098000 | -4.837566000 | -1.108294000 |

107

thf_TS1_cis_1,2 E = -2044.707117 a.u. Imaginary frequency=327i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.205361000 | -0.340356000 | 1.499763000 |
| P | 2.654392000 | -0.240385000 | 0.325637000 |
| P | -2.805689000 | -0.333293000 | 0.048848000 |
| Si | 0.011143000 | 4.490403000 | -0.624642000 |
| C | 0.025844000 | 2.588684000 | -0.667938000 |
| H | -0.879664000 | 2.326499000 | -0.075757000 |
| H | 0.916535000 | 2.291163000 | -0.073442000 |
| C | 1.437002000 | 5.249641000 | -1.602156000 |
| H | 2.408379000 | 4.835715000 | -1.304618000 |
| H | 1.472721000 | 6.327727000 | -1.401218000 |
| H | 1.329420000 | 5.131942000 | -2.686573000 |
| C | -1.633653000 | 5.132778000 | -1.297703000 |
| H | -1.785804000 | 4.921046000 | -2.362908000 |
| H | -1.674263000 | 6.223075000 | -1.182599000 |
| H | -2.484984000 | 4.719022000 | -0.743390000 |
| C | 0.170425000 | 5.012859000 | 1.182130000 |
| H | -0.618297000 | 4.570943000 | 1.802508000 |
| H | 0.098670000 | 6.103417000 | 1.280017000 |
| H | 1.136722000 | 4.707820000 | 1.601013000 |
| C | 3.713949000 | -1.388378000 | -0.664750000 |
| C | 3.965192000 | -2.723511000 | -0.324499000 |
| H | 3.567091000 | -3.137354000 | 0.596326000 |
| C | 4.740178000 | -3.531527000 | -1.158912000 |
| H | 4.937038000 | -4.561647000 | -0.873154000 |
| C | 5.271425000 | -3.020910000 | -2.341900000 |
| H | 5.882617000 | -3.649789000 | -2.983364000 |
| C | 5.016885000 | -1.695346000 | -2.696334000 |
| H | 5.427664000 | -1.287764000 | -3.616386000 |
| C | 4.237349000 | -0.888916000 | -1.869626000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.041333000 | 0.141073000 | -2.158253000 |
| C | 3.795792000 | 1.077902000 | 0.946054000 |
| C | 3.245934000 | 2.027521000 | 1.820849000 |
| H | 2.204409000 | 1.950902000 | 2.126309000 |
| C | 4.036521000 | 3.055047000 | 2.328950000 |
| H | 3.604344000 | 3.778410000 | 3.015343000 |
| C | 5.380132000 | 3.151066000 | 1.963891000 |
| H | 5.996362000 | 3.953219000 | 2.360393000 |
| C | 5.930163000 | 2.209345000 | 1.097301000 |
| H | 6.978910000 | 2.270866000 | 0.819130000 |
| C | 5.144143000 | 1.174159000 | 0.588830000 |
| H | 5.592764000 | 0.439648000 | -0.073014000 |
| C | 2.119516000 | -1.125261000 | 1.838100000 |
| C | 0.748609000 | -1.074714000 | 2.215742000 |
| C | 0.383511000 | -1.826997000 | 3.359340000 |
| H | -0.660897000 | -1.844625000 | 3.655530000 |
| C | 1.316592000 | -2.515898000 | 4.117296000 |
| H | 0.983783000 | -3.073514000 | 4.989412000 |
| C | 2.674139000 | -2.488956000 | 3.780345000 |
| H | 3.412080000 | -2.997480000 | 4.393295000 |
| C | 3.058102000 | -1.794121000 | 2.643104000 |
| H | 4.110807000 | -1.747839000 | 2.374200000 |
| C | -1.227597000 | 0.269928000 | 2.246299000 |
| C | -0.989802000 | 0.870557000 | 3.502072000 |
| H | 0.007864000 | 0.820155000 | 3.928794000 |
| C | -2.001019000 | 1.521518000 | 4.196364000 |
| H | -1.775428000 | 1.975119000 | 5.158463000 |
| C | -3.292180000 | 1.611676000 | 3.668620000 |
| H | -4.080177000 | 2.122867000 | 4.213496000 |
| C | -3.550437000 | 1.041079000 | 2.428087000 |
| H | -4.545537000 | 1.110219000 | 1.996861000 |
| C | -2.541740000 | 0.373918000 | 1.720545000 |
| C | -4.315604000 | 0.506767000 | -0.596255000 |
| C | -5.593866000 | -0.054575000 | -0.482243000 |
| H | -5.724758000 | -1.023366000 | -0.009412000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.705828000 | 0.627795000 | -0.975414000 |
| H | -7.692859000 | 0.182762000 | -0.882470000 |
| C | -6.554771000 | 1.874329000 | -1.580556000 |
| H | -7.423250000 | 2.402178000 | -1.964790000 |
| C | -5.285586000 | 2.442286000 | -1.692430000 |
| H | -5.161294000 | 3.413886000 | -2.163012000 |
| C | -4.172131000 | 1.760154000 | -1.207715000 |
| H | -3.187074000 | 2.209667000 | -1.302059000 |
| C | -3.335432000 | -2.085049000 | 0.295680000 |
| C | -3.433612000 | -2.663439000 | 1.565423000 |
| H | -3.231656000 | -2.064669000 | 2.449073000 |
| C | -3.806466000 | -4.002011000 | 1.698710000 |
| H | -3.885268000 | -4.441777000 | 2.689425000 |
| C | -4.091024000 | -4.767879000 | 0.569525000 |
| H | -4.389991000 | -5.806987000 | 0.677166000 |
| C | -4.001039000 | -4.194395000 | -0.700592000 |
| H | -4.237210000 | -4.783509000 | -1.583085000 |
| C | -3.616761000 | -2.862387000 | -0.839142000 |
| H | -3.556959000 | -2.419003000 | -1.831294000 |
| C | 1.823161000 | 1.171153000 | -3.922929000 |
| C | 1.190780000 | 2.048507000 | -3.127995000 |
| H | 2.875327000 | 1.298678000 | -4.161364000 |
| H | 1.313427000 | 0.346421000 | -4.412607000 |
| H | 1.756288000 | 2.883534000 | -2.724607000 |
| C | -0.245173000 | 1.994799000 | -2.760643000 |
| C | -1.000057000 | 0.813910000 | -2.966751000 |
| H | -2.075432000 | 0.899121000 | -3.093812000 |
| H | -0.542368000 | 0.013022000 | -3.550128000 |
| Y | -0.045713000 | 0.145818000 | -0.782183000 |
| H | -0.765362000 | 2.945342000 | -2.825493000 |
| O | 0.288514000 | -2.085385000 | -1.533757000 |
| C | 0.694271000 | -2.540586000 | -2.859119000 |
| C | 0.124913000 | -3.237995000 | -0.642136000 |
| C | 0.997201000 | -4.024081000 | -2.706407000 |
| H | -0.143444000 | -2.358231000 | -3.540850000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.559904000 | -1.949136000 | -3.166609000 |
| C | 0.059918000 | -4.437914000 | -1.570064000 |
| H | 0.993409000 | -3.270370000 | 0.022173000 |
| H | -0.780004000 | -3.074679000 | -0.055640000 |
| H | 2.042854000 | -4.169929000 | -2.417449000 |
| H | 0.816390000 | -4.572501000 | -3.635165000 |
| H | 0.375768000 | -5.356728000 | -1.068155000 |
| H | -0.962468000 | -4.581583000 | -1.935982000 |

107

thf_P1_cis_1,2 E = -2044.751773 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.031542000 | 0.118471000 | 1.436340000 |
| P | 2.713537000 | -0.534509000 | 0.160843000 |
| P | -2.605644000 | -0.603004000 | 0.241137000 |
| Si | -0.239998000 | 5.365194000 | -0.516111000 |
| C | 0.690038000 | 3.713322000 | -0.774017000 |
| H | 0.522749000 | 3.080842000 | 0.114368000 |
| H | 1.755805000 | 3.991017000 | -0.750790000 |
| C | 0.225445000 | 6.535978000 | -1.923543000 |
| H | 1.309016000 | 6.699007000 | -1.972865000 |
| H | -0.245837000 | 7.515894000 | -1.778881000 |
| H | -0.100275000 | 6.163368000 | -2.902227000 |
| C | -2.113865000 | 5.153688000 | -0.460372000 |
| H | -2.518667000 | 4.817783000 | -1.421993000 |
| H | -2.592363000 | 6.111879000 | -0.221496000 |
| H | -2.418295000 | 4.432257000 | 0.307000000 |
| C | 0.362307000 | 6.076226000 | 1.126464000 |
| H | 0.108112000 | 5.416693000 | 1.965001000 |
| H | -0.097870000 | 7.051807000 | 1.324755000 |
| H | 1.449572000 | 6.221130000 | 1.132650000 |
| C | 3.228265000 | -2.202913000 | -0.448154000 |
| C | 3.038117000 | -3.371903000 | 0.299544000 |
| H | 2.646150000 | -3.312101000 | 1.310667000 |
| C | 3.363947000 | -4.616267000 | -0.243591000 |
| H | 3.220101000 | -5.514169000 | 0.351743000 |
| C | 3.885324000 | -4.708751000 | -1.533035000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.149711000 | -5.677772000 | -1.947601000 |
| C | 4.077984000 | -3.548381000 | -2.286280000 |
| H | 4.494049000 | -3.610132000 | -3.288573000 |
| C | 3.743507000 | -2.305869000 | -1.751870000 |
| H | 3.904380000 | -1.408832000 | -2.345871000 |
| C | 4.263015000 | 0.471625000 | 0.150859000 |
| C | 4.134479000 | 1.851056000 | 0.367742000 |
| H | 3.150479000 | 2.291098000 | 0.513824000 |
| C | 5.264033000 | 2.664277000 | 0.415464000 |
| H | 5.154124000 | 3.731190000 | 0.590651000 |
| C | 6.532150000 | 2.110325000 | 0.237201000 |
| H | 7.413203000 | 2.745238000 | 0.270031000 |
| C | 6.665691000 | 0.740366000 | 0.019941000 |
| H | 7.651529000 | 0.302767000 | -0.112878000 |
| C | 5.537738000 | -0.079639000 | -0.021196000 |
| H | 5.657761000 | -1.146663000 | -0.184001000 |
| C | 2.281901000 | -0.744237000 | 1.922611000 |
| C | 0.973885000 | -0.382370000 | 2.341335000 |
| C | 0.672808000 | -0.583806000 | 3.708811000 |
| H | -0.320234000 | -0.338986000 | 4.071166000 |
| C | 1.615353000 | -1.072358000 | 4.601168000 |
| H | 1.334762000 | -1.206731000 | 5.643063000 |
| C | 2.911185000 | -1.387648000 | 4.181980000 |
| H | 3.652421000 | -1.753622000 | 4.885759000 |
| C | 3.228848000 | -1.219990000 | 2.841833000 |
| H | 4.232342000 | -1.451893000 | 2.492002000 |
| C | -1.017674000 | 0.911657000 | 1.950488000 |
| C | -0.783444000 | 1.965176000 | 2.857409000 |
| H | 0.231513000 | 2.141338000 | 3.203001000 |
| C | -1.822530000 | 2.766490000 | 3.313330000 |
| H | -1.609024000 | 3.568052000 | 4.015979000 |
| C | -3.130657000 | 2.559427000 | 2.866456000 |
| H | -3.941575000 | 3.188766000 | 3.221123000 |
| C | -3.384058000 | 1.537758000 | 1.958103000 |
| H | -4.395702000 | 1.375256000 | 1.596888000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.349288000 | 0.706915000 | 1.509019000 |
| C | -4.266332000 | -0.272999000 | -0.487008000 |
| C | -5.440627000 | -0.800002000 | 0.067926000 |
| H | -5.391074000 | -1.430466000 | 0.951203000 |
| C | -6.676248000 | -0.520240000 | -0.513600000 |
| H | -7.581682000 | -0.933025000 | -0.076885000 |
| C | -6.751484000 | 0.287124000 | -1.648371000 |
| H | -7.716298000 | 0.502768000 | -2.099274000 |
| C | -5.586982000 | 0.817173000 | -2.203729000 |
| H | -5.641548000 | 1.448782000 | -3.086486000 |
| C | -4.348541000 | 0.535189000 | -1.629825000 |
| H | -3.444855000 | 0.955939000 | -2.063738000 |
| C | -2.818023000 | -2.191633000 | 1.158589000 |
| C | -2.624848000 | -2.291009000 | 2.539422000 |
| H | -2.392935000 | -1.402299000 | 3.118022000 |
| C | -2.742300000 | -3.526519000 | 3.177439000 |
| H | -2.593525000 | -3.591928000 | 4.251901000 |
| C | -3.059038000 | -4.668875000 | 2.445115000 |
| H | -3.156166000 | -5.628259000 | 2.945825000 |
| C | -3.263271000 | -4.575465000 | 1.067223000 |
| H | -3.527873000 | -5.460164000 | 0.493778000 |
| C | -3.137218000 | -3.345489000 | 0.426397000 |
| H | -3.319402000 | -3.276885000 | -0.644336000 |
| C | 1.523828000 | 0.977694000 | -3.249636000 |
| C | 1.578893000 | 2.099500000 | -2.509139000 |
| H | 2.424907000 | 0.459286000 | -3.566395000 |
| H | 0.583431000 | 0.617517000 | -3.666328000 |
| H | 2.564873000 | 2.460727000 | -2.209674000 |
| C | 0.380183000 | 2.917574000 | -2.062896000 |
| C | -0.858940000 | 2.010922000 | -1.889113000 |
| H | -1.633952000 | 2.552879000 | -1.333949000 |
| H | -1.298212000 | 1.779943000 | -2.875664000 |
| Y | 0.016307000 | 0.056296000 | -0.848073000 |
| H | 0.228820000 | 3.651954000 | -2.875834000 |
| O | -0.272077000 | -1.864402000 | -2.216653000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.170542000 | -1.856508000 | -3.364843000 |
| C | 0.084053000 | -3.246672000 | -1.876881000 |
| C | -0.978045000 | -3.214984000 | -4.015599000 |
| H | -2.194190000 | -1.711349000 | -3.000192000 |
| H | -0.892410000 | -1.014533000 | -4.003468000 |
| C | -0.753885000 | -4.119830000 | -2.801885000 |
| H | 1.156581000 | -3.356633000 | -2.052546000 |
| H | -0.134293000 | -3.397929000 | -0.816760000 |
| H | -0.095385000 | -3.206718000 | -4.664854000 |
| H | -1.843519000 | -3.507213000 | -4.616579000 |
| H | -0.239111000 | -5.051337000 | -3.052014000 |
| H | -1.709516000 | -4.375825000 | -2.332409000 |

94

C1_cis E = -1812.394692 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.349985000 | -1.492581000 | -0.579383000 |
| P | 2.717261000 | 0.031392000 | 0.257286000 |
| P | -2.383198000 | -0.544819000 | 0.126190000 |
| Si | -1.357225000 | 3.981136000 | 0.850687000 |
| C | -0.267914000 | 2.448261000 | 0.928587000 |
| H | -0.449039000 | 1.992424000 | 1.917303000 |
| H | 0.782598000 | 2.811764000 | 0.973839000 |
| C | -3.024299000 | 3.669355000 | 1.681010000 |
| H | -3.571063000 | 2.830624000 | 1.235109000 |
| H | -3.662233000 | 4.559147000 | 1.611388000 |
| H | -2.895682000 | 3.437737000 | 2.744895000 |
| C | -0.520081000 | 5.447647000 | 1.706573000 |
| H | -0.320958000 | 5.224707000 | 2.761903000 |
| H | -1.147145000 | 6.347372000 | 1.670201000 |
| H | 0.440285000 | 5.696884000 | 1.237087000 |
| C | -1.706418000 | 4.525088000 | -0.941656000 |
| H | -0.790454000 | 4.749872000 | -1.505708000 |
| H | -2.303939000 | 5.445460000 | -0.946243000 |
| H | -2.284328000 | 3.773714000 | -1.496387000 |
| C | 4.329281000 | 0.916135000 | 0.187018000 |
| C | 4.336048000 | 2.295369000 | -0.057237000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.396619000 | 2.826690000 | -0.191088000 |
| C | 5.539057000 | 2.999963000 | -0.094739000 |
| H | 5.534318000 | 4.071193000 | -0.277194000 |
| C | 6.742877000 | 2.331250000 | 0.119818000 |
| H | 7.680559000 | 2.879549000 | 0.096482000 |
| C | 6.743298000 | 0.960264000 | 0.382428000 |
| H | 7.680086000 | 0.441172000 | 0.565620000 |
| C | 5.543451000 | 0.254304000 | 0.421963000 |
| H | 5.550563000 | -0.808139000 | 0.650998000 |
| C | 2.819112000 | -1.025973000 | 1.759580000 |
| C | 2.484644000 | -0.441480000 | 2.988807000 |
| H | 2.157236000 | 0.595436000 | 3.030818000 |
| C | 2.580863000 | -1.184713000 | 4.163364000 |
| H | 2.326099000 | -0.725874000 | 5.114861000 |
| C | 3.002330000 | -2.513726000 | 4.116428000 |
| H | 3.074898000 | -3.093002000 | 5.032761000 |
| C | 3.330779000 | -3.098820000 | 2.894030000 |
| H | 3.660490000 | -4.133609000 | 2.856506000 |
| C | 3.240164000 | -2.359331000 | 1.715458000 |
| H | 3.496516000 | -2.819150000 | 0.764817000 |
| C | 2.681631000 | -1.119312000 | -1.184995000 |
| C | 1.443269000 | -1.784711000 | -1.407651000 |
| C | 1.349550000 | -2.647188000 | -2.522508000 |
| H | 0.415692000 | -3.175718000 | -2.695058000 |
| C | 2.423226000 | -2.823554000 | -3.384688000 |
| H | 2.322340000 | -3.494932000 | -4.233770000 |
| C | 3.625986000 | -2.137938000 | -3.176288000 |
| H | 4.463262000 | -2.277429000 | -3.853923000 |
| C | 3.747134000 | -1.288202000 | -2.082118000 |
| H | 4.682668000 | -0.763541000 | -1.908170000 |
| C | -0.451843000 | -2.531255000 | -0.098462000 |
| C | 0.019090000 | -3.851239000 | 0.053324000 |
| H | 1.040984000 | -4.085977000 | -0.227830000 |
| C | -0.794508000 | -4.848417000 | 0.576643000 |
| H | -0.394450000 | -5.853460000 | 0.685672000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.103076000 | -4.572993000 | 0.979921000 |
| H | -2.731971000 | -5.353784000 | 1.396587000 |
| C | -2.583892000 | -3.275185000 | 0.849216000 |
| H | -3.594326000 | -3.036520000 | 1.172316000 |
| C | -1.782440000 | -2.264211000 | 0.305884000 |
| C | -3.339407000 | -0.239684000 | 1.673266000 |
| C | -2.611067000 | -0.047134000 | 2.856033000 |
| H | -1.523790000 | -0.061579000 | 2.837144000 |
| C | -3.273700000 | 0.146368000 | 4.064515000 |
| H | -2.700950000 | 0.289736000 | 4.976847000 |
| C | -4.668797000 | 0.160809000 | 4.103180000 |
| H | -5.185534000 | 0.317913000 | 5.045917000 |
| C | -5.396926000 | -0.029289000 | 2.930910000 |
| H | -6.483289000 | -0.025286000 | 2.956261000 |
| C | -4.737901000 | -0.232644000 | 1.717773000 |
| H | -5.317504000 | -0.389106000 | 0.812846000 |
| C | -3.634078000 | -0.569926000 | -1.234591000 |
| C | -4.329781000 | 0.614617000 | -1.528623000 |
| H | -4.182057000 | 1.501118000 | -0.915073000 |
| C | -5.227116000 | 0.659345000 | -2.593606000 |
| H | -5.772924000 | 1.576057000 | -2.801158000 |
| C | -5.425952000 | -0.471312000 | -3.388955000 |
| H | -6.124348000 | -0.435799000 | -4.220513000 |
| C | -4.732192000 | -1.647109000 | -3.107099000 |
| H | -4.890490000 | -2.532565000 | -3.717089000 |
| C | -3.841725000 | -1.700540000 | -2.033145000 |
| H | -3.317809000 | -2.625513000 | -1.809899000 |
| C | -1.295225000 | 1.332963000 | -3.330034000 |
| C | -0.109282000 | 0.713188000 | -3.510813000 |
| H | -1.374443000 | 2.386016000 | -3.061508000 |
| H | -2.229228000 | 0.809718000 | -3.509412000 |
| C | 1.219559000 | 1.297511000 | -3.270153000 |
| C | 1.474923000 | 2.468826000 | -2.647262000 |
| H | 2.496224000 | 2.809317000 | -2.511062000 |
| H | 0.690846000 | 3.157058000 | -2.324810000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.106653000 | -0.321433000 | -3.848979000 |
| Y | 0.103321000 | 0.769189000 | -0.656397000 |
| H | 2.061239000 | 0.684664000 | -3.586520000 |

94

TS1_cis E = -1812.384252 a.u. Imaginary frequency=108i

| | | | |
|----|--------------|--------------|--------------|
| N | 0.439686000 | -1.632654000 | -0.600562000 |
| P | 2.717946000 | 0.101941000 | 0.200391000 |
| P | -2.271451000 | -0.738025000 | 0.142212000 |
| Si | -1.611566000 | 4.216712000 | 0.563662000 |
| C | -0.613410000 | 2.668511000 | 0.152288000 |
| H | -0.801105000 | 1.964866000 | 0.998345000 |
| H | 0.460712000 | 2.954169000 | 0.200555000 |
| C | -3.464621000 | 3.871805000 | 0.426201000 |
| H | -3.786311000 | 3.693959000 | -0.607158000 |
| H | -4.038381000 | 4.730743000 | 0.795511000 |
| H | -3.754931000 | 3.002339000 | 1.028284000 |
| C | -1.233445000 | 4.752264000 | 2.336676000 |
| H | -1.509818000 | 3.973005000 | 3.057536000 |
| H | -1.791830000 | 5.658635000 | 2.602412000 |
| H | -0.167229000 | 4.970882000 | 2.473355000 |
| C | -1.128443000 | 5.623655000 | -0.604350000 |
| H | -0.043883000 | 5.790875000 | -0.612109000 |
| H | -1.594103000 | 6.559897000 | -0.273003000 |
| H | -1.452931000 | 5.456992000 | -1.638340000 |
| C | 4.310344000 | 1.016213000 | 0.101251000 |
| C | 4.340480000 | 2.270203000 | -0.521053000 |
| H | 3.426121000 | 2.697505000 | -0.925367000 |
| C | 5.534488000 | 2.983553000 | -0.613176000 |
| H | 5.548326000 | 3.957285000 | -1.095204000 |
| C | 6.705004000 | 2.451126000 | -0.074888000 |
| H | 7.635370000 | 3.008372000 | -0.140622000 |
| C | 6.680214000 | 1.208152000 | 0.559074000 |
| H | 7.590003000 | 0.796862000 | 0.987652000 |
| C | 5.488920000 | 0.491911000 | 0.651109000 |
| H | 5.473356000 | -0.468963000 | 1.158674000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.742538000 | -0.719521000 | 1.847555000 |
| C | 2.434891000 | 0.061760000 | 2.970705000 |
| H | 2.194958000 | 1.117257000 | 2.854721000 |
| C | 2.455967000 | -0.504704000 | 4.243110000 |
| H | 2.225610000 | 0.107409000 | 5.110949000 |
| C | 2.773599000 | -1.854429000 | 4.400851000 |
| H | 2.787197000 | -2.296718000 | 5.393154000 |
| C | 3.075660000 | -2.634479000 | 3.285654000 |
| H | 3.325859000 | -3.684871000 | 3.407261000 |
| C | 3.061701000 | -2.071409000 | 2.009822000 |
| H | 3.299413000 | -2.681922000 | 1.143374000 |
| C | 2.808664000 | -1.235347000 | -1.069798000 |
| C | 1.608829000 | -1.952471000 | -1.321040000 |
| C | 1.617929000 | -2.912943000 | -2.352696000 |
| H | 0.705362000 | -3.467512000 | -2.554678000 |
| C | 2.763025000 | -3.151682000 | -3.101357000 |
| H | 2.740523000 | -3.899303000 | -3.890131000 |
| C | 3.935359000 | -2.430012000 | -2.855881000 |
| H | 4.829937000 | -2.617437000 | -3.442647000 |
| C | 3.950139000 | -1.470239000 | -1.850035000 |
| H | 4.858193000 | -0.906339000 | -1.655667000 |
| C | -0.287597000 | -2.661695000 | 0.003503000 |
| C | 0.238196000 | -3.947942000 | 0.244356000 |
| H | 1.250728000 | -4.178450000 | -0.070819000 |
| C | -0.511670000 | -4.921613000 | 0.893353000 |
| H | -0.068082000 | -5.899037000 | 1.066767000 |
| C | -1.810115000 | -4.660014000 | 1.335028000 |
| H | -2.388401000 | -5.423473000 | 1.846243000 |
| C | -2.347282000 | -3.396652000 | 1.114656000 |
| H | -3.351669000 | -3.166681000 | 1.461622000 |
| C | -1.608513000 | -2.410687000 | 0.452411000 |
| C | -3.256689000 | -0.309104000 | 1.638926000 |
| C | -2.557335000 | 0.124868000 | 2.774891000 |
| H | -1.471947000 | 0.204049000 | 2.753199000 |
| C | -3.241740000 | 0.433507000 | 3.947536000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.690248000 | 0.762990000 | 4.823969000 |
| C | -4.631951000 | 0.321343000 | 3.994983000 |
| H | -5.166736000 | 0.567404000 | 4.908140000 |
| C | -5.332270000 | -0.109336000 | 2.869847000 |
| H | -6.414242000 | -0.204050000 | 2.903989000 |
| C | -4.650474000 | -0.426896000 | 1.694675000 |
| H | -5.206964000 | -0.767007000 | 0.826216000 |
| C | -3.489168000 | -0.914758000 | -1.235529000 |
| C | -4.276436000 | 0.191134000 | -1.595978000 |
| H | -4.226234000 | 1.108557000 | -1.013598000 |
| C | -5.146556000 | 0.110790000 | -2.680922000 |
| H | -5.764726000 | 0.965905000 | -2.941639000 |
| C | -5.227627000 | -1.066375000 | -3.427600000 |
| H | -5.905371000 | -1.127595000 | -4.274589000 |
| C | -4.443949000 | -2.164595000 | -3.077984000 |
| H | -4.511438000 | -3.086331000 | -3.649716000 |
| C | -3.578495000 | -2.093619000 | -1.985268000 |
| H | -2.982735000 | -2.958442000 | -1.707710000 |
| C | -1.302339000 | 2.496156000 | -2.410725000 |
| C | -0.973300000 | 1.338558000 | -3.080468000 |
| H | -0.638291000 | 3.352874000 | -2.385934000 |
| H | -2.329453000 | 2.686272000 | -2.126135000 |
| C | 0.370733000 | 1.008363000 | -3.529285000 |
| C | 1.513078000 | 1.625960000 | -3.125207000 |
| H | 2.484819000 | 1.286723000 | -3.467272000 |
| H | 1.496963000 | 2.557229000 | -2.555682000 |
| H | -1.761559000 | 0.617242000 | -3.292259000 |
| Y | 0.103283000 | 0.613473000 | -0.840230000 |
| H | 0.465811000 | 0.118371000 | -4.150405000 |

94

P1_cis E = -1812.430133 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.152756000 | -1.849091000 | -0.524112000 |
| P | 2.615546000 | -0.245277000 | 0.087368000 |
| P | -2.459495000 | -0.547962000 | 0.102813000 |
| Si | -0.286264000 | 4.723806000 | 0.392885000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.367932000 | 3.024002000 | -0.518477000 |
| H | -0.935778000 | 2.372118000 | 0.176289000 |
| H | 0.691696000 | 2.701367000 | -0.551255000 |
| C | -2.045836000 | 5.329510000 | 0.675453000 |
| H | -2.581869000 | 5.502266000 | -0.265094000 |
| H | -2.035948000 | 6.281759000 | 1.219516000 |
| H | -2.628992000 | 4.617497000 | 1.271903000 |
| C | 0.588478000 | 4.423520000 | 2.034382000 |
| H | 0.038455000 | 3.711306000 | 2.661562000 |
| H | 0.673997000 | 5.357606000 | 2.602518000 |
| H | 1.605560000 | 4.038816000 | 1.888639000 |
| C | 0.689476000 | 5.925815000 | -0.676479000 |
| H | 1.707663000 | 5.566180000 | -0.868797000 |
| H | 0.776462000 | 6.897804000 | -0.175921000 |
| H | 0.205490000 | 6.101769000 | -1.644132000 |
| C | 4.267105000 | 0.515444000 | -0.191955000 |
| C | 4.408400000 | 1.449075000 | -1.228516000 |
| H | 3.555364000 | 1.702318000 | -1.853988000 |
| C | 5.642096000 | 2.048256000 | -1.471201000 |
| H | 5.744079000 | 2.766752000 | -2.280018000 |
| C | 6.740595000 | 1.731047000 | -0.671553000 |
| H | 7.701213000 | 2.204098000 | -0.855660000 |
| C | 6.603861000 | 0.809781000 | 0.365896000 |
| H | 7.457196000 | 0.562168000 | 0.991305000 |
| C | 5.373261000 | 0.200429000 | 0.607256000 |
| H | 5.275769000 | -0.514604000 | 1.419094000 |
| C | 2.672267000 | -0.945978000 | 1.787392000 |
| C | 2.372314000 | -0.095452000 | 2.860971000 |
| H | 2.115169000 | 0.946311000 | 2.677878000 |
| C | 2.422296000 | -0.573502000 | 4.168688000 |
| H | 2.196340000 | 0.092221000 | 4.997329000 |
| C | 2.762732000 | -1.904429000 | 4.411758000 |
| H | 2.798136000 | -2.278320000 | 5.431267000 |
| C | 3.059534000 | -2.754049000 | 3.346692000 |
| H | 3.328757000 | -3.789790000 | 3.535046000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.016478000 | -2.279298000 | 2.036325000 |
| H | 3.252195000 | -2.943445000 | 1.209543000 |
| C | 2.530263000 | -1.692336000 | -1.065711000 |
| C | 1.279489000 | -2.353771000 | -1.203253000 |
| C | 1.195010000 | -3.435351000 | -2.102975000 |
| H | 0.241154000 | -3.942919000 | -2.219084000 |
| C | 2.300525000 | -3.842994000 | -2.836324000 |
| H | 2.207925000 | -4.680216000 | -3.523210000 |
| C | 3.523037000 | -3.174470000 | -2.710439000 |
| H | 4.385405000 | -3.493261000 | -3.288611000 |
| C | 3.630090000 | -2.099846000 | -1.836695000 |
| H | 4.577882000 | -1.579359000 | -1.733295000 |
| C | -0.674866000 | -2.690191000 | 0.221387000 |
| C | -0.284042000 | -3.976890000 | 0.641679000 |
| H | 0.692375000 | -4.355672000 | 0.356419000 |
| C | -1.118804000 | -4.757961000 | 1.431604000 |
| H | -0.780725000 | -5.743662000 | 1.741611000 |
| C | -2.369121000 | -4.290783000 | 1.842063000 |
| H | -3.014491000 | -4.902956000 | 2.464476000 |
| C | -2.770697000 | -3.020409000 | 1.444570000 |
| H | -3.735765000 | -2.633708000 | 1.763309000 |
| C | -1.948427000 | -2.226242000 | 0.637003000 |
| C | -3.168602000 | 0.229855000 | 1.621549000 |
| C | -2.265426000 | 0.635478000 | 2.616182000 |
| H | -1.196952000 | 0.465983000 | 2.488569000 |
| C | -2.726436000 | 1.217793000 | 3.793910000 |
| H | -2.018821000 | 1.516894000 | 4.562656000 |
| C | -4.095102000 | 1.411695000 | 3.987475000 |
| H | -4.455946000 | 1.869279000 | 4.904416000 |
| C | -4.996980000 | 1.009227000 | 3.004929000 |
| H | -6.064286000 | 1.147877000 | 3.154962000 |
| C | -4.539636000 | 0.417725000 | 1.826365000 |
| H | -5.254528000 | 0.100011000 | 1.073344000 |
| C | -3.871590000 | -0.786758000 | -1.059430000 |
| C | -4.588811000 | 0.335100000 | -1.505413000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.353309000 | 1.323987000 | -1.118095000 |
| C | -5.620551000 | 0.189106000 | -2.429195000 |
| H | -6.178797000 | 1.062123000 | -2.756648000 |
| C | -5.934517000 | -1.074081000 | -2.933689000 |
| H | -6.736627000 | -1.186498000 | -3.657824000 |
| C | -5.218773000 | -2.189210000 | -2.503592000 |
| H | -5.461720000 | -3.175503000 | -2.889624000 |
| C | -4.192979000 | -2.050630000 | -1.567627000 |
| H | -3.650620000 | -2.927738000 | -1.227461000 |
| C | -1.030928000 | 3.090151000 | -1.922423000 |
| C | -1.411029000 | 1.794268000 | -2.635471000 |
| H | -0.365431000 | 3.675559000 | -2.572771000 |
| H | -1.948965000 | 3.678825000 | -1.817722000 |
| C | -0.532238000 | 1.074586000 | -3.435688000 |
| C | 0.875174000 | 1.082566000 | -3.295797000 |
| H | 1.476651000 | 0.478164000 | -3.969808000 |
| H | 1.355136000 | 2.015231000 | -2.978849000 |
| H | -2.472917000 | 1.615982000 | -2.779169000 |
| Y | 0.059078000 | 0.303344000 | -1.066115000 |
| H | -0.968949000 | 0.275103000 | -4.040238000 |

94

C1_trans E = -1812.397824 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.006108000 | -0.526254000 | 1.460594000 |
| P | 2.658574000 | -0.219107000 | 0.072195000 |
| P | -2.406243000 | -0.804189000 | -0.237856000 |
| Si | -1.544799000 | 4.284373000 | 0.213334000 |
| C | -0.181693000 | 3.006019000 | 0.418767000 |
| H | 0.002417000 | 2.919802000 | 1.507195000 |
| H | 0.740187000 | 3.453657000 | -0.007632000 |
| C | -1.920491000 | 4.553018000 | -1.629322000 |
| H | -1.050039000 | 4.959009000 | -2.160473000 |
| H | -2.737006000 | 5.274253000 | -1.758162000 |
| H | -2.225734000 | 3.628361000 | -2.138475000 |
| C | -3.124405000 | 3.712051000 | 1.078861000 |
| H | -3.534939000 | 2.795123000 | 0.639665000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.902247000 | 4.483404000 | 1.017918000 |
| H | -2.942630000 | 3.511054000 | 2.141546000 |
| C | -1.034070000 | 5.953666000 | 0.941454000 |
| H | -0.832266000 | 5.868989000 | 2.016395000 |
| H | -1.819481000 | 6.708772000 | 0.811269000 |
| H | -0.123435000 | 6.337185000 | 0.464669000 |
| C | 3.333461000 | -1.233943000 | -1.315161000 |
| C | 2.867467000 | -2.540698000 | -1.519012000 |
| H | 2.198269000 | -2.999066000 | -0.795848000 |
| C | 3.282136000 | -3.268364000 | -2.634277000 |
| H | 2.923758000 | -4.284733000 | -2.774028000 |
| C | 4.162617000 | -2.703855000 | -3.556276000 |
| H | 4.490928000 | -3.276324000 | -4.419286000 |
| C | 4.631183000 | -1.404594000 | -3.359518000 |
| H | 5.329067000 | -0.963466000 | -4.066299000 |
| C | 4.216330000 | -0.669851000 | -2.249524000 |
| H | 4.604281000 | 0.334393000 | -2.096745000 |
| C | 4.057635000 | 0.822137000 | 0.666657000 |
| C | 3.763168000 | 2.086009000 | 1.195202000 |
| H | 2.738686000 | 2.451057000 | 1.206933000 |
| C | 4.779693000 | 2.883716000 | 1.718833000 |
| H | 4.540469000 | 3.860960000 | 2.129302000 |
| C | 6.097216000 | 2.428986000 | 1.710863000 |
| H | 6.890124000 | 3.051824000 | 2.115634000 |
| C | 6.398011000 | 1.173993000 | 1.180353000 |
| H | 7.424417000 | 0.817398000 | 1.171804000 |
| C | 5.385147000 | 0.370954000 | 0.661478000 |
| H | 5.633365000 | -0.601329000 | 0.245144000 |
| C | 2.277603000 | -1.413278000 | 1.408951000 |
| C | 0.972769000 | -1.396026000 | 1.966084000 |
| C | 0.704101000 | -2.318665000 | 2.999857000 |
| H | -0.287027000 | -2.346226000 | 3.440617000 |
| C | 1.679174000 | -3.192732000 | 3.460138000 |
| H | 1.430677000 | -3.886652000 | 4.259339000 |
| C | 2.962653000 | -3.196961000 | 2.908638000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.723622000 | -3.879923000 | 3.273339000 |
| C | 3.247031000 | -2.306481000 | 1.881699000 |
| H | 4.239678000 | -2.298910000 | 1.439182000 |
| C | -1.166177000 | -0.270751000 | 2.200489000 |
| C | -1.136392000 | 0.140071000 | 3.547490000 |
| H | -0.175607000 | 0.216461000 | 4.049149000 |
| C | -2.309003000 | 0.447820000 | 4.223877000 |
| H | -2.259925000 | 0.761791000 | 5.263294000 |
| C | -3.545975000 | 0.374305000 | 3.574859000 |
| H | -4.460368000 | 0.620243000 | 4.106732000 |
| C | -3.599814000 | -0.012251000 | 2.241274000 |
| H | -4.557477000 | -0.063879000 | 1.731362000 |
| C | -2.426944000 | -0.353430000 | 1.552099000 |
| C | -4.108161000 | -0.491892000 | -0.861202000 |
| C | -5.130206000 | -1.439175000 | -0.709896000 |
| H | -4.925548000 | -2.388156000 | -0.221844000 |
| C | -6.408776000 | -1.168941000 | -1.193447000 |
| H | -7.196321000 | -1.907981000 | -1.074322000 |
| C | -6.677061000 | 0.043173000 | -1.830071000 |
| H | -7.674674000 | 0.248866000 | -2.208084000 |
| C | -5.663949000 | 0.988336000 | -1.987244000 |
| H | -5.868393000 | 1.931521000 | -2.486359000 |
| C | -4.382587000 | 0.719532000 | -1.509636000 |
| H | -3.596614000 | 1.460182000 | -1.641563000 |
| C | -2.195564000 | -2.630709000 | -0.336848000 |
| C | -2.215226000 | -3.453564000 | 0.793607000 |
| H | -2.365009000 | -3.021505000 | 1.778671000 |
| C | -2.051373000 | -4.831971000 | 0.655027000 |
| H | -2.070812000 | -5.466636000 | 1.536801000 |
| C | -1.871017000 | -5.394598000 | -0.607430000 |
| H | -1.748479000 | -6.469181000 | -0.711552000 |
| C | -1.854931000 | -4.577539000 | -1.738923000 |
| H | -1.724061000 | -5.013257000 | -2.725840000 |
| C | -2.011202000 | -3.200239000 | -1.605127000 |
| H | -2.011534000 | -2.571434000 | -2.493488000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.402884000 | 3.167653000 | -3.243530000 |
| C | 1.192137000 | 2.585667000 | -3.231952000 |
| H | 2.513864000 | 4.246850000 | -3.287898000 |
| H | 3.318316000 | 2.580800000 | -3.223879000 |
| H | 0.293380000 | 3.200120000 | -3.267776000 |
| C | 1.014024000 | 1.142840000 | -3.198608000 |
| C | -0.187079000 | 0.514565000 | -3.182542000 |
| H | -0.253562000 | -0.569657000 | -3.233257000 |
| H | -1.121854000 | 1.069619000 | -3.272738000 |
| Y | -0.026644000 | 0.817102000 | -0.326422000 |
| H | 1.922065000 | 0.537589000 | -3.197942000 |

94

TS1_trans E = -1812.381695 a.u. Imaginary frequency=198i

| | | | |
|----|--------------|--------------|--------------|
| N | 0.351851000 | -1.715543000 | 0.019993000 |
| P | 2.749319000 | 0.049122000 | 0.117610000 |
| P | -2.415287000 | -0.637065000 | 0.122095000 |
| Si | -1.258721000 | 4.326512000 | -0.041166000 |
| C | -0.496704000 | 2.606120000 | -0.303175000 |
| H | -0.820220000 | 2.029762000 | 0.593343000 |
| H | 0.605012000 | 2.743869000 | -0.240188000 |
| C | -3.136692000 | 4.253326000 | -0.204916000 |
| H | -3.469964000 | 4.025636000 | -1.224323000 |
| H | -3.571018000 | 5.224756000 | 0.062114000 |
| H | -3.569971000 | 3.504496000 | 0.468221000 |
| C | -0.815941000 | 4.901843000 | 1.702651000 |
| H | -1.221285000 | 4.225932000 | 2.465216000 |
| H | -1.225787000 | 5.900634000 | 1.898690000 |
| H | 0.269782000 | 4.960365000 | 1.847432000 |
| C | -0.535426000 | 5.552540000 | -1.283916000 |
| H | 0.561681000 | 5.528944000 | -1.290591000 |
| H | -0.832187000 | 6.572314000 | -1.009573000 |
| H | -0.885336000 | 5.386516000 | -2.309449000 |
| C | 4.347399000 | 0.779681000 | -0.430830000 |
| C | 4.408665000 | 1.402744000 | -1.684996000 |
| H | 3.521393000 | 1.450701000 | -2.312912000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.601868000 | 1.959039000 | -2.139471000 |
| H | 5.639796000 | 2.438241000 | -3.114074000 |
| C | 6.742827000 | 1.908309000 | -1.338193000 |
| H | 7.672469000 | 2.348279000 | -1.688261000 |
| C | 6.687237000 | 1.297955000 | -0.085901000 |
| H | 7.573413000 | 1.259772000 | 0.541659000 |
| C | 5.495976000 | 0.734349000 | 0.369450000 |
| H | 5.461212000 | 0.264429000 | 1.348290000 |
| C | 2.860201000 | -0.064041000 | 1.950598000 |
| C | 2.530143000 | 1.070667000 | 2.705145000 |
| H | 2.219225000 | 1.987560000 | 2.207749000 |
| C | 2.613708000 | 1.035429000 | 4.095442000 |
| H | 2.362890000 | 1.919939000 | 4.674754000 |
| C | 3.018178000 | -0.133946000 | 4.740332000 |
| H | 3.080098000 | -0.162363000 | 5.824706000 |
| C | 3.344438000 | -1.265398000 | 3.993405000 |
| H | 3.662812000 | -2.175645000 | 4.494292000 |
| C | 3.266812000 | -1.234248000 | 2.601487000 |
| H | 3.523811000 | -2.116959000 | 2.022369000 |
| C | 2.743692000 | -1.680113000 | -0.518475000 |
| C | 1.500063000 | -2.362673000 | -0.480933000 |
| C | 1.450972000 | -3.662509000 | -1.023371000 |
| H | 0.506890000 | -4.200243000 | -1.004115000 |
| C | 2.578814000 | -4.253254000 | -1.578828000 |
| H | 2.507174000 | -5.255900000 | -1.992659000 |
| C | 3.795640000 | -3.566102000 | -1.621150000 |
| H | 4.676132000 | -4.030311000 | -2.055697000 |
| C | 3.870211000 | -2.280075000 | -1.097312000 |
| H | 4.811119000 | -1.737165000 | -1.125452000 |
| C | -0.446465000 | -2.409452000 | 0.934799000 |
| C | 0.038252000 | -3.469486000 | 1.729629000 |
| H | 1.072696000 | -3.780300000 | 1.624808000 |
| C | -0.777165000 | -4.110828000 | 2.653567000 |
| H | -0.361797000 | -4.918879000 | 3.250791000 |
| C | -2.107280000 | -3.724986000 | 2.834880000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.738960000 | -4.227469000 | 3.560895000 |
| C | -2.605058000 | -2.674552000 | 2.073072000 |
| H | -3.633015000 | -2.346770000 | 2.206955000 |
| C | -1.796932000 | -2.025859000 | 1.131568000 |
| C | -3.599449000 | 0.253149000 | 1.221775000 |
| C | -4.976428000 | 0.302674000 | 0.981529000 |
| H | -5.402101000 | -0.207345000 | 0.122607000 |
| C | -5.814455000 | 0.998711000 | 1.854337000 |
| H | -6.883327000 | 1.027741000 | 1.660863000 |
| C | -5.288033000 | 1.643701000 | 2.971116000 |
| H | -5.943907000 | 2.181807000 | 3.649794000 |
| C | -3.915354000 | 1.590276000 | 3.220506000 |
| H | -3.500007000 | 2.081223000 | 4.096518000 |
| C | -3.074241000 | 0.903567000 | 2.349230000 |
| H | -2.008578000 | 0.852893000 | 2.564960000 |
| C | -3.427377000 | -1.375744000 | -1.234921000 |
| C | -3.568579000 | -2.760879000 | -1.378578000 |
| H | -3.120528000 | -3.429160000 | -0.648994000 |
| C | -4.293170000 | -3.282688000 | -2.450716000 |
| H | -4.401095000 | -4.359272000 | -2.551696000 |
| C | -4.884327000 | -2.430938000 | -3.382367000 |
| H | -5.451763000 | -2.841267000 | -4.213046000 |
| C | -4.750080000 | -1.048402000 | -3.244164000 |
| H | -5.215485000 | -0.379542000 | -3.963241000 |
| C | -4.018066000 | -0.522870000 | -2.181670000 |
| H | -3.926535000 | 0.556682000 | -2.076577000 |
| C | -1.058553000 | 2.301725000 | -2.554408000 |
| C | -0.756971000 | 1.072581000 | -3.141571000 |
| H | -2.090866000 | 2.568610000 | -2.364134000 |
| H | -0.385254000 | 3.140426000 | -2.703814000 |
| H | -1.533961000 | 0.309218000 | -3.233067000 |
| C | 0.595972000 | 0.728537000 | -3.522825000 |
| C | 1.102080000 | -0.534797000 | -3.542002000 |
| H | 2.140615000 | -0.728172000 | -3.789505000 |
| H | 0.461614000 | -1.411586000 | -3.433047000 |

| | | | |
|---|-------------|-------------|--------------|
| Y | 0.103149000 | 0.358285000 | -0.935030000 |
| H | 1.286528000 | 1.562777000 | -3.674612000 |

94

P1_trans E = -1812.423255 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.178016000 | -2.037957000 | -0.156410000 |
| P | 2.595674000 | -0.307223000 | 0.090806000 |
| P | -2.422291000 | -0.670845000 | 0.133486000 |
| Si | -0.348469000 | 5.181678000 | 0.236582000 |
| C | -0.505671000 | 3.440409000 | -0.547756000 |
| H | -1.281066000 | 2.896108000 | 0.016918000 |
| H | 0.455339000 | 2.922742000 | -0.358250000 |
| C | -2.012323000 | 6.061095000 | 0.127047000 |
| H | -2.333695000 | 6.204563000 | -0.911452000 |
| H | -1.956390000 | 7.054546000 | 0.588366000 |
| H | -2.799515000 | 5.501666000 | 0.646940000 |
| C | 0.149202000 | 4.948783000 | 2.042770000 |
| H | -0.590856000 | 4.352521000 | 2.590237000 |
| H | 0.232569000 | 5.915523000 | 2.553775000 |
| H | 1.122109000 | 4.449517000 | 2.133442000 |
| C | 0.980575000 | 6.156499000 | -0.679951000 |
| H | 1.949198000 | 5.641787000 | -0.656860000 |
| H | 1.123943000 | 7.141808000 | -0.220136000 |
| H | 0.714962000 | 6.324986000 | -1.730297000 |
| C | 4.198709000 | 0.446460000 | -0.397927000 |
| C | 4.245594000 | 1.215765000 | -1.569114000 |
| H | 3.346551000 | 1.363225000 | -2.165243000 |
| C | 5.442281000 | 1.795727000 | -1.982650000 |
| H | 5.470815000 | 2.387509000 | -2.893465000 |
| C | 6.597995000 | 1.624557000 | -1.220024000 |
| H | 7.530261000 | 2.083586000 | -1.537043000 |
| C | 6.555223000 | 0.870014000 | -0.048115000 |
| H | 7.453500000 | 0.739055000 | 0.548906000 |
| C | 5.361606000 | 0.279194000 | 0.364190000 |
| H | 5.335244000 | -0.305766000 | 1.279226000 |
| C | 2.713156000 | -0.664880000 | 1.887461000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.388434000 | 0.361511000 | 2.785114000 |
| H | 2.069819000 | 1.333484000 | 2.413248000 |
| C | 2.486251000 | 0.145175000 | 4.157776000 |
| H | 2.239611000 | 0.945271000 | 4.850352000 |
| C | 2.898302000 | -1.097497000 | 4.640082000 |
| H | 2.970582000 | -1.267154000 | 5.710779000 |
| C | 3.217740000 | -2.121728000 | 3.749263000 |
| H | 3.540975000 | -3.088931000 | 4.124355000 |
| C | 3.127329000 | -1.909776000 | 2.374135000 |
| H | 3.379522000 | -2.709082000 | 1.682806000 |
| C | 2.527955000 | -1.935595000 | -0.786059000 |
| C | 1.291988000 | -2.642723000 | -0.760518000 |
| C | 1.219370000 | -3.876045000 | -1.442170000 |
| H | 0.279530000 | -4.420928000 | -1.434079000 |
| C | 2.316361000 | -4.379375000 | -2.124893000 |
| H | 2.232343000 | -5.330622000 | -2.643941000 |
| C | 3.519756000 | -3.664871000 | -2.168837000 |
| H | 4.373841000 | -4.061436000 | -2.709859000 |
| C | 3.617981000 | -2.446462000 | -1.510926000 |
| H | 4.551967000 | -1.892199000 | -1.535856000 |
| C | -0.667724000 | -2.749695000 | 0.692278000 |
| C | -0.293800000 | -3.944133000 | 1.338036000 |
| H | 0.690952000 | -4.362692000 | 1.154460000 |
| C | -1.158504000 | -4.578837000 | 2.222091000 |
| H | -0.835330000 | -5.495311000 | 2.709488000 |
| C | -2.421083000 | -4.051539000 | 2.502292000 |
| H | -3.088713000 | -4.550264000 | 3.198100000 |
| C | -2.807401000 | -2.869353000 | 1.879697000 |
| H | -3.781693000 | -2.437036000 | 2.094260000 |
| C | -1.953215000 | -2.225155000 | 0.978656000 |
| C | -3.292158000 | 0.342710000 | 1.403228000 |
| C | -4.683326000 | 0.486422000 | 1.446684000 |
| H | -5.308317000 | -0.000455000 | 0.703897000 |
| C | -5.274390000 | 1.254864000 | 2.450392000 |
| H | -6.355538000 | 1.360147000 | 2.477924000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.486315000 | 1.876966000 | 3.416490000 |
| H | -4.951045000 | 2.471898000 | 4.197819000 |
| C | -3.098737000 | 1.730394000 | 3.381938000 |
| H | -2.480730000 | 2.205687000 | 4.138970000 |
| C | -2.503008000 | 0.972796000 | 2.377104000 |
| H | -1.421096000 | 0.852707000 | 2.366706000 |
| C | -3.685351000 | -1.122994000 | -1.133235000 |
| C | -3.946913000 | -2.459403000 | -1.458841000 |
| H | -3.460664000 | -3.258114000 | -0.906434000 |
| C | -4.842231000 | -2.766953000 | -2.483554000 |
| H | -5.042804000 | -3.807114000 | -2.725681000 |
| C | -5.483581000 | -1.749152000 | -3.187161000 |
| H | -6.183187000 | -1.992993000 | -3.981758000 |
| C | -5.229072000 | -0.414845000 | -2.866210000 |
| H | -5.731248000 | 0.382885000 | -3.406727000 |
| C | -4.328890000 | -0.101158000 | -1.850912000 |
| H | -4.147640000 | 0.942516000 | -1.602060000 |
| C | -0.825022000 | 3.400651000 | -2.056582000 |
| C | -0.976949000 | 1.992623000 | -2.572010000 |
| H | -1.740688000 | 3.974878000 | -2.250581000 |
| H | -0.023903000 | 3.905008000 | -2.612889000 |
| H | -1.947516000 | 1.510794000 | -2.400766000 |
| C | -0.064475000 | 1.343671000 | -3.374822000 |
| C | -0.025476000 | -0.070606000 | -3.595057000 |
| H | 0.714253000 | -0.461863000 | -4.290328000 |
| H | -0.993546000 | -0.587090000 | -3.665632000 |
| Y | 0.080374000 | -0.045408000 | -1.176125000 |
| H | 0.833237000 | 1.907712000 | -3.650819000 |

94

C1_1,2 E = -1812.389632 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.081867000 | 0.236645000 | 1.557394000 |
| P | 2.361045000 | 0.501135000 | -0.038335000 |
| P | -2.350677000 | 0.401884000 | -0.432423000 |
| Si | 1.017611000 | -3.734321000 | -1.953320000 |
| C | 1.232148000 | -3.335035000 | -0.142105000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.291709000 | -3.211695000 | 0.127712000 |
| H | 0.859722000 | -4.165791000 | 0.473091000 |
| C | 0.026960000 | -2.251437000 | -2.741094000 |
| H | -1.006261000 | -2.100525000 | -2.371509000 |
| H | -0.116190000 | -2.480643000 | -3.804650000 |
| H | 0.559790000 | -1.281672000 | -2.749854000 |
| C | 2.605274000 | -3.839302000 | -2.964599000 |
| H | 3.199293000 | -2.919835000 | -2.906235000 |
| H | 2.389063000 | -4.028606000 | -4.023217000 |
| H | 3.231784000 | -4.663413000 | -2.602410000 |
| C | -0.044914000 | -5.262339000 | -2.266337000 |
| H | 0.479568000 | -6.160269000 | -1.917536000 |
| H | -0.249490000 | -5.394225000 | -3.335782000 |
| H | -1.011220000 | -5.231464000 | -1.748339000 |
| C | 4.104723000 | 0.227823000 | -0.573721000 |
| C | 4.528187000 | -1.079895000 | -0.851075000 |
| H | 3.838005000 | -1.911709000 | -0.741051000 |
| C | 5.836751000 | -1.325531000 | -1.259692000 |
| H | 6.154813000 | -2.343780000 | -1.466444000 |
| C | 6.731327000 | -0.265645000 | -1.410913000 |
| H | 7.750131000 | -0.455830000 | -1.737014000 |
| C | 6.314076000 | 1.037398000 | -1.146067000 |
| H | 7.006628000 | 1.866440000 | -1.263422000 |
| C | 5.007553000 | 1.287434000 | -0.726842000 |
| H | 4.695870000 | 2.306977000 | -0.521592000 |
| C | 2.137829000 | 2.325564000 | -0.072541000 |
| C | 1.719107000 | 2.921939000 | -1.268542000 |
| H | 1.486659000 | 2.308217000 | -2.135895000 |
| C | 1.605688000 | 4.308129000 | -1.355128000 |
| H | 1.285577000 | 4.763986000 | -2.287464000 |
| C | 1.896514000 | 5.103443000 | -0.247124000 |
| H | 1.806645000 | 6.184255000 | -0.314981000 |
| C | 2.303883000 | 4.511992000 | 0.948693000 |
| H | 2.531833000 | 5.129991000 | 1.812964000 |
| C | 2.428259000 | 3.126672000 | 1.038454000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.757400000 | 2.670570000 | 1.967908000 |
| C | 2.326546000 | 0.019182000 | 1.749195000 |
| C | 1.046107000 | -0.032552000 | 2.360545000 |
| C | 0.964027000 | -0.450897000 | 3.702593000 |
| H | -0.012826000 | -0.514124000 | 4.172515000 |
| C | 2.110095000 | -0.787817000 | 4.412429000 |
| H | 2.024413000 | -1.100632000 | 5.449940000 |
| C | 3.366448000 | -0.741116000 | 3.801033000 |
| H | 4.258763000 | -1.007502000 | 4.360102000 |
| C | 3.469803000 | -0.351141000 | 2.470317000 |
| H | 4.442865000 | -0.316012000 | 1.989100000 |
| C | -1.056436000 | 1.151670000 | 1.942364000 |
| C | -0.933889000 | 1.970013000 | 3.085804000 |
| H | -0.036056000 | 1.903223000 | 3.691199000 |
| C | -1.935703000 | 2.858809000 | 3.452212000 |
| H | -1.800701000 | 3.466078000 | 4.343880000 |
| C | -3.103913000 | 2.979862000 | 2.697074000 |
| H | -3.892192000 | 3.664776000 | 2.993972000 |
| C | -3.232040000 | 2.212575000 | 1.545176000 |
| H | -4.130326000 | 2.301492000 | 0.938906000 |
| C | -2.227488000 | 1.317728000 | 1.149902000 |
| C | -2.075375000 | 1.643815000 | -1.779943000 |
| C | -1.756404000 | 1.165997000 | -3.060919000 |
| H | -1.666259000 | 0.096587000 | -3.240664000 |
| C | -1.573665000 | 2.050096000 | -4.124014000 |
| H | -1.339159000 | 1.665549000 | -5.113101000 |
| C | -1.696681000 | 3.422992000 | -3.914482000 |
| H | -1.559266000 | 4.114235000 | -4.741592000 |
| C | -1.996653000 | 3.905709000 | -2.640470000 |
| H | -2.091541000 | 4.975085000 | -2.471996000 |
| C | -2.181635000 | 3.024726000 | -1.576248000 |
| H | -2.404825000 | 3.414621000 | -0.588287000 |
| C | -4.131517000 | -0.073795000 | -0.600275000 |
| C | -4.754926000 | -0.105674000 | -1.853927000 |
| H | -4.228446000 | 0.240976000 | -2.738468000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.068527000 | -0.556889000 | -1.974297000 |
| H | -6.543726000 | -0.566359000 | -2.951489000 |
| C | -6.773243000 | -0.982677000 | -0.849416000 |
| H | -7.797924000 | -1.330227000 | -0.946414000 |
| C | -6.160616000 | -0.949351000 | 0.402595000 |
| H | -6.707804000 | -1.264719000 | 1.287014000 |
| C | -4.846818000 | -0.500392000 | 0.528475000 |
| H | -4.388825000 | -0.449475000 | 1.512709000 |
| C | -2.108326000 | -3.083410000 | 0.657507000 |
| C | -1.648509000 | -3.223140000 | 1.922862000 |
| H | -3.051661000 | -2.585148000 | 0.445232000 |
| H | -1.634635000 | -3.627733000 | -0.159030000 |
| H | -0.736995000 | -3.796882000 | 2.093077000 |
| C | -2.309018000 | -2.702289000 | 3.106696000 |
| C | -1.875485000 | -2.959047000 | 4.350247000 |
| H | -2.406689000 | -2.595403000 | 5.224912000 |
| H | -0.984798000 | -3.557270000 | 4.530275000 |
| Y | 0.064468000 | -1.259069000 | -0.090580000 |
| H | -3.213135000 | -2.114910000 | 2.956236000 |

94

TS1_1,2 E = -1812.367425 a.u. Imaginary frequency=312i

| | | | |
|----|--------------|--------------|--------------|
| N | 0.110855000 | -0.680584000 | 1.428267000 |
| P | -2.269805000 | -0.715313000 | -0.272350000 |
| P | 2.630072000 | -0.169322000 | -0.093136000 |
| Si | -0.690959000 | 3.504952000 | -2.018697000 |
| C | -1.454269000 | 3.082082000 | -0.342885000 |
| H | -2.188871000 | 2.252767000 | -0.362689000 |
| H | -2.063803000 | 3.938470000 | -0.048925000 |
| C | 0.626152000 | 2.177522000 | -2.463250000 |
| H | 1.529579000 | 2.162185000 | -1.827718000 |
| H | 1.018796000 | 2.451626000 | -3.450730000 |
| H | 0.260681000 | 1.145908000 | -2.608099000 |
| C | -1.937130000 | 3.532811000 | -3.430406000 |
| H | -2.397662000 | 2.552185000 | -3.597299000 |
| H | -1.454706000 | 3.836893000 | -4.367956000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.741227000 | 4.249461000 | -3.225982000 |
| C | 0.218595000 | 5.146485000 | -1.894096000 |
| H | -0.465625000 | 5.957810000 | -1.617910000 |
| H | 0.668466000 | 5.415748000 | -2.857269000 |
| H | 1.024421000 | 5.122732000 | -1.150687000 |
| C | -4.027788000 | -0.501968000 | -0.797136000 |
| C | -4.391819000 | 0.629378000 | -1.537743000 |
| H | -3.644302000 | 1.372432000 | -1.801232000 |
| C | -5.711003000 | 0.809273000 | -1.952515000 |
| H | -5.981370000 | 1.690861000 | -2.527432000 |
| C | -6.675650000 | -0.146086000 | -1.639076000 |
| H | -7.702626000 | -0.010273000 | -1.966855000 |
| C | -6.319272000 | -1.283024000 | -0.912266000 |
| H | -7.067296000 | -2.034438000 | -0.674329000 |
| C | -5.003178000 | -1.463335000 | -0.493729000 |
| H | -4.732407000 | -2.358679000 | 0.059312000 |
| C | -1.975351000 | -2.525839000 | -0.455087000 |
| C | -1.635254000 | -3.001038000 | -1.728314000 |
| H | -1.520066000 | -2.307219000 | -2.558510000 |
| C | -1.455881000 | -4.366188000 | -1.941457000 |
| H | -1.203116000 | -4.728141000 | -2.934394000 |
| C | -1.601776000 | -5.263687000 | -0.883583000 |
| H | -1.461366000 | -6.328285000 | -1.049905000 |
| C | -1.930693000 | -4.793596000 | 0.387296000 |
| H | -2.046518000 | -5.490468000 | 1.213091000 |
| C | -2.119950000 | -3.429088000 | 0.603459000 |
| H | -2.384405000 | -3.069324000 | 1.594026000 |
| C | -2.285893000 | -0.398652000 | 1.553515000 |
| C | -1.028051000 | -0.479393000 | 2.215361000 |
| C | -0.990650000 | -0.243917000 | 3.608346000 |
| H | -0.036890000 | -0.304379000 | 4.125136000 |
| C | -2.149347000 | 0.059381000 | 4.309140000 |
| H | -2.096017000 | 0.228318000 | 5.381682000 |
| C | -3.378197000 | 0.166078000 | 3.645678000 |
| H | -4.280968000 | 0.408790000 | 4.198686000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.439927000 | -0.053216000 | 2.274907000 |
| H | -4.393478000 | 0.013558000 | 1.759333000 |
| C | 1.139662000 | -1.524098000 | 1.833493000 |
| C | 0.970781000 | -2.536084000 | 2.802471000 |
| H | -0.000537000 | -2.668981000 | 3.268428000 |
| C | 2.021357000 | -3.369074000 | 3.163922000 |
| H | 1.851733000 | -4.134520000 | 3.917212000 |
| C | 3.281768000 | -3.240129000 | 2.574944000 |
| H | 4.102222000 | -3.887240000 | 2.869319000 |
| C | 3.464757000 | -2.267862000 | 1.599288000 |
| H | 4.436872000 | -2.151929000 | 1.126144000 |
| C | 2.415071000 | -1.421769000 | 1.221660000 |
| C | 2.742430000 | -1.115095000 | -1.678897000 |
| C | 3.084471000 | -0.434356000 | -2.859421000 |
| H | 3.347379000 | 0.620703000 | -2.826886000 |
| C | 3.126604000 | -1.109579000 | -4.076668000 |
| H | 3.411822000 | -0.576418000 | -4.979786000 |
| C | 2.811502000 | -2.468303000 | -4.133755000 |
| H | 2.846993000 | -2.995438000 | -5.083249000 |
| C | 2.460142000 | -3.146643000 | -2.968558000 |
| H | 2.220198000 | -4.205781000 | -3.004812000 |
| C | 2.424704000 | -2.477183000 | -1.744704000 |
| H | 2.159101000 | -3.017900000 | -0.841470000 |
| C | 4.308162000 | 0.551413000 | 0.170646000 |
| C | 5.426982000 | 0.174143000 | -0.581377000 |
| H | 5.332572000 | -0.560449000 | -1.375461000 |
| C | 6.673586000 | 0.739040000 | -0.310959000 |
| H | 7.536668000 | 0.438619000 | -0.898944000 |
| C | 6.814662000 | 1.676876000 | 0.709977000 |
| H | 7.787446000 | 2.113923000 | 0.917598000 |
| C | 5.704557000 | 2.049680000 | 1.468654000 |
| H | 5.809613000 | 2.774488000 | 2.271450000 |
| C | 4.456805000 | 1.493807000 | 1.198761000 |
| H | 3.600751000 | 1.779630000 | 1.804685000 |
| C | 0.743017000 | 2.697496000 | 1.770263000 |

| | | | |
|---|--------------|-------------|-------------|
| C | -0.372431000 | 3.544294000 | 1.486626000 |
| H | 0.722239000 | 2.154459000 | 2.716473000 |
| H | 1.725425000 | 3.087892000 | 1.497196000 |
| H | -0.158987000 | 4.499267000 | 1.011921000 |
| C | -1.509198000 | 3.565850000 | 2.424265000 |
| C | -2.214304000 | 4.666520000 | 2.707417000 |
| H | -3.003301000 | 4.658181000 | 3.453668000 |
| H | -2.013342000 | 5.619631000 | 2.221209000 |
| Y | 0.025956000 | 1.138366000 | 0.092475000 |
| H | -1.725463000 | 2.633782000 | 2.946341000 |

94

P1_1,2 E = -1812.398652 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.226874000 | -1.479632000 | -1.090461000 |
| P | 2.685388000 | -0.255186000 | 0.053170000 |
| P | -2.433014000 | -0.729849000 | 0.109226000 |
| Si | -0.287520000 | 4.138555000 | 1.247907000 |
| C | 0.080107000 | 4.023083000 | -0.611340000 |
| H | 1.121561000 | 3.679149000 | -0.725132000 |
| H | 0.081359000 | 5.040727000 | -1.025419000 |
| C | -0.198404000 | 2.354382000 | 1.944675000 |
| H | -1.039321000 | 1.702506000 | 1.644116000 |
| H | -0.284353000 | 2.379215000 | 3.038213000 |
| H | 0.779994000 | 1.876067000 | 1.759832000 |
| C | 1.048481000 | 5.149497000 | 2.101188000 |
| H | 2.047068000 | 4.723518000 | 1.945923000 |
| H | 0.875133000 | 5.207372000 | 3.182371000 |
| H | 1.064879000 | 6.176665000 | 1.717604000 |
| C | -2.001518000 | 4.831545000 | 1.582010000 |
| H | -2.056399000 | 5.880189000 | 1.266754000 |
| H | -2.245793000 | 4.794786000 | 2.650382000 |
| H | -2.781367000 | 4.289279000 | 1.035841000 |
| C | 4.223216000 | 0.755652000 | 0.016390000 |
| C | 4.226102000 | 1.933969000 | -0.746007000 |
| H | 3.349926000 | 2.212217000 | -1.329386000 |
| C | 5.357876000 | 2.743714000 | -0.782127000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 5.355117000 | 3.649200000 | -1.382995000 |
| C | 6.491096000 | 2.393185000 | -0.045947000 |
| H | 7.372202000 | 3.028369000 | -0.069797000 |
| C | 6.490640000 | 1.227936000 | 0.717973000 |
| H | 7.371778000 | 0.950219000 | 1.289878000 |
| C | 5.362616000 | 0.407393000 | 0.749912000 |
| H | 5.373450000 | -0.501653000 | 1.343997000 |
| C | 2.980063000 | -1.612259000 | 1.255379000 |
| C | 2.707534000 | -1.373170000 | 2.609569000 |
| H | 2.327702000 | -0.404867000 | 2.929733000 |
| C | 2.934871000 | -2.370410000 | 3.555689000 |
| H | 2.728472000 | -2.177236000 | 4.604893000 |
| C | 3.423988000 | -3.613615000 | 3.153893000 |
| H | 3.597611000 | -4.392719000 | 3.891058000 |
| C | 3.691251000 | -3.856737000 | 1.806749000 |
| H | 4.074305000 | -4.824038000 | 1.493239000 |
| C | 3.472396000 | -2.860346000 | 0.856703000 |
| H | 3.684459000 | -3.052504000 | -0.191351000 |
| C | 2.567797000 | -1.027311000 | -1.619263000 |
| C | 1.311233000 | -1.578198000 | -1.985236000 |
| C | 1.180126000 | -2.130769000 | -3.274197000 |
| H | 0.220005000 | -2.544522000 | -3.569885000 |
| C | 2.250514000 | -2.141154000 | -4.157927000 |
| H | 2.121649000 | -2.572254000 | -5.147315000 |
| C | 3.482276000 | -1.587168000 | -3.793462000 |
| H | 4.316346000 | -1.596233000 | -4.488965000 |
| C | 3.632359000 | -1.023026000 | -2.532726000 |
| H | 4.584429000 | -0.587538000 | -2.243091000 |
| C | -0.572079000 | -2.594595000 | -0.829117000 |
| C | -0.140644000 | -3.914737000 | -1.076187000 |
| H | 0.849024000 | -4.079620000 | -1.489968000 |
| C | -0.954211000 | -5.003871000 | -0.794196000 |
| H | -0.584693000 | -6.005323000 | -1.000284000 |
| C | -2.229220000 | -4.830937000 | -0.249646000 |
| H | -2.865464000 | -5.685137000 | -0.039679000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.666817000 | -3.541147000 | 0.022220000 |
| H | -3.654482000 | -3.386588000 | 0.449528000 |
| C | -1.857207000 | -2.431361000 | -0.250798000 |
| C | -2.847237000 | -0.694756000 | 1.906818000 |
| C | -3.647821000 | 0.344247000 | 2.408219000 |
| H | -4.104390000 | 1.060296000 | 1.728561000 |
| C | -3.888512000 | 0.448406000 | 3.776351000 |
| H | -4.524929000 | 1.245620000 | 4.151193000 |
| C | -3.321656000 | -0.471180000 | 4.660336000 |
| H | -3.513578000 | -0.390555000 | 5.726715000 |
| C | -2.517513000 | -1.498108000 | 4.169300000 |
| H | -2.081452000 | -2.223202000 | 4.851302000 |
| C | -2.278792000 | -1.613096000 | 2.799376000 |
| H | -1.664970000 | -2.427734000 | 2.425728000 |
| C | -4.028955000 | -0.516443000 | -0.783712000 |
| C | -5.258581000 | -0.901449000 | -0.233331000 |
| H | -5.308571000 | -1.292073000 | 0.779246000 |
| C | -6.427172000 | -0.774911000 | -0.981977000 |
| H | -7.377545000 | -1.075278000 | -0.549174000 |
| C | -6.378401000 | -0.268112000 | -2.280576000 |
| H | -7.291998000 | -0.171398000 | -2.860606000 |
| C | -5.157454000 | 0.117213000 | -2.832913000 |
| H | -5.114699000 | 0.516218000 | -3.842536000 |
| C | -3.986717000 | -0.001891000 | -2.086455000 |
| H | -3.039512000 | 0.302532000 | -2.526132000 |
| C | -0.064360000 | 2.106084000 | -2.286205000 |
| C | -0.870218000 | 3.124193000 | -1.456751000 |
| H | 0.804932000 | 2.574889000 | -2.761794000 |
| H | -0.685097000 | 1.664576000 | -3.082530000 |
| H | -1.550774000 | 2.559199000 | -0.751662000 |
| C | -1.830183000 | 3.938647000 | -2.283877000 |
| C | -3.161239000 | 3.889810000 | -2.214243000 |
| H | -3.787559000 | 4.491237000 | -2.867196000 |
| H | -3.677259000 | 3.241018000 | -1.507938000 |
| Y | 0.034715000 | 0.651145000 | -0.490860000 |

H -1.347344000 4.594765000 -3.010361000

94

C1_cis_1,2 E = -1812.396139 a.u.

N 0.173309000 -1.527969000 -0.441824000

P 2.693264000 -0.117975000 0.173611000

P -2.535345000 -0.380107000 0.147538000

Si -0.520700000 4.155110000 0.600950000

C -0.259015000 2.346381000 1.023041000

H -1.087264000 2.050106000 1.686669000

H 0.656925000 2.292770000 1.642334000

C -1.988510000 4.340576000 -0.591984000

H -1.809674000 3.856182000 -1.562631000

H -2.202710000 5.396466000 -0.798357000

H -2.897982000 3.901353000 -0.162206000

C -0.879020000 5.207544000 2.129036000

H -1.787635000 4.865340000 2.639354000

H -1.019383000 6.264759000 1.871116000

H -0.054482000 5.147528000 2.849931000

C 1.030272000 4.858065000 -0.241102000

H 1.899666000 4.792378000 0.425628000

H 0.896255000 5.916479000 -0.496457000

H 1.287998000 4.332757000 -1.171031000

C 4.358739000 0.629435000 -0.062240000

C 4.450405000 1.941318000 -0.544697000

H 3.546322000 2.506558000 -0.759318000

C 5.696123000 2.542800000 -0.721836000

H 5.757023000 3.563417000 -1.089892000

C 6.858391000 1.839781000 -0.409996000

H 7.829387000 2.308964000 -0.542185000

C 6.774716000 0.539009000 0.089210000

H 7.679378000 -0.004501000 0.347686000

C 5.532150000 -0.064128000 0.268287000

H 5.475012000 -1.068556000 0.679390000

C 2.786479000 -0.972687000 1.802469000

C 2.525501000 -0.216961000 2.953524000

| | | | |
|---|--------------|--------------|--------------|
| H | 2.256879000 | 0.833700000 | 2.869492000 |
| C | 2.615824000 | -0.806895000 | 4.212442000 |
| H | 2.416387000 | -0.214390000 | 5.101211000 |
| C | 2.959580000 | -2.153739000 | 4.329702000 |
| H | 3.027789000 | -2.613673000 | 5.311704000 |
| C | 3.216742000 | -2.909462000 | 3.186476000 |
| H | 3.487574000 | -3.958096000 | 3.276037000 |
| C | 3.130525000 | -2.323974000 | 1.923985000 |
| H | 3.332786000 | -2.918229000 | 1.036871000 |
| C | 2.533632000 | -1.456717000 | -1.088146000 |
| C | 1.239008000 | -2.026133000 | -1.218595000 |
| C | 1.051802000 | -3.022907000 | -2.198066000 |
| H | 0.070217000 | -3.478981000 | -2.297712000 |
| C | 2.096603000 | -3.424446000 | -3.022631000 |
| H | 1.922485000 | -4.196164000 | -3.768118000 |
| C | 3.359224000 | -2.836343000 | -2.907505000 |
| H | 4.172871000 | -3.146912000 | -3.556363000 |
| C | 3.569672000 | -1.853701000 | -1.944469000 |
| H | 4.551097000 | -1.398475000 | -1.844213000 |
| C | -0.655999000 | -2.439765000 | 0.221822000 |
| C | -0.225779000 | -3.733745000 | 0.579364000 |
| H | 0.780140000 | -4.048108000 | 0.320078000 |
| C | -1.056774000 | -4.603320000 | 1.274776000 |
| H | -0.685853000 | -5.590380000 | 1.539335000 |
| C | -2.345641000 | -4.219757000 | 1.650349000 |
| H | -2.989576000 | -4.898867000 | 2.200748000 |
| C | -2.788320000 | -2.944728000 | 1.314992000 |
| H | -3.783060000 | -2.622071000 | 1.612418000 |
| C | -1.969212000 | -2.062634000 | 0.600207000 |
| C | -3.516302000 | 0.174648000 | 1.611042000 |
| C | -2.848992000 | 0.285220000 | 2.840715000 |
| H | -1.797974000 | 0.017404000 | 2.920272000 |
| C | -3.533028000 | 0.714304000 | 3.974609000 |
| H | -3.007874000 | 0.789312000 | 4.922997000 |
| C | -4.886547000 | 1.044973000 | 3.893720000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -5.418929000 | 1.381947000 | 4.778838000 |
| C | -5.553677000 | 0.934580000 | 2.676061000 |
| H | -6.610092000 | 1.180071000 | 2.607976000 |
| C | -4.874746000 | 0.499859000 | 1.536845000 |
| H | -5.413044000 | 0.405618000 | 0.598687000 |
| C | -3.766066000 | -0.585858000 | -1.216121000 |
| C | -4.290242000 | 0.572864000 | -1.812920000 |
| H | -4.013098000 | 1.555072000 | -1.433606000 |
| C | -5.182935000 | 0.476251000 | -2.878670000 |
| H | -5.594921000 | 1.378931000 | -3.322273000 |
| C | -5.546413000 | -0.777674000 | -3.373369000 |
| H | -6.238524000 | -0.853739000 | -4.207416000 |
| C | -5.022014000 | -1.930997000 | -2.791860000 |
| H | -5.306567000 | -2.909195000 | -3.170297000 |
| C | -4.137715000 | -1.839278000 | -1.715511000 |
| H | -3.740847000 | -2.743343000 | -1.263032000 |
| C | -0.972024000 | -0.046677000 | -3.333664000 |
| C | -0.819492000 | 1.296651000 | -3.286486000 |
| H | -0.133701000 | -0.740940000 | -3.381994000 |
| H | -1.964138000 | -0.484708000 | -3.377550000 |
| C | 0.454723000 | 2.023185000 | -3.195670000 |
| C | 1.687262000 | 1.474204000 | -3.108655000 |
| H | 2.568935000 | 2.103479000 | -3.041157000 |
| H | 1.869832000 | 0.402185000 | -3.180468000 |
| H | -1.715515000 | 1.915336000 | -3.301279000 |
| Y | 0.058209000 | 0.735465000 | -0.642261000 |
| H | 0.372099000 | 3.108811000 | -3.171683000 |

94

TS1_cis_1,2 E = -1812.366083 a.u. Imaginary frequency=318i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.084449000 | 0.361231000 | 1.556888000 |
| P | 2.260376000 | 0.669251000 | -0.187318000 |
| P | -2.481817000 | 0.294061000 | -0.240656000 |
| Si | 1.000762000 | -3.428765000 | -2.125626000 |
| C | 1.316770000 | -3.302051000 | -0.256013000 |
| H | 2.072885000 | -2.555195000 | 0.066894000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.785443000 | -4.250300000 | 0.019549000 |
| C | -0.202303000 | -2.026612000 | -2.658605000 |
| H | -1.205672000 | -2.066792000 | -2.197736000 |
| H | -0.401022000 | -2.185060000 | -3.726402000 |
| H | 0.194746000 | -0.997157000 | -2.617186000 |
| C | 2.556300000 | -3.256771000 | -3.167338000 |
| H | 3.040262000 | -2.282669000 | -3.036538000 |
| H | 2.320860000 | -3.374168000 | -4.232685000 |
| H | 3.287478000 | -4.031121000 | -2.906368000 |
| C | 0.125800000 | -5.054203000 | -2.482344000 |
| H | 0.724139000 | -5.909068000 | -2.145053000 |
| H | -0.028679000 | -5.173203000 | -3.561596000 |
| H | -0.857026000 | -5.122587000 | -2.001812000 |
| C | 4.012338000 | 0.535611000 | -0.765447000 |
| C | 4.565996000 | -0.737844000 | -0.970679000 |
| H | 3.981772000 | -1.630477000 | -0.759407000 |
| C | 5.871774000 | -0.877406000 | -1.434911000 |
| H | 6.289734000 | -1.870023000 | -1.580220000 |
| C | 6.636793000 | 0.254383000 | -1.718148000 |
| H | 7.653189000 | 0.146853000 | -2.086623000 |
| C | 6.091045000 | 1.522109000 | -1.528578000 |
| H | 6.681016000 | 2.407984000 | -1.747715000 |
| C | 4.787770000 | 1.665701000 | -1.052254000 |
| H | 4.378433000 | 2.660243000 | -0.904926000 |
| C | 1.924540000 | 2.479250000 | -0.159881000 |
| C | 1.337138000 | 3.061279000 | -1.289703000 |
| H | 1.048191000 | 2.442227000 | -2.136196000 |
| C | 1.122715000 | 4.437907000 | -1.336717000 |
| H | 0.670854000 | 4.882018000 | -2.219004000 |
| C | 1.481228000 | 5.237478000 | -0.252258000 |
| H | 1.311967000 | 6.310315000 | -0.287974000 |
| C | 2.057712000 | 4.660276000 | 0.879646000 |
| H | 2.338268000 | 5.281872000 | 1.725748000 |
| C | 2.283244000 | 3.285934000 | 0.927285000 |
| H | 2.742286000 | 2.841783000 | 1.806389000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.333373000 | 0.182707000 | 1.603323000 |
| C | 1.091210000 | 0.132365000 | 2.293677000 |
| C | 1.096631000 | -0.244739000 | 3.652270000 |
| H | 0.151511000 | -0.296445000 | 4.185086000 |
| C | 2.285234000 | -0.547106000 | 4.302900000 |
| H | 2.264610000 | -0.825900000 | 5.353301000 |
| C | 3.501957000 | -0.507960000 | 3.614771000 |
| H | 4.430128000 | -0.744001000 | 4.127348000 |
| C | 3.520996000 | -0.154226000 | 2.270220000 |
| H | 4.466240000 | -0.111270000 | 1.736737000 |
| C | -1.095547000 | 1.200146000 | 2.012946000 |
| C | -0.956881000 | 2.049328000 | 3.131109000 |
| H | -0.010819000 | 2.080741000 | 3.661631000 |
| C | -2.007125000 | 2.848789000 | 3.563926000 |
| H | -1.860112000 | 3.484756000 | 4.433443000 |
| C | -3.239211000 | 2.843717000 | 2.906259000 |
| H | -4.062885000 | 3.455625000 | 3.260812000 |
| C | -3.385736000 | 2.046932000 | 1.776557000 |
| H | -4.331449000 | 2.037667000 | 1.239674000 |
| C | -2.332287000 | 1.247860000 | 1.314215000 |
| C | -2.481554000 | 1.531874000 | -1.616844000 |
| C | -2.375212000 | 1.059466000 | -2.934903000 |
| H | -2.306301000 | -0.008773000 | -3.129012000 |
| C | -2.381945000 | 1.947025000 | -4.009534000 |
| H | -2.312607000 | 1.567166000 | -5.025472000 |
| C | -2.482207000 | 3.319017000 | -3.778060000 |
| H | -2.490475000 | 4.012709000 | -4.614422000 |
| C | -2.574062000 | 3.795993000 | -2.471261000 |
| H | -2.653599000 | 4.863759000 | -2.285423000 |
| C | -2.570845000 | 2.910696000 | -1.393569000 |
| H | -2.636363000 | 3.295079000 | -0.380678000 |
| C | -4.192284000 | -0.406792000 | -0.220441000 |
| C | -5.073547000 | -0.276997000 | -1.299465000 |
| H | -4.792041000 | 0.303138000 | -2.173213000 |
| C | -6.332759000 | -0.876237000 | -1.250748000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -7.012622000 | -0.761585000 | -2.090735000 |
| C | -6.722019000 | -1.606663000 | -0.130117000 |
| H | -7.704666000 | -2.068799000 | -0.094459000 |
| C | -5.849078000 | -1.733892000 | 0.951157000 |
| H | -6.150054000 | -2.291817000 | 1.833834000 |
| C | -4.590234000 | -1.140880000 | 0.906937000 |
| H | -3.925435000 | -1.230134000 | 1.762047000 |
| C | -1.436786000 | -2.969482000 | 1.007519000 |
| C | -0.310617000 | -3.849494000 | 1.011312000 |
| H | -1.719598000 | -2.514137000 | 1.957813000 |
| H | -2.286950000 | -3.253985000 | 0.386862000 |
| H | -0.386728000 | -4.714912000 | 0.355671000 |
| C | 0.472267000 | -4.117232000 | 2.244183000 |
| C | 0.107480000 | -3.777339000 | 3.485238000 |
| H | 0.725203000 | -4.047054000 | 4.336802000 |
| H | -0.816688000 | -3.250399000 | 3.704248000 |
| Y | -0.052039000 | -1.270645000 | 0.027885000 |
| H | 1.395754000 | -4.678817000 | 2.113801000 |

94

P1_cis_1,2 E = -1812.405394 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.299220000 | -0.113540000 | 1.399706000 |
| P | 1.811456000 | -1.529550000 | -0.154229000 |
| P | -2.757965000 | 0.360522000 | -0.209309000 |
| Si | 3.788911000 | 3.923611000 | 0.186407000 |
| C | 2.871254000 | 2.417046000 | -0.568595000 |
| H | 2.424461000 | 1.852777000 | 0.272581000 |
| H | 3.657971000 | 1.765080000 | -0.977044000 |
| C | 4.705883000 | 4.802679000 | -1.208340000 |
| H | 5.410619000 | 4.134072000 | -1.717440000 |
| H | 5.283318000 | 5.647698000 | -0.814104000 |
| H | 4.021925000 | 5.206605000 | -1.964578000 |
| C | 2.609227000 | 5.121176000 | 1.039229000 |
| H | 1.902663000 | 5.577109000 | 0.336469000 |
| H | 3.176394000 | 5.935744000 | 1.506852000 |
| H | 2.029244000 | 4.630939000 | 1.830479000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.014615000 | 3.236936000 | 1.445939000 |
| H | 4.504822000 | 2.705308000 | 2.259197000 |
| H | 5.596967000 | 4.046449000 | 1.902082000 |
| H | 5.726923000 | 2.543416000 | 0.982962000 |
| C | 0.970400000 | -2.757801000 | -1.252370000 |
| C | 0.151761000 | -3.779653000 | -0.755529000 |
| H | 0.022545000 | -3.897157000 | 0.316268000 |
| C | -0.489622000 | -4.651731000 | -1.635643000 |
| H | -1.114052000 | -5.447703000 | -1.239244000 |
| C | -0.324726000 | -4.512553000 | -3.013106000 |
| H | -0.819317000 | -5.200090000 | -3.693840000 |
| C | 0.483023000 | -3.491996000 | -3.517492000 |
| H | 0.622104000 | -3.384564000 | -4.590017000 |
| C | 1.120622000 | -2.613865000 | -2.643334000 |
| H | 1.766213000 | -1.833917000 | -3.043645000 |
| C | 3.609854000 | -1.910364000 | -0.259695000 |
| C | 4.496664000 | -1.051372000 | 0.406402000 |
| H | 4.118033000 | -0.198796000 | 0.965026000 |
| C | 5.866700000 | -1.296037000 | 0.372635000 |
| H | 6.546018000 | -0.631223000 | 0.899194000 |
| C | 6.365047000 | -2.390674000 | -0.335331000 |
| H | 7.434780000 | -2.578329000 | -0.364389000 |
| C | 5.487965000 | -3.244557000 | -1.000965000 |
| H | 5.870599000 | -4.102387000 | -1.547293000 |
| C | 4.113051000 | -3.010211000 | -0.963601000 |
| H | 3.438902000 | -3.689032000 | -1.477484000 |
| C | 1.297001000 | -1.939881000 | 1.551192000 |
| C | 0.261254000 | -1.159013000 | 2.130482000 |
| C | -0.178703000 | -1.526825000 | 3.418690000 |
| H | -0.991909000 | -0.975660000 | 3.880018000 |
| C | 0.407754000 | -2.583055000 | 4.104878000 |
| H | 0.043730000 | -2.832127000 | 5.098558000 |
| C | 1.448707000 | -3.323003000 | 3.539869000 |
| H | 1.910718000 | -4.139733000 | 4.085858000 |
| C | 1.879889000 | -2.997990000 | 2.258777000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.685415000 | -3.564993000 | 1.798517000 |
| C | -1.120678000 | 0.852667000 | 2.011497000 |
| C | -0.752018000 | 1.539765000 | 3.185839000 |
| H | 0.172534000 | 1.262981000 | 3.684956000 |
| C | -1.546035000 | 2.557678000 | 3.695817000 |
| H | -1.239835000 | 3.069693000 | 4.604405000 |
| C | -2.722422000 | 2.939992000 | 3.042176000 |
| H | -3.338534000 | 3.739473000 | 3.443088000 |
| C | -3.099559000 | 2.288874000 | 1.874735000 |
| H | -4.010133000 | 2.583513000 | 1.361029000 |
| C | -2.325092000 | 1.237015000 | 1.361512000 |
| C | -4.100412000 | 1.364711000 | -0.969112000 |
| C | -5.441891000 | 0.967457000 | -0.928640000 |
| H | -5.725495000 | 0.048884000 | -0.423524000 |
| C | -6.420025000 | 1.751440000 | -1.540445000 |
| H | -7.459118000 | 1.435621000 | -1.506158000 |
| C | -6.069278000 | 2.933840000 | -2.189352000 |
| H | -6.834356000 | 3.541419000 | -2.664657000 |
| C | -4.733445000 | 3.336163000 | -2.229881000 |
| H | -4.455318000 | 4.257934000 | -2.733718000 |
| C | -3.751800000 | 2.552288000 | -1.629750000 |
| H | -2.713044000 | 2.876003000 | -1.663140000 |
| C | -3.531031000 | -1.235119000 | 0.270111000 |
| C | -4.063523000 | -1.444684000 | 1.547603000 |
| H | -4.000942000 | -0.662809000 | 2.299216000 |
| C | -4.677977000 | -2.658009000 | 1.853936000 |
| H | -5.090783000 | -2.816596000 | 2.846492000 |
| C | -4.768837000 | -3.661445000 | 0.889537000 |
| H | -5.253078000 | -4.603818000 | 1.130677000 |
| C | -4.239241000 | -3.455337000 | -0.384488000 |
| H | -4.310551000 | -4.234514000 | -1.138400000 |
| C | -3.615467000 | -2.248523000 | -0.693929000 |
| H | -3.201058000 | -2.095642000 | -1.688010000 |
| C | 0.656637000 | 1.257809000 | -3.406497000 |
| C | 1.747727000 | 1.630356000 | -2.705863000 |

| | | | |
|---|--------------|-------------|--------------|
| H | 0.713133000 | 0.513175000 | -4.196152000 |
| H | -0.300682000 | 1.772613000 | -3.297029000 |
| H | 2.696546000 | 1.141966000 | -2.937164000 |
| C | 1.795832000 | 2.720631000 | -1.642103000 |
| C | 0.420653000 | 2.965353000 | -0.985673000 |
| H | 0.530822000 | 3.613218000 | -0.109994000 |
| H | -0.266475000 | 3.477318000 | -1.676188000 |
| Y | 0.027645000 | 0.669797000 | -0.667347000 |
| H | 2.128104000 | 3.606586000 | -2.215492000 |

117

theta3_thf_C2_cis_1,4 E = -2200.65044 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.074057000 | 1.123144000 | 1.137977000 |
| P | -2.888157000 | -1.055870000 | 0.058300000 |
| P | 1.767884000 | 1.794199000 | 0.329602000 |
| Si | 4.901170000 | -4.051259000 | -1.378612000 |
| C | 3.983531000 | -2.567251000 | -2.145100000 |
| H | 3.628542000 | -2.871149000 | -3.140668000 |
| H | 4.708810000 | -1.758752000 | -2.319252000 |
| C | 3.701515000 | -5.499869000 | -1.185143000 |
| H | 2.875968000 | -5.262568000 | -0.502227000 |
| H | 4.213323000 | -6.381559000 | -0.780769000 |
| H | 3.263061000 | -5.788425000 | -2.148268000 |
| C | 6.311296000 | -4.531822000 | -2.534749000 |
| H | 5.938243000 | -4.807087000 | -3.528493000 |
| H | 6.869878000 | -5.390603000 | -2.143389000 |
| H | 7.022490000 | -3.707171000 | -2.664040000 |
| C | 5.593613000 | -3.581354000 | 0.317443000 |
| H | 6.279453000 | -2.728838000 | 0.244579000 |
| H | 6.150263000 | -4.416997000 | 0.758759000 |
| H | 4.797592000 | -3.309548000 | 1.021898000 |
| C | -4.188847000 | -1.569113000 | -1.149353000 |
| C | -4.003210000 | -1.269383000 | -2.504728000 |
| H | -3.091197000 | -0.772387000 | -2.821604000 |
| C | -4.969297000 | -1.614100000 | -3.447708000 |
| H | -4.810846000 | -1.380702000 | -4.497458000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.131043000 | -2.272531000 | -3.045744000 |
| H | -6.882246000 | -2.549433000 | -3.780281000 |
| C | -6.321834000 | -2.582087000 | -1.699729000 |
| H | -7.223590000 | -3.098477000 | -1.381813000 |
| C | -5.357880000 | -2.234067000 | -0.754313000 |
| H | -5.515230000 | -2.486947000 | 0.290296000 |
| C | -3.151799000 | -2.226356000 | 1.466954000 |
| C | -2.942938000 | -3.597111000 | 1.248218000 |
| H | -2.676285000 | -3.958201000 | 0.256492000 |
| C | -3.102964000 | -4.508235000 | 2.289125000 |
| H | -2.948921000 | -5.568324000 | 2.106228000 |
| C | -3.462956000 | -4.060856000 | 3.561508000 |
| H | -3.586376000 | -4.772189000 | 4.373469000 |
| C | -3.672291000 | -2.701337000 | 3.785029000 |
| H | -3.964744000 | -2.349677000 | 4.770948000 |
| C | -3.519710000 | -1.785205000 | 2.742933000 |
| H | -3.703032000 | -0.728818000 | 2.918331000 |
| C | -3.436598000 | 0.583482000 | 0.683838000 |
| C | -2.436749000 | 1.462402000 | 1.178072000 |
| C | -2.870910000 | 2.731623000 | 1.627239000 |
| H | -2.131551000 | 3.435312000 | 1.998100000 |
| C | -4.207075000 | 3.103994000 | 1.589934000 |
| H | -4.491414000 | 4.094138000 | 1.938118000 |
| C | -5.179797000 | 2.229890000 | 1.096654000 |
| H | -6.225508000 | 2.520718000 | 1.063716000 |
| C | -4.781978000 | 0.977857000 | 0.644515000 |
| H | -5.524303000 | 0.289136000 | 0.250325000 |
| C | -0.286910000 | 1.595403000 | 2.200909000 |
| C | -0.786079000 | 1.659666000 | 3.522328000 |
| H | -1.812539000 | 1.357625000 | 3.707644000 |
| C | -0.003693000 | 2.099275000 | 4.582204000 |
| H | -0.432854000 | 2.128343000 | 5.580926000 |
| C | 1.322372000 | 2.490448000 | 4.379257000 |
| H | 1.933929000 | 2.839216000 | 5.205961000 |
| C | 1.848373000 | 2.415570000 | 3.094285000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.883215000 | 2.697290000 | 2.918977000 |
| C | 1.070177000 | 1.973261000 | 2.015785000 |
| C | 3.593016000 | 1.648966000 | 0.579606000 |
| C | 4.496266000 | 2.592681000 | 0.077327000 |
| H | 4.137564000 | 3.466822000 | -0.456914000 |
| C | 5.868107000 | 2.424130000 | 0.269652000 |
| H | 6.558354000 | 3.166058000 | -0.122851000 |
| C | 6.350002000 | 1.320260000 | 0.968848000 |
| H | 7.418392000 | 1.194412000 | 1.121614000 |
| C | 5.453806000 | 0.379556000 | 1.478156000 |
| H | 5.820956000 | -0.481294000 | 2.030154000 |
| C | 4.084568000 | 0.536943000 | 1.279839000 |
| H | 3.398897000 | -0.197468000 | 1.695597000 |
| C | 1.560208000 | 3.435530000 | -0.495068000 |
| C | 1.165529000 | 4.581275000 | 0.204953000 |
| H | 0.968111000 | 4.522229000 | 1.271628000 |
| C | 1.033701000 | 5.799332000 | -0.462865000 |
| H | 0.730164000 | 6.684970000 | 0.089030000 |
| C | 1.304256000 | 5.885424000 | -1.828272000 |
| H | 1.211996000 | 6.838166000 | -2.342594000 |
| C | 1.701118000 | 4.746913000 | -2.532067000 |
| H | 1.924214000 | 4.811984000 | -3.594042000 |
| C | 1.818038000 | 3.524834000 | -1.871526000 |
| H | 2.130643000 | 2.639771000 | -2.422580000 |
| C | 2.442746000 | -2.213637000 | 3.609834000 |
| C | 1.413969000 | -1.393152000 | 3.353190000 |
| H | 1.311842000 | -0.465406000 | 3.913539000 |
| C | 0.336535000 | -1.707883000 | 2.413224000 |
| C | 0.478996000 | -2.389214000 | 1.256811000 |
| H | -0.397967000 | -2.743294000 | 0.715867000 |
| H | 1.450076000 | -2.752090000 | 0.932225000 |
| Y | -0.160328000 | -0.150395000 | -0.638849000 |
| H | -0.660030000 | -1.374017000 | 2.699546000 |
| O | -1.135257000 | 1.409126000 | -2.197311000 |
| C | -1.223392000 | 1.301997000 | -3.649552000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.792887000 | 2.658392000 | -1.774396000 |
| C | -2.294741000 | 2.293768000 | -4.064384000 |
| H | -0.247268000 | 1.569535000 | -4.069644000 |
| H | -1.453744000 | 0.264862000 | -3.898105000 |
| C | -2.079243000 | 3.421782000 | -3.056201000 |
| H | -2.708777000 | 2.377917000 | -1.251684000 |
| H | -1.118309000 | 3.171893000 | -1.089577000 |
| H | -3.292324000 | 1.855057000 | -3.948780000 |
| H | -2.175321000 | 2.609807000 | -5.104632000 |
| H | -2.949953000 | 4.074450000 | -2.948045000 |
| H | -1.219848000 | 4.037799000 | -3.341101000 |
| H | 3.200993000 | -1.952797000 | 4.342831000 |
| H | 2.537248000 | -3.185090000 | 3.130166000 |
| C | 2.788907000 | -2.013073000 | -1.339044000 |
| C | 2.060975000 | -0.945477000 | -2.131026000 |
| H | 2.103027000 | -2.837596000 | -1.110866000 |
| H | 3.161758000 | -1.625600000 | -0.381494000 |
| H | 2.713681000 | -0.165174000 | -2.523545000 |
| C | 0.875507000 | -1.159760000 | -2.823888000 |
| C | -0.226774000 | -1.955669000 | -2.431154000 |
| H | 0.684435000 | -0.456584000 | -3.636562000 |
| H | -1.047984000 | -2.091414000 | -3.130436000 |
| H | -0.047176000 | -2.835426000 | -1.805423000 |

117

theta3_thf_TS2_cis_1,4 E = -2200.633721 a.u. Imaginary frequency=148i

| | | | |
|----|--------------|--------------|--------------|
| N | -1.344113000 | -1.401583000 | -0.868437000 |
| P | -2.913279000 | 1.072747000 | -0.019369000 |
| P | 1.538024000 | -2.097278000 | -0.222338000 |
| Si | 5.663486000 | 4.288472000 | 0.264059000 |
| C | 4.249851000 | 3.508398000 | 1.281454000 |
| H | 3.644440000 | 4.319190000 | 1.710994000 |
| H | 4.690714000 | 2.977086000 | 2.137590000 |
| C | 4.927607000 | 5.396038000 | -1.076999000 |
| H | 4.322797000 | 4.831199000 | -1.797582000 |
| H | 5.719157000 | 5.898610000 | -1.645800000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.290247000 | 6.176677000 | -0.644064000 |
| C | 6.730614000 | 5.305659000 | 1.438357000 |
| H | 6.146626000 | 6.090027000 | 1.934595000 |
| H | 7.551239000 | 5.796818000 | 0.901790000 |
| H | 7.177359000 | 4.679581000 | 2.220064000 |
| C | 6.693683000 | 2.919254000 | -0.534464000 |
| H | 7.097514000 | 2.228135000 | 0.215793000 |
| H | 7.544964000 | 3.342357000 | -1.081124000 |
| H | 6.106318000 | 2.334499000 | -1.253705000 |
| C | -3.688124000 | 1.865521000 | 1.464105000 |
| C | -2.945565000 | 1.963198000 | 2.648557000 |
| H | -1.931054000 | 1.575211000 | 2.681119000 |
| C | -3.498255000 | 2.546510000 | 3.787990000 |
| H | -2.909385000 | 2.620393000 | 4.698654000 |
| C | -4.799593000 | 3.044739000 | 3.755481000 |
| H | -5.229673000 | 3.504601000 | 4.640976000 |
| C | -5.544951000 | 2.959235000 | 2.579812000 |
| H | -6.558229000 | 3.350501000 | 2.547032000 |
| C | -4.994110000 | 2.377488000 | 1.439617000 |
| H | -5.578273000 | 2.336389000 | 0.524733000 |
| C | -3.764750000 | 1.944215000 | -1.415457000 |
| C | -3.752529000 | 3.347340000 | -1.461674000 |
| H | -3.312667000 | 3.917390000 | -0.645999000 |
| C | -4.332378000 | 4.023316000 | -2.532923000 |
| H | -4.326539000 | 5.110002000 | -2.550626000 |
| C | -4.923984000 | 3.308328000 | -3.575357000 |
| H | -5.376023000 | 3.836400000 | -4.410347000 |
| C | -4.941370000 | 1.915680000 | -3.535397000 |
| H | -5.411538000 | 1.352960000 | -4.337535000 |
| C | -4.366782000 | 1.234432000 | -2.461101000 |
| H | -4.401581000 | 0.149067000 | -2.429369000 |
| C | -3.555829000 | -0.644128000 | -0.086785000 |
| C | -2.683168000 | -1.661916000 | -0.558754000 |
| C | -3.220789000 | -2.970919000 | -0.622063000 |
| H | -2.590479000 | -3.779948000 | -0.977632000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.522985000 | -3.251053000 | -0.236499000 |
| H | -4.883023000 | -4.275402000 | -0.296238000 |
| C | -5.364171000 | -2.240745000 | 0.237709000 |
| H | -6.381883000 | -2.459563000 | 0.546236000 |
| C | -4.867021000 | -0.946790000 | 0.307407000 |
| H | -5.505038000 | -0.149880000 | 0.679623000 |
| C | -0.744472000 | -2.216695000 | -1.846432000 |
| C | -1.428004000 | -2.565232000 | -3.032924000 |
| H | -2.458100000 | -2.241751000 | -3.152312000 |
| C | -0.814647000 | -3.292830000 | -4.043249000 |
| H | -1.375175000 | -3.534598000 | -4.942918000 |
| C | 0.517235000 | -3.694209000 | -3.917309000 |
| H | 1.005301000 | -4.256569000 | -4.707803000 |
| C | 1.215071000 | -3.360252000 | -2.762106000 |
| H | 2.254060000 | -3.659961000 | -2.666617000 |
| C | 0.604187000 | -2.646177000 | -1.722249000 |
| C | 3.324175000 | -2.395376000 | -0.599350000 |
| C | 3.849980000 | -3.693745000 | -0.697037000 |
| H | 3.204013000 | -4.554884000 | -0.549080000 |
| C | 5.202445000 | -3.887151000 | -0.967214000 |
| H | 5.596621000 | -4.896933000 | -1.043679000 |
| C | 6.049874000 | -2.790574000 | -1.132341000 |
| H | 7.105324000 | -2.945042000 | -1.339151000 |
| C | 5.542136000 | -1.498187000 | -1.018736000 |
| H | 6.199945000 | -0.640554000 | -1.130519000 |
| C | 4.187096000 | -1.304160000 | -0.750030000 |
| H | 3.799056000 | -0.295349000 | -0.645810000 |
| C | 1.230116000 | -3.418313000 | 1.044335000 |
| C | 0.169797000 | -4.323152000 | 0.934247000 |
| H | -0.492936000 | -4.278051000 | 0.075849000 |
| C | -0.024152000 | -5.304189000 | 1.908231000 |
| H | -0.846959000 | -6.006781000 | 1.805543000 |
| C | 0.842176000 | -5.395743000 | 2.996582000 |
| H | 0.697097000 | -6.168405000 | 3.746673000 |
| C | 1.905186000 | -4.498074000 | 3.111530000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.594028000 | -4.571685000 | 3.949055000 |
| C | 2.095545000 | -3.512605000 | 2.145011000 |
| H | 2.945635000 | -2.839104000 | 2.230754000 |
| C | 1.732649000 | 0.559243000 | -2.462969000 |
| C | 0.465575000 | 0.516846000 | -2.968713000 |
| H | 0.188938000 | -0.342898000 | -3.574773000 |
| C | -0.585036000 | 1.434768000 | -2.617832000 |
| C | -0.308158000 | 2.683872000 | -2.074516000 |
| H | -1.118752000 | 3.385146000 | -1.917556000 |
| H | 0.669601000 | 3.122156000 | -2.241553000 |
| Y | -0.030709000 | 0.446300000 | -0.265819000 |
| H | -1.610547000 | 1.164358000 | -2.851166000 |
| O | -0.417927000 | -0.407420000 | 2.135129000 |
| C | 0.520668000 | -0.353216000 | 3.242554000 |
| C | -1.485832000 | -1.353527000 | 2.475689000 |
| C | -0.236899000 | -0.884217000 | 4.446760000 |
| H | 1.381942000 | -0.985455000 | 3.000265000 |
| H | 0.852696000 | 0.678678000 | 3.364103000 |
| C | -1.101512000 | -1.971167000 | 3.812233000 |
| H | -2.416652000 | -0.783135000 | 2.537386000 |
| H | -1.558329000 | -2.079894000 | 1.668625000 |
| H | -0.858053000 | -0.096455000 | 4.888954000 |
| H | 0.437828000 | -1.262135000 | 5.220344000 |
| H | -1.983399000 | -2.223789000 | 4.407927000 |
| H | -0.517024000 | -2.883473000 | 3.659401000 |
| H | 2.471701000 | -0.179472000 | -2.750745000 |
| H | 2.105748000 | 1.420551000 | -1.902993000 |
| C | 3.326073000 | 2.544498000 | 0.503303000 |
| C | 2.212427000 | 2.045109000 | 1.377543000 |
| H | 2.924158000 | 3.051213000 | -0.382744000 |
| H | 3.930645000 | 1.702853000 | 0.139782000 |
| H | 2.530759000 | 1.487825000 | 2.257575000 |
| C | 0.896743000 | 2.415174000 | 1.291593000 |
| C | 0.233881000 | 3.128775000 | 0.225895000 |
| H | 0.244869000 | 2.075862000 | 2.100011000 |

| | | | |
|---|--------------|-------------|--------------|
| H | -0.738123000 | 3.536287000 | 0.497901000 |
| H | 0.849630000 | 3.853488000 | -0.299252000 |

117

theta3_thf_P2_cis_1,4 E = -2200.685665 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 1.646617000 | 1.351032000 | -0.708390000 |
| P | 2.724220000 | -1.385164000 | -0.023490000 |
| P | -1.099437000 | 2.506622000 | -0.183474000 |
| Si | -6.361807000 | -3.657547000 | 0.167167000 |
| C | -4.677768000 | -3.169382000 | 0.926733000 |
| H | -4.250237000 | -4.058993000 | 1.411127000 |
| H | -4.866290000 | -2.446930000 | 1.735268000 |
| C | -6.090861000 | -4.930653000 | -1.199498000 |
| H | -5.507490000 | -4.525616000 | -2.035459000 |
| H | -7.050840000 | -5.266912000 | -1.609423000 |
| H | -5.567599000 | -5.818741000 | -0.824579000 |
| C | -7.413626000 | -4.394593000 | 1.547336000 |
| H | -6.944892000 | -5.288661000 | 1.975707000 |
| H | -8.401687000 | -4.689691000 | 1.174113000 |
| H | -7.571802000 | -3.678568000 | 2.362876000 |
| C | -7.198249000 | -2.119160000 | -0.541018000 |
| H | -7.330613000 | -1.343343000 | 0.223094000 |
| H | -8.192882000 | -2.365988000 | -0.931534000 |
| H | -6.625648000 | -1.684284000 | -1.369517000 |
| C | 3.308362000 | -2.510245000 | 1.325306000 |
| C | 2.502119000 | -2.679560000 | 2.459099000 |
| H | 1.552428000 | -2.155018000 | 2.526609000 |
| C | 2.907201000 | -3.509098000 | 3.503611000 |
| H | 2.270127000 | -3.635403000 | 4.375347000 |
| C | 4.123368000 | -4.185866000 | 3.424162000 |
| H | 4.438472000 | -4.837615000 | 4.234377000 |
| C | 4.930377000 | -4.030150000 | 2.297593000 |
| H | 5.877438000 | -4.558561000 | 2.228701000 |
| C | 4.527043000 | -3.200430000 | 1.252563000 |
| H | 5.157587000 | -3.098776000 | 0.374038000 |
| C | 3.564410000 | -2.069962000 | -1.524836000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.375340000 | -3.419434000 | -1.860251000 |
| H | 2.786897000 | -4.065984000 | -1.213228000 |
| C | 3.954490000 | -3.948202000 | -3.010782000 |
| H | 3.810411000 | -4.997821000 | -3.253095000 |
| C | 4.718045000 | -3.133245000 | -3.848375000 |
| H | 5.167860000 | -3.545610000 | -4.747329000 |
| C | 4.906103000 | -1.791912000 | -3.523324000 |
| H | 5.507052000 | -1.154193000 | -4.166223000 |
| C | 4.335404000 | -1.260745000 | -2.365523000 |
| H | 4.505078000 | -0.219196000 | -2.109640000 |
| C | 3.588810000 | 0.215992000 | 0.268267000 |
| C | 2.945258000 | 1.397471000 | -0.185007000 |
| C | 3.644476000 | 2.613142000 | -0.024212000 |
| H | 3.183972000 | 3.533402000 | -0.369185000 |
| C | 4.896325000 | 2.657396000 | 0.575342000 |
| H | 5.396059000 | 3.616474000 | 0.687987000 |
| C | 5.507425000 | 1.492184000 | 1.043083000 |
| H | 6.483679000 | 1.527542000 | 1.517217000 |
| C | 4.846097000 | 0.280031000 | 0.881324000 |
| H | 5.313903000 | -0.635945000 | 1.231969000 |
| C | 1.273760000 | 2.321270000 | -1.662519000 |
| C | 2.111214000 | 2.636353000 | -2.751434000 |
| H | 3.084559000 | 2.158099000 | -2.813731000 |
| C | 1.709609000 | 3.525668000 | -3.739075000 |
| H | 2.378736000 | 3.741434000 | -4.568168000 |
| C | 0.448708000 | 4.123727000 | -3.682203000 |
| H | 0.127300000 | 4.811429000 | -4.458908000 |
| C | -0.395707000 | 3.828301000 | -2.617864000 |
| H | -1.379129000 | 4.287090000 | -2.573099000 |
| C | 0.004295000 | 2.953278000 | -1.598977000 |
| C | -2.793134000 | 3.090998000 | -0.638222000 |
| C | -3.125015000 | 4.454371000 | -0.619503000 |
| H | -2.379343000 | 5.192638000 | -0.337207000 |
| C | -4.413611000 | 4.869274000 | -0.948045000 |
| H | -4.658231000 | 5.927975000 | -0.933013000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -5.387296000 | 3.930113000 | -1.289501000 |
| H | -6.392542000 | 4.256015000 | -1.542459000 |
| C | -5.070083000 | 2.573125000 | -1.297410000 |
| H | -5.827358000 | 1.837262000 | -1.554453000 |
| C | -3.780448000 | 2.155512000 | -0.970379000 |
| H | -3.538484000 | 1.097188000 | -0.975782000 |
| C | -0.653637000 | 3.704484000 | 1.160424000 |
| C | 0.415793000 | 4.599298000 | 1.054814000 |
| H | 1.009789000 | 4.625166000 | 0.146314000 |
| C | 0.706159000 | 5.477397000 | 2.100747000 |
| H | 1.536406000 | 6.172049000 | 2.003811000 |
| C | -0.073630000 | 5.477532000 | 3.255282000 |
| H | 0.147117000 | 6.169757000 | 4.063189000 |
| C | -1.148977000 | 4.593286000 | 3.364812000 |
| H | -1.772519000 | 4.600599000 | 4.255317000 |
| C | -1.432533000 | 3.707076000 | 2.328062000 |
| H | -2.284403000 | 3.035140000 | 2.416310000 |
| C | -1.495119000 | -0.073054000 | -2.329346000 |
| C | -0.327787000 | -0.730035000 | -2.787420000 |
| H | 0.415223000 | -0.093259000 | -3.277798000 |
| C | 0.104674000 | -1.995477000 | -2.420374000 |
| C | -0.839202000 | -3.139957000 | -2.106962000 |
| H | -0.627194000 | -3.949121000 | -2.820558000 |
| H | -1.868482000 | -2.823358000 | -2.312865000 |
| Y | 0.023103000 | -0.177579000 | -0.301714000 |
| H | 1.102377000 | -2.282511000 | -2.741514000 |
| O | 0.107292000 | -0.008439000 | 2.175697000 |
| C | -0.794322000 | -0.422699000 | 3.236822000 |
| C | 1.155735000 | 0.853219000 | 2.739490000 |
| C | -0.068889000 | -0.111545000 | 4.536451000 |
| H | -1.724497000 | 0.151216000 | 3.143882000 |
| H | -1.009206000 | -1.486363000 | 3.104948000 |
| C | 0.724799000 | 1.142215000 | 4.168225000 |
| H | 2.094644000 | 0.294488000 | 2.694012000 |
| H | 1.230075000 | 1.743344000 | 2.113257000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.605567000 | -0.932078000 | 4.805669000 |
| H | -0.764762000 | 0.043525000 | 5.365771000 |
| H | 1.585132000 | 1.310798000 | 4.821810000 |
| H | 0.087467000 | 2.031237000 | 4.203159000 |
| H | -1.762388000 | 0.872869000 | -2.791540000 |
| H | -2.349288000 | -0.686545000 | -2.028779000 |
| C | -3.648959000 | -2.584570000 | -0.062213000 |
| C | -2.364554000 | -2.252629000 | 0.639068000 |
| H | -3.470999000 | -3.288651000 | -0.880542000 |
| H | -4.062685000 | -1.671826000 | -0.515381000 |
| H | -2.489520000 | -1.586373000 | 1.495280000 |
| C | -1.138092000 | -2.764890000 | 0.402259000 |
| C | -0.774309000 | -3.741501000 | -0.691683000 |
| H | -0.345064000 | -2.533806000 | 1.124391000 |
| H | 0.235395000 | -4.122325000 | -0.501933000 |
| H | -1.444341000 | -4.611352000 | -0.643988000 |

117

theta3_thf_C2_cis_1,2 E = -2200.653446 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.121150000 | 1.078201000 | 1.258746000 |
| P | -2.809221000 | -1.007925000 | -0.086768000 |
| P | 1.527646000 | 2.189078000 | 0.289398000 |
| Si | 5.297462000 | -4.091853000 | -0.902947000 |
| C | 4.041016000 | -2.961640000 | -1.785741000 |
| H | 3.509503000 | -3.567213000 | -2.534214000 |
| H | 4.606825000 | -2.212865000 | -2.361249000 |
| C | 4.400260000 | -5.561630000 | -0.125365000 |
| H | 3.658665000 | -5.244198000 | 0.617371000 |
| H | 5.107125000 | -6.229785000 | 0.381208000 |
| H | 3.875338000 | -6.153421000 | -0.885203000 |
| C | 6.528495000 | -4.710326000 | -2.191801000 |
| H | 6.023154000 | -5.259551000 | -2.995256000 |
| H | 7.263989000 | -5.388372000 | -1.742377000 |
| H | 7.081184000 | -3.882667000 | -2.652556000 |
| C | 6.212758000 | -3.122315000 | 0.438352000 |
| H | 6.732820000 | -2.252458000 | 0.018297000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 6.970157000 | -3.749389000 | 0.924226000 |
| H | 5.538043000 | -2.761833000 | 1.224295000 |
| C | -3.898595000 | -1.425433000 | -1.517625000 |
| C | -3.419335000 | -1.225457000 | -2.819171000 |
| H | -2.411924000 | -0.846559000 | -2.971934000 |
| C | -4.218669000 | -1.523233000 | -3.922496000 |
| H | -3.833910000 | -1.369899000 | -4.927422000 |
| C | -5.503097000 | -2.031249000 | -3.736337000 |
| H | -6.124864000 | -2.268264000 | -4.595264000 |
| C | -5.983525000 | -2.248533000 | -2.444739000 |
| H | -6.980035000 | -2.655181000 | -2.295130000 |
| C | -5.186431000 | -1.953316000 | -1.340823000 |
| H | -5.562109000 | -2.151334000 | -0.340643000 |
| C | -3.226785000 | -2.332125000 | 1.138560000 |
| C | -3.182555000 | -3.676137000 | 0.736803000 |
| H | -2.940016000 | -3.931986000 | -0.291392000 |
| C | -3.476621000 | -4.690895000 | 1.645398000 |
| H | -3.456947000 | -5.727488000 | 1.319197000 |
| C | -3.799456000 | -4.377320000 | 2.967211000 |
| H | -4.029509000 | -5.169595000 | 3.674266000 |
| C | -3.835853000 | -3.044415000 | 3.373596000 |
| H | -4.097431000 | -2.793808000 | 4.398231000 |
| C | -3.555157000 | -2.023862000 | 2.463830000 |
| H | -3.615132000 | -0.985995000 | 2.779315000 |
| C | -3.448017000 | 0.539822000 | 0.658697000 |
| C | -2.491573000 | 1.374216000 | 1.300542000 |
| C | -2.993739000 | 2.545371000 | 1.916198000 |
| H | -2.305891000 | 3.206719000 | 2.433464000 |
| C | -4.342013000 | 2.874430000 | 1.877864000 |
| H | -4.674847000 | 3.791016000 | 2.359115000 |
| C | -5.264211000 | 2.054921000 | 1.223809000 |
| H | -6.317238000 | 2.316793000 | 1.187081000 |
| C | -4.803249000 | 0.890391000 | 0.622556000 |
| H | -5.506252000 | 0.240075000 | 0.109514000 |
| C | -0.326564000 | 1.589627000 | 2.302590000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.729294000 | 1.483581000 | 3.651842000 |
| H | -1.702191000 | 1.052183000 | 3.870676000 |
| C | 0.083957000 | 1.910907000 | 4.692133000 |
| H | -0.260939000 | 1.804675000 | 5.717625000 |
| C | 1.343073000 | 2.455018000 | 4.428854000 |
| H | 1.986649000 | 2.782725000 | 5.239807000 |
| C | 1.767636000 | 2.565911000 | 3.110075000 |
| H | 2.752307000 | 2.972809000 | 2.901568000 |
| C | 0.951448000 | 2.155023000 | 2.046251000 |
| C | 3.349694000 | 2.462769000 | 0.370491000 |
| C | 3.904968000 | 3.697800000 | 0.741170000 |
| H | 3.257622000 | 4.538512000 | 0.975716000 |
| C | 5.287528000 | 3.855175000 | 0.799261000 |
| H | 5.708578000 | 4.814250000 | 1.088780000 |
| C | 6.129554000 | 2.787432000 | 0.483688000 |
| H | 7.207779000 | 2.914566000 | 0.528143000 |
| C | 5.586120000 | 1.562790000 | 0.101455000 |
| H | 6.237931000 | 0.732814000 | -0.156941000 |
| C | 4.201688000 | 1.403235000 | 0.040770000 |
| H | 3.777334000 | 0.456441000 | -0.279686000 |
| C | 0.927754000 | 3.806712000 | -0.391460000 |
| C | -0.151925000 | 4.488950000 | 0.177947000 |
| H | -0.632720000 | 4.094293000 | 1.066840000 |
| C | -0.600777000 | 5.688493000 | -0.376085000 |
| H | -1.434893000 | 6.212692000 | 0.082912000 |
| C | 0.027713000 | 6.221848000 | -1.500442000 |
| H | -0.314266000 | 7.162750000 | -1.922871000 |
| C | 1.109297000 | 5.549160000 | -2.072029000 |
| H | 1.616179000 | 5.966892000 | -2.938094000 |
| C | 1.553979000 | 4.346211000 | -1.525892000 |
| H | 2.415931000 | 3.847230000 | -1.963402000 |
| C | 1.424911000 | -1.347060000 | 2.077600000 |
| C | 0.327966000 | -2.066077000 | 2.403654000 |
| H | -0.534723000 | -1.536586000 | 2.810939000 |
| C | 0.194914000 | -3.520608000 | 2.296654000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.213102000 | -4.380889000 | 2.440637000 |
| H | 1.057392000 | -5.453902000 | 2.375862000 |
| H | 2.222416000 | -4.045877000 | 2.667617000 |
| Y | -0.029311000 | -0.285805000 | -0.326677000 |
| H | -0.813009000 | -3.904237000 | 2.153824000 |
| O | -0.699215000 | 1.090494000 | -2.166531000 |
| C | 0.098379000 | 1.416724000 | -3.341841000 |
| C | -1.854885000 | 1.998336000 | -2.100791000 |
| C | -0.860567000 | 2.138455000 | -4.269988000 |
| H | 0.922945000 | 2.064067000 | -3.026620000 |
| H | 0.500070000 | 0.485767000 | -3.743897000 |
| C | -1.703484000 | 2.947773000 | -3.282544000 |
| H | -2.751746000 | 1.378386000 | -2.175184000 |
| H | -1.833118000 | 2.497625000 | -1.132026000 |
| H | -1.478778000 | 1.419233000 | -4.819434000 |
| H | -0.333614000 | 2.763038000 | -4.996782000 |
| H | -2.675754000 | 3.239923000 | -3.689064000 |
| H | -1.171105000 | 3.854440000 | -2.979946000 |
| H | 1.496906000 | -0.296304000 | 2.349500000 |
| H | 2.315350000 | -1.824512000 | 1.678550000 |
| C | 3.004850000 | -2.236273000 | -0.901814000 |
| C | 2.055974000 | -1.407886000 | -1.756740000 |
| H | 2.439969000 | -2.976917000 | -0.321490000 |
| H | 3.542337000 | -1.617176000 | -0.171380000 |
| H | 2.571841000 | -0.753779000 | -2.462468000 |
| C | 0.820559000 | -1.901936000 | -2.192834000 |
| C | -0.121479000 | -2.620246000 | -1.441510000 |
| H | 0.440385000 | -1.498554000 | -3.136125000 |
| H | -1.016788000 | -2.988578000 | -1.933193000 |
| H | 0.198661000 | -3.201283000 | -0.571989000 |

117

theta3_thf_TS2_cis_1,2 E = -2200.63101 a.u. Imaginary frequency=220i

| | | | |
|---|--------------|--------------|--------------|
| N | 1.329819000 | -1.303716000 | -0.987158000 |
| P | -1.489684000 | -2.223780000 | -0.160313000 |
| P | 2.829250000 | 1.195084000 | -0.130071000 |

| | | | |
|----|--------------|--------------|--------------|
| Si | -5.844105000 | 4.101372000 | 0.509196000 |
| C | -4.032438000 | 3.828363000 | 1.044454000 |
| H | -4.029319000 | 3.137644000 | 1.899448000 |
| H | -3.642621000 | 4.782629000 | 1.428548000 |
| C | -6.583450000 | 2.456089000 | -0.058329000 |
| H | -6.078501000 | 2.065627000 | -0.950690000 |
| H | -7.643532000 | 2.574100000 | -0.313380000 |
| H | -6.519666000 | 1.693587000 | 0.728029000 |
| C | -6.794960000 | 4.754841000 | 2.001084000 |
| H | -6.769548000 | 4.047241000 | 2.838551000 |
| H | -7.848174000 | 4.930928000 | 1.751188000 |
| H | -6.378881000 | 5.705189000 | 2.356453000 |
| C | -5.915184000 | 5.351661000 | -0.903834000 |
| H | -5.459067000 | 6.307726000 | -0.619308000 |
| H | -6.954658000 | 5.557905000 | -1.186404000 |
| H | -5.401574000 | 4.991221000 | -1.803569000 |
| C | -2.369935000 | -2.943661000 | 1.306931000 |
| C | -1.975442000 | -2.550667000 | 2.593610000 |
| H | -1.180034000 | -1.820968000 | 2.711788000 |
| C | -2.588053000 | -3.091986000 | 3.721572000 |
| H | -2.271641000 | -2.777426000 | 4.712935000 |
| C | -3.610622000 | -4.029814000 | 3.580487000 |
| H | -4.093197000 | -4.447977000 | 4.459559000 |
| C | -4.010327000 | -4.426832000 | 2.306182000 |
| H | -4.803671000 | -5.159899000 | 2.186876000 |
| C | -3.394857000 | -3.890170000 | 1.175161000 |
| H | -3.716645000 | -4.212034000 | 0.189711000 |
| C | -2.596930000 | -2.702466000 | -1.562881000 |
| C | -3.888396000 | -2.154398000 | -1.614996000 |
| H | -4.240569000 | -1.507128000 | -0.814114000 |
| C | -4.736010000 | -2.446961000 | -2.680230000 |
| H | -5.737367000 | -2.025270000 | -2.704352000 |
| C | -4.300211000 | -3.279130000 | -3.713296000 |
| H | -4.960594000 | -3.504592000 | -4.546077000 |
| C | -3.018073000 | -3.822287000 | -3.669602000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.675668000 | -4.476535000 | -4.467010000 |
| C | -2.168198000 | -3.538858000 | -2.598523000 |
| H | -1.174929000 | -3.977092000 | -2.566892000 |
| C | 0.006527000 | -3.279430000 | -0.340218000 |
| C | 1.221299000 | -2.683466000 | -0.771914000 |
| C | 2.338682000 | -3.543127000 | -0.895795000 |
| H | 3.287475000 | -3.125384000 | -1.217665000 |
| C | 2.259586000 | -4.897534000 | -0.607639000 |
| H | 3.149373000 | -5.513832000 | -0.711755000 |
| C | 1.060383000 | -5.468001000 | -0.172858000 |
| H | 0.996819000 | -6.527348000 | 0.056712000 |
| C | -0.052193000 | -4.648360000 | -0.038539000 |
| H | -0.992250000 | -5.072524000 | 0.304885000 |
| C | 2.271696000 | -0.873562000 | -1.941703000 |
| C | 2.412806000 | -1.536734000 | -3.180875000 |
| H | 1.818162000 | -2.427442000 | -3.362537000 |
| C | 3.272605000 | -1.070015000 | -4.165362000 |
| H | 3.345657000 | -1.606409000 | -5.108147000 |
| C | 4.020858000 | 0.090818000 | -3.958842000 |
| H | 4.685981000 | 0.467813000 | -4.730040000 |
| C | 3.899328000 | 0.764198000 | -2.749035000 |
| H | 4.469130000 | 1.674395000 | -2.592584000 |
| C | 3.054715000 | 0.294202000 | -1.733231000 |
| C | 3.493446000 | 2.903675000 | -0.384554000 |
| C | 4.859692000 | 3.148528000 | -0.596593000 |
| H | 5.563807000 | 2.321126000 | -0.619976000 |
| C | 5.326019000 | 4.451259000 | -0.753337000 |
| H | 6.385052000 | 4.627154000 | -0.921614000 |
| C | 4.440406000 | 5.527806000 | -0.683674000 |
| H | 4.808178000 | 6.543282000 | -0.802304000 |
| C | 3.087689000 | 5.298506000 | -0.442466000 |
| H | 2.398135000 | 6.134945000 | -0.363825000 |
| C | 2.619421000 | 3.993125000 | -0.289590000 |
| H | 1.568275000 | 3.820590000 | -0.074974000 |
| C | 4.134107000 | 0.498017000 | 0.989423000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.823117000 | -0.682541000 | 0.694324000 |
| H | 4.610942000 | -1.217298000 | -0.226772000 |
| C | 5.804358000 | -1.161736000 | 1.564127000 |
| H | 6.338156000 | -2.076265000 | 1.319393000 |
| C | 6.113333000 | -0.462509000 | 2.729693000 |
| H | 6.886652000 | -0.830478000 | 3.398408000 |
| C | 5.433768000 | 0.720091000 | 3.027765000 |
| H | 5.678964000 | 1.279028000 | 3.927136000 |
| C | 4.446262000 | 1.194293000 | 2.167074000 |
| H | 3.942710000 | 2.130883000 | 2.397383000 |
| C | -0.632398000 | 3.014982000 | -1.625635000 |
| C | 0.195130000 | 2.033478000 | -2.187582000 |
| H | 1.249257000 | 2.246510000 | -2.338780000 |
| C | -0.355384000 | 0.845572000 | -2.775190000 |
| C | -1.583452000 | 0.330803000 | -2.462980000 |
| H | -1.949253000 | -0.569174000 | -2.940084000 |
| H | -2.321006000 | 0.901708000 | -1.892186000 |
| Y | -0.048609000 | 0.359675000 | -0.166322000 |
| H | 0.303638000 | 0.260987000 | -3.413827000 |
| O | 0.861950000 | -0.471594000 | 2.117118000 |
| C | 0.954558000 | 0.318287000 | 3.327084000 |
| C | 1.627641000 | -1.706464000 | 2.296244000 |
| C | 1.373130000 | -0.651344000 | 4.419986000 |
| H | 1.706586000 | 1.103369000 | 3.178293000 |
| H | -0.017458000 | 0.780586000 | 3.512328000 |
| C | 2.299776000 | -1.598749000 | 3.658457000 |
| H | 0.919809000 | -2.538673000 | 2.247184000 |
| H | 2.331623000 | -1.788402000 | 1.470267000 |
| H | 0.500394000 | -1.186505000 | 4.811818000 |
| H | 1.862883000 | -0.142665000 | 5.255352000 |
| H | 2.399549000 | -2.576961000 | 4.137428000 |
| H | 3.297948000 | -1.161376000 | 3.561551000 |
| H | -0.198592000 | 3.983871000 | -1.407109000 |
| H | -1.668572000 | 3.033060000 | -1.945155000 |
| C | -3.087267000 | 3.299394000 | -0.050872000 |

| | | | |
|---|--------------|-------------|--------------|
| C | -1.670764000 | 3.109532000 | 0.453181000 |
| H | -3.483620000 | 2.356828000 | -0.455045000 |
| H | -3.084202000 | 4.010582000 | -0.886595000 |
| H | -1.133230000 | 4.039272000 | 0.631187000 |
| C | -1.386408000 | 2.106635000 | 1.418555000 |
| C | -2.002076000 | 0.877973000 | 1.576687000 |
| H | -0.533257000 | 2.320289000 | 2.070831000 |
| H | -1.803362000 | 0.264741000 | 2.447273000 |
| H | -2.908984000 | 0.629555000 | 1.027545000 |

117

theta3_thf_P2_cis_1,2 E = -2200.682955 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 2.155067000 | 0.745867000 | -0.598862000 |
| P | 2.083212000 | -2.243210000 | -0.067639000 |
| P | 0.024120000 | 2.813113000 | -0.090958000 |
| Si | -7.593037000 | -2.108641000 | 0.252521000 |
| C | -5.865159000 | -1.312968000 | 0.418931000 |
| H | -5.349447000 | -1.827568000 | 1.243396000 |
| H | -6.007148000 | -0.272383000 | 0.750570000 |
| C | -7.405757000 | -3.921400000 | -0.241266000 |
| H | -6.927609000 | -4.034182000 | -1.221716000 |
| H | -8.385533000 | -4.410610000 | -0.300913000 |
| H | -6.806631000 | -4.479115000 | 0.489113000 |
| C | -8.449841000 | -1.985197000 | 1.929735000 |
| H | -7.889743000 | -2.514955000 | 2.709942000 |
| H | -9.453375000 | -2.425907000 | 1.891646000 |
| H | -8.563413000 | -0.942599000 | 2.250746000 |
| C | -8.596983000 | -1.184033000 | -1.052066000 |
| H | -8.706098000 | -0.122017000 | -0.800273000 |
| H | -9.606344000 | -1.605483000 | -1.132594000 |
| H | -8.140519000 | -1.246649000 | -2.047246000 |
| C | 2.145272000 | -3.510730000 | 1.280741000 |
| C | 1.325010000 | -3.335284000 | 2.403112000 |
| H | 0.673593000 | -2.466816000 | 2.454191000 |
| C | 1.339743000 | -4.258601000 | 3.447309000 |
| H | 0.696434000 | -4.112838000 | 4.311551000 |

| | | | |
|---|-------------|--------------|--------------|
| C | 2.170935000 | -5.375684000 | 3.377344000 |
| H | 2.180371000 | -6.100073000 | 4.187093000 |
| C | 2.983061000 | -5.565605000 | 2.259687000 |
| H | 3.627955000 | -6.438032000 | 2.197182000 |
| C | 2.970528000 | -4.642451000 | 1.215049000 |
| H | 3.595937000 | -4.811253000 | 0.342927000 |
| C | 2.575227000 | -3.223637000 | -1.556199000 |
| C | 1.766204000 | -4.301464000 | -1.945192000 |
| H | 0.900541000 | -4.579192000 | -1.347115000 |
| C | 2.075613000 | -5.037985000 | -3.085349000 |
| H | 1.447077000 | -5.876660000 | -3.372872000 |
| C | 3.189394000 | -4.699802000 | -3.856126000 |
| H | 3.428710000 | -5.273152000 | -4.747482000 |
| C | 3.994651000 | -3.628475000 | -3.475998000 |
| H | 4.867494000 | -3.365518000 | -4.067776000 |
| C | 3.692124000 | -2.892350000 | -2.329133000 |
| H | 4.332347000 | -2.067169000 | -2.031424000 |
| C | 3.509672000 | -1.117676000 | 0.245491000 |
| C | 3.376197000 | 0.243325000 | -0.136069000 |
| C | 4.503334000 | 1.075611000 | 0.031843000 |
| H | 4.432111000 | 2.118112000 | -0.262499000 |
| C | 5.686121000 | 0.594892000 | 0.576977000 |
| H | 6.528478000 | 1.271484000 | 0.698554000 |
| C | 5.795946000 | -0.737510000 | 0.982029000 |
| H | 6.717981000 | -1.112056000 | 1.416471000 |
| C | 4.705145000 | -1.581725000 | 0.810031000 |
| H | 4.781656000 | -2.623250000 | 1.110842000 |
| C | 2.151475000 | 1.749547000 | -1.580397000 |
| C | 3.032134000 | 1.718121000 | -2.682793000 |
| H | 3.787016000 | 0.938275000 | -2.723389000 |
| C | 2.929545000 | 2.640599000 | -3.713638000 |
| H | 3.617929000 | 2.581897000 | -4.552955000 |
| C | 1.936101000 | 3.624349000 | -3.690935000 |
| H | 1.846835000 | 4.338266000 | -4.504412000 |
| C | 1.065634000 | 3.685675000 | -2.609591000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.297652000 | 4.452846000 | -2.586689000 |
| C | 1.173057000 | 2.782160000 | -1.541758000 |
| C | -1.280166000 | 4.056700000 | -0.499047000 |
| C | -0.985999000 | 5.427763000 | -0.558442000 |
| H | 0.026828000 | 5.775711000 | -0.373460000 |
| C | -1.989954000 | 6.350345000 | -0.841694000 |
| H | -1.750457000 | 7.409258000 | -0.888485000 |
| C | -3.299432000 | 5.918306000 | -1.057422000 |
| H | -4.081503000 | 6.640710000 | -1.274567000 |
| C | -3.603832000 | 4.560647000 | -0.983324000 |
| H | -4.624301000 | 4.220806000 | -1.139238000 |
| C | -2.599019000 | 3.634769000 | -0.702462000 |
| H | -2.841508000 | 2.578093000 | -0.637901000 |
| C | 0.958213000 | 3.704202000 | 1.239824000 |
| C | 2.291094000 | 4.100891000 | 1.097348000 |
| H | 2.819436000 | 3.896852000 | 0.171211000 |
| C | 2.936768000 | 4.781998000 | 2.130833000 |
| H | 3.971568000 | 5.090114000 | 2.006595000 |
| C | 2.255393000 | 5.081311000 | 3.308681000 |
| H | 2.756994000 | 5.620739000 | 4.107423000 |
| C | 0.920596000 | 4.698339000 | 3.453407000 |
| H | 0.377543000 | 4.945823000 | 4.361999000 |
| C | 0.277415000 | 4.007780000 | 2.428570000 |
| H | -0.769443000 | 3.732521000 | 2.542825000 |
| C | -2.908108000 | -0.615203000 | -2.104296000 |
| C | -1.737468000 | 0.349168000 | -2.253845000 |
| H | -2.034179000 | 1.379802000 | -2.443789000 |
| C | -0.533389000 | -0.040912000 | -2.870609000 |
| C | 0.117686000 | -1.263242000 | -2.731321000 |
| H | 1.079158000 | -1.416324000 | -3.209781000 |
| H | -0.432425000 | -2.178543000 | -2.509563000 |
| Y | 0.072640000 | -0.109394000 | -0.360139000 |
| H | 0.071447000 | 0.771631000 | -3.281134000 |
| O | 0.197332000 | -0.056613000 | 2.131451000 |
| C | -0.865475000 | -0.040173000 | 3.118622000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.463307000 | 0.319402000 | 2.773926000 |
| C | -0.168241000 | -0.059833000 | 4.469521000 |
| H | -1.458335000 | 0.872379000 | 2.979513000 |
| H | -1.500404000 | -0.912234000 | 2.945432000 |
| C | 1.097519000 | 0.750274000 | 4.186551000 |
| H | 2.108135000 | -0.563900000 | 2.762034000 |
| H | 1.918568000 | 1.110532000 | 2.177294000 |
| H | 0.083634000 | -1.086935000 | 4.756724000 |
| H | -0.791079000 | 0.371209000 | 5.258479000 |
| H | 1.905366000 | 0.542545000 | 4.893673000 |
| H | 0.885076000 | 1.823469000 | 4.214804000 |
| H | -3.641358000 | -0.365279000 | -2.885705000 |
| H | -2.593972000 | -1.640847000 | -2.336237000 |
| C | -5.006526000 | -1.341902000 | -0.849922000 |
| C | -3.647988000 | -0.595229000 | -0.760859000 |
| H | -4.801623000 | -2.380744000 | -1.143526000 |
| H | -5.560716000 | -0.888053000 | -1.682328000 |
| H | -3.878746000 | 0.450915000 | -0.509046000 |
| C | -2.835574000 | -1.160983000 | 0.373327000 |
| C | -1.921147000 | -2.147535000 | 0.299693000 |
| H | -3.082194000 | -0.776156000 | 1.363281000 |
| H | -1.470068000 | -2.573611000 | 1.193565000 |
| H | -1.680602000 | -2.644792000 | -0.638425000 |

117

theta3_thf_C2_trans_1,4 E = -2200.657535 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.201371000 | 1.213045000 | 1.106703000 |
| P | -3.003231000 | -0.974631000 | 0.089966000 |
| P | 1.685239000 | 1.761459000 | 0.325624000 |
| Si | 5.050873000 | -3.740553000 | -1.435328000 |
| C | 3.431084000 | -3.032407000 | -2.144903000 |
| H | 2.725375000 | -3.860618000 | -2.302456000 |
| H | 3.666570000 | -2.659148000 | -3.153557000 |
| C | 4.779910000 | -4.385692000 | 0.321248000 |
| H | 4.484186000 | -3.582455000 | 1.006456000 |
| H | 5.698426000 | -4.835814000 | 0.717277000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.000417000 | -5.157491000 | 0.348642000 |
| C | 5.590582000 | -5.160833000 | -2.554720000 |
| H | 4.841455000 | -5.961355000 | -2.580778000 |
| H | 6.532675000 | -5.602687000 | -2.208078000 |
| H | 5.747538000 | -4.820554000 | -3.585417000 |
| C | 6.383219000 | -2.401247000 | -1.424102000 |
| H | 6.579492000 | -2.029917000 | -2.437493000 |
| H | 7.329818000 | -2.793871000 | -1.032781000 |
| H | 6.102270000 | -1.540786000 | -0.805355000 |
| C | -4.180803000 | -1.514756000 | -1.222872000 |
| C | -3.870363000 | -1.229076000 | -2.559746000 |
| H | -2.945454000 | -0.709693000 | -2.801360000 |
| C | -4.737127000 | -1.606761000 | -3.583275000 |
| H | -4.486188000 | -1.383731000 | -4.617115000 |
| C | -5.919438000 | -2.282511000 | -3.281788000 |
| H | -6.592364000 | -2.584393000 | -4.079616000 |
| C | -6.232407000 | -2.576427000 | -1.955260000 |
| H | -7.151239000 | -3.105176000 | -1.716509000 |
| C | -5.368991000 | -2.196353000 | -0.928499000 |
| H | -5.617503000 | -2.437495000 | 0.101203000 |
| C | -3.360561000 | -2.108318000 | 1.503646000 |
| C | -3.097630000 | -3.478468000 | 1.349896000 |
| H | -2.729383000 | -3.860536000 | 0.400675000 |
| C | -3.324193000 | -4.358514000 | 2.404948000 |
| H | -3.128523000 | -5.419535000 | 2.273844000 |
| C | -3.802835000 | -3.879304000 | 3.625881000 |
| H | -3.977160000 | -4.566705000 | 4.449087000 |
| C | -4.061708000 | -2.519359000 | 3.784277000 |
| H | -4.441632000 | -2.143102000 | 4.730384000 |
| C | -3.843813000 | -1.633996000 | 2.727561000 |
| H | -4.060270000 | -0.576820000 | 2.851876000 |
| C | -3.560967000 | 0.688086000 | 0.619061000 |
| C | -2.558181000 | 1.577306000 | 1.089346000 |
| C | -2.987034000 | 2.873671000 | 1.457863000 |
| H | -2.249970000 | 3.587620000 | 1.813454000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.318194000 | 3.257439000 | 1.369848000 |
| H | -4.597291000 | 4.268285000 | 1.657613000 |
| C | -5.292775000 | 2.369633000 | 0.905618000 |
| H | -6.333335000 | 2.671527000 | 0.834188000 |
| C | -4.900772000 | 1.090544000 | 0.530891000 |
| H | -5.641212000 | 0.387842000 | 0.157108000 |
| C | -0.429125000 | 1.733844000 | 2.156270000 |
| C | -0.952466000 | 1.878554000 | 3.462173000 |
| H | -1.987381000 | 1.603232000 | 3.641804000 |
| C | -0.181015000 | 2.355845000 | 4.512130000 |
| H | -0.626317000 | 2.443316000 | 5.500202000 |
| C | 1.156316000 | 2.709007000 | 4.313685000 |
| H | 1.760221000 | 3.087472000 | 5.132960000 |
| C | 1.705060000 | 2.557617000 | 3.045975000 |
| H | 2.747710000 | 2.813121000 | 2.878221000 |
| C | 0.938252000 | 2.075389000 | 1.975294000 |
| C | 3.502237000 | 1.701508000 | 0.654454000 |
| C | 4.337133000 | 2.812562000 | 0.477282000 |
| H | 3.932076000 | 3.749471000 | 0.107372000 |
| C | 5.695943000 | 2.725973000 | 0.780552000 |
| H | 6.333076000 | 3.594597000 | 0.637571000 |
| C | 6.232833000 | 1.537422000 | 1.271396000 |
| H | 7.291279000 | 1.473683000 | 1.508316000 |
| C | 5.405538000 | 0.429714000 | 1.457971000 |
| H | 5.815291000 | -0.500524000 | 1.842021000 |
| C | 4.050271000 | 0.508336000 | 1.144577000 |
| H | 3.419424000 | -0.363272000 | 1.294623000 |
| C | 1.471911000 | 3.324211000 | -0.641038000 |
| C | 0.733180000 | 4.404443000 | -0.147754000 |
| H | 0.287836000 | 4.345858000 | 0.841328000 |
| C | 0.588404000 | 5.563736000 | -0.911940000 |
| H | 0.019189000 | 6.400694000 | -0.516031000 |
| C | 1.187470000 | 5.657665000 | -2.167505000 |
| H | 1.086427000 | 6.567299000 | -2.753312000 |
| C | 1.929591000 | 4.583893000 | -2.664575000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.411503000 | 4.656736000 | -3.636208000 |
| C | 2.063241000 | 3.419439000 | -1.910674000 |
| H | 2.658436000 | 2.593918000 | -2.296690000 |
| C | 3.420008000 | -2.315161000 | 3.641485000 |
| C | 2.307596000 | -2.545989000 | 2.926267000 |
| H | 2.149746000 | -3.523032000 | 2.470504000 |
| C | 1.251246000 | -1.561437000 | 2.768580000 |
| C | 0.062096000 | -1.804295000 | 2.174739000 |
| H | -0.739410000 | -1.070772000 | 2.243054000 |
| H | -0.195921000 | -2.792447000 | 1.799522000 |
| Y | -0.249650000 | -0.308305000 | -0.465863000 |
| H | 1.425821000 | -0.580130000 | 3.211198000 |
| O | -0.976705000 | 1.078726000 | -2.271470000 |
| C | -0.393873000 | 1.179012000 | -3.607126000 |
| C | -1.921416000 | 2.193146000 | -2.076842000 |
| C | -1.342814000 | 2.072566000 | -4.384223000 |
| H | 0.598285000 | 1.628321000 | -3.505971000 |
| H | -0.300556000 | 0.170715000 | -4.010154000 |
| C | -1.786182000 | 3.068184000 | -3.312904000 |
| H | -2.917217000 | 1.752810000 | -1.980193000 |
| H | -1.652288000 | 2.694856000 | -1.148052000 |
| H | -2.195632000 | 1.495591000 | -4.760041000 |
| H | -0.848394000 | 2.546777000 | -5.236792000 |
| H | -2.728192000 | 3.568452000 | -3.554523000 |
| H | -1.019237000 | 3.834090000 | -3.159357000 |
| H | 4.174992000 | -3.082982000 | 3.781870000 |
| H | 3.597188000 | -1.356057000 | 4.123573000 |
| C | 2.712245000 | -1.906824000 | -1.366630000 |
| C | 1.569232000 | -1.340141000 | -2.192757000 |
| H | 2.364362000 | -2.303479000 | -0.400468000 |
| H | 3.422449000 | -1.106985000 | -1.127415000 |
| H | 1.902099000 | -0.738978000 | -3.040161000 |
| C | 0.348012000 | -1.997815000 | -2.357232000 |
| C | -0.358267000 | -2.723709000 | -1.384117000 |
| H | -0.235977000 | -1.729499000 | -3.242039000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.296923000 | -3.193390000 | -1.662404000 |
| H | 0.188646000 | -3.230850000 | -0.585972000 |

117

theta3_thf_TS2_trans_1,4 E = -2200.626351 a.u. Imaginary frequency=249i

| | | | |
|----|--------------|--------------|--------------|
| N | -1.389220000 | -1.501963000 | -0.842024000 |
| P | -2.904067000 | 1.028960000 | -0.060940000 |
| P | 1.492295000 | -2.189036000 | -0.259538000 |
| Si | 5.456917000 | 4.272210000 | 0.286223000 |
| C | 3.971710000 | 3.356611000 | 1.054014000 |
| H | 3.354323000 | 4.092305000 | 1.589962000 |
| H | 4.358105000 | 2.676556000 | 1.828483000 |
| C | 4.844848000 | 5.563310000 | -0.951801000 |
| H | 4.328889000 | 5.105128000 | -1.804619000 |
| H | 5.682576000 | 6.143832000 | -1.356842000 |
| H | 4.152948000 | 6.273401000 | -0.482286000 |
| C | 6.409318000 | 5.121999000 | 1.675504000 |
| H | 5.781947000 | 5.846341000 | 2.208777000 |
| H | 7.277406000 | 5.665402000 | 1.283213000 |
| H | 6.779688000 | 4.398543000 | 2.411809000 |
| C | 6.583764000 | 3.037612000 | -0.598756000 |
| H | 6.899495000 | 2.229446000 | 0.072415000 |
| H | 7.490989000 | 3.531458000 | -0.967248000 |
| H | 6.088446000 | 2.582833000 | -1.465509000 |
| C | -3.733502000 | 1.975319000 | 1.289077000 |
| C | -3.055038000 | 2.152692000 | 2.502450000 |
| H | -2.053291000 | 1.748740000 | 2.626137000 |
| C | -3.653780000 | 2.842370000 | 3.555445000 |
| H | -3.115405000 | 2.977310000 | 4.489870000 |
| C | -4.935738000 | 3.369328000 | 3.404602000 |
| H | -5.400839000 | 3.913047000 | 4.222198000 |
| C | -5.616785000 | 3.202482000 | 2.199193000 |
| H | -6.615327000 | 3.612959000 | 2.075750000 |
| C | -5.021611000 | 2.510885000 | 1.145446000 |
| H | -5.558678000 | 2.397437000 | 0.207957000 |
| C | -3.651695000 | 1.708067000 | -1.610188000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.693630000 | 3.096042000 | -1.814682000 |
| H | -3.368913000 | 3.773463000 | -1.028337000 |
| C | -4.183390000 | 3.616093000 | -3.010680000 |
| H | -4.225939000 | 4.692752000 | -3.152685000 |
| C | -4.623455000 | 2.758449000 | -4.019930000 |
| H | -5.004169000 | 3.165497000 | -4.952516000 |
| C | -4.582388000 | 1.379407000 | -3.823381000 |
| H | -4.935044000 | 0.707051000 | -4.600889000 |
| C | -4.101438000 | 0.853651000 | -2.623733000 |
| H | -4.092465000 | -0.221402000 | -2.468829000 |
| C | -3.539232000 | -0.688957000 | 0.061123000 |
| C | -2.688899000 | -1.745093000 | -0.366566000 |
| C | -3.198725000 | -3.057222000 | -0.221543000 |
| H | -2.582836000 | -3.896854000 | -0.526757000 |
| C | -4.460855000 | -3.303667000 | 0.300917000 |
| H | -4.801382000 | -4.332032000 | 0.395291000 |
| C | -5.284156000 | -2.253987000 | 0.713052000 |
| H | -6.271656000 | -2.444794000 | 1.121991000 |
| C | -4.808413000 | -0.954749000 | 0.591869000 |
| H | -5.429194000 | -0.125625000 | 0.920002000 |
| C | -0.864772000 | -2.481424000 | -1.716930000 |
| C | -1.622583000 | -2.970778000 | -2.799919000 |
| H | -2.640484000 | -2.613364000 | -2.927515000 |
| C | -1.097616000 | -3.888706000 | -3.700909000 |
| H | -1.712212000 | -4.236045000 | -4.527602000 |
| C | 0.212201000 | -4.349979000 | -3.559614000 |
| H | 0.628974000 | -5.062514000 | -4.265225000 |
| C | 0.985595000 | -3.870301000 | -2.508435000 |
| H | 2.014252000 | -4.203588000 | -2.409643000 |
| C | 0.465131000 | -2.952817000 | -1.586782000 |
| C | 3.250902000 | -2.377305000 | -0.792251000 |
| C | 3.909609000 | -3.615803000 | -0.753063000 |
| H | 3.389974000 | -4.498652000 | -0.390438000 |
| C | 5.237622000 | -3.718422000 | -1.160984000 |
| H | 5.737233000 | -4.682918000 | -1.129148000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.925873000 | -2.587840000 | -1.602768000 |
| H | 6.962810000 | -2.670595000 | -1.916605000 |
| C | 5.285200000 | -1.350571000 | -1.628801000 |
| H | 5.822410000 | -0.464359000 | -1.955453000 |
| C | 3.955362000 | -1.246088000 | -1.221516000 |
| H | 3.465152000 | -0.276353000 | -1.224211000 |
| C | 1.410377000 | -3.367734000 | 1.168753000 |
| C | 0.443576000 | -4.375234000 | 1.251840000 |
| H | -0.271365000 | -4.508486000 | 0.445057000 |
| C | 0.411835000 | -5.231449000 | 2.354507000 |
| H | -0.337736000 | -6.017004000 | 2.402581000 |
| C | 1.347437000 | -5.094292000 | 3.378874000 |
| H | 1.328889000 | -5.770603000 | 4.229151000 |
| C | 2.317793000 | -4.093175000 | 3.300696000 |
| H | 3.060651000 | -3.990351000 | 4.087512000 |
| C | 2.346200000 | -3.231974000 | 2.205993000 |
| H | 3.124858000 | -2.474726000 | 2.141323000 |
| C | 0.945012000 | -0.046231000 | -2.871360000 |
| C | 1.018482000 | 1.278704000 | -2.549113000 |
| H | 1.993536000 | 1.744502000 | -2.408331000 |
| C | -0.138867000 | 2.090861000 | -2.289085000 |
| C | -0.088975000 | 3.396616000 | -1.860318000 |
| H | -0.993288000 | 3.990028000 | -1.802342000 |
| H | 0.847034000 | 3.941209000 | -1.893465000 |
| Y | -0.055572000 | 0.323537000 | -0.213812000 |
| H | -1.118572000 | 1.654593000 | -2.506204000 |
| O | -0.281970000 | -0.326854000 | 2.171169000 |
| C | 0.636075000 | -0.088878000 | 3.278886000 |
| C | -1.308166000 | -1.284752000 | 2.603147000 |
| C | -0.101736000 | -0.558338000 | 4.519578000 |
| H | 1.541588000 | -0.679457000 | 3.104201000 |
| H | 0.890966000 | 0.972451000 | 3.289587000 |
| C | -0.882247000 | -1.757759000 | 3.983932000 |
| H | -2.263151000 | -0.752176000 | 2.625027000 |
| H | -1.353408000 | -2.080917000 | 1.861168000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.780676000 | 0.221369000 | 4.884086000 |
| H | 0.587369000 | -0.816509000 | 5.328637000 |
| H | -1.744846000 | -2.022103000 | 4.602208000 |
| H | -0.232291000 | -2.634795000 | 3.905350000 |
| H | 1.835653000 | -0.630221000 | -3.074407000 |
| H | -0.006219000 | -0.510378000 | -3.125641000 |
| C | 3.077755000 | 2.557360000 | 0.082685000 |
| C | 1.906386000 | 1.896132000 | 0.776447000 |
| H | 2.715262000 | 3.227371000 | -0.707857000 |
| H | 3.693591000 | 1.800783000 | -0.421107000 |
| H | 2.202917000 | 1.127505000 | 1.496578000 |
| C | 0.729390000 | 2.601972000 | 1.089292000 |
| C | 0.240534000 | 3.793991000 | 0.565997000 |
| H | 0.029833000 | 2.107364000 | 1.778284000 |
| H | -0.731506000 | 4.154935000 | 0.887739000 |
| H | 0.918714000 | 4.543480000 | 0.171635000 |

117

theta3_thf_P2_trans_1,4 E = -2200.683403 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 2.022624000 | 1.046643000 | -0.650057000 |
| P | 2.381633000 | -1.874901000 | -0.039528000 |
| P | -0.453241000 | 2.758201000 | -0.238233000 |
| Si | -7.039752000 | -2.685919000 | 0.099420000 |
| C | -5.356660000 | -2.337355000 | 0.931929000 |
| H | -5.107687000 | -3.189110000 | 1.581038000 |
| H | -5.483630000 | -1.474973000 | 1.604158000 |
| C | -6.872481000 | -4.156933000 | -1.072269000 |
| H | -6.174235000 | -3.953491000 | -1.893319000 |
| H | -7.840307000 | -4.403655000 | -1.525270000 |
| H | -6.520258000 | -5.053242000 | -0.547235000 |
| C | -8.286786000 | -3.073988000 | 1.459073000 |
| H | -7.992306000 | -3.961030000 | 2.032580000 |
| H | -9.279631000 | -3.270838000 | 1.037070000 |
| H | -8.389002000 | -2.240449000 | 2.164370000 |
| C | -7.585474000 | -1.155838000 | -0.865502000 |
| H | -7.667971000 | -0.276833000 | -0.214415000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -8.569492000 | -1.317239000 | -1.322075000 |
| H | -6.890239000 | -0.909528000 | -1.677588000 |
| C | 2.653770000 | -3.193557000 | 1.223946000 |
| C | 1.866255000 | -3.181796000 | 2.383832000 |
| H | 1.110741000 | -2.410282000 | 2.515938000 |
| C | 2.046430000 | -4.147517000 | 3.372348000 |
| H | 1.428868000 | -4.130239000 | 4.266668000 |
| C | 3.011101000 | -5.141136000 | 3.208287000 |
| H | 3.148267000 | -5.898609000 | 3.975064000 |
| C | 3.795552000 | -5.163419000 | 2.055674000 |
| H | 4.547676000 | -5.936525000 | 1.923481000 |
| C | 3.620249000 | -4.196335000 | 1.066811000 |
| H | 4.231625000 | -4.226731000 | 0.169472000 |
| C | 3.008266000 | -2.620062000 | -1.612321000 |
| C | 2.440821000 | -3.816605000 | -2.077344000 |
| H | 1.683482000 | -4.327612000 | -1.487409000 |
| C | 2.858031000 | -4.371588000 | -3.284337000 |
| H | 2.419987000 | -5.304720000 | -3.628540000 |
| C | 3.835370000 | -3.731775000 | -4.048239000 |
| H | 4.157966000 | -4.163801000 | -4.991500000 |
| C | 4.399517000 | -2.541557000 | -3.594091000 |
| H | 5.167241000 | -2.043623000 | -4.180309000 |
| C | 3.991781000 | -1.987202000 | -2.380309000 |
| H | 4.450382000 | -1.069428000 | -2.024628000 |
| C | 3.591650000 | -0.551470000 | 0.355884000 |
| C | 3.260556000 | 0.767508000 | -0.053429000 |
| C | 4.206393000 | 1.777377000 | 0.230184000 |
| H | 3.993626000 | 2.798049000 | -0.071555000 |
| C | 5.397625000 | 1.496324000 | 0.887453000 |
| H | 6.092706000 | 2.307447000 | 1.090660000 |
| C | 5.703837000 | 0.196544000 | 1.295064000 |
| H | 6.634154000 | -0.021490000 | 1.810741000 |
| C | 4.792956000 | -0.818096000 | 1.022525000 |
| H | 5.014533000 | -1.837052000 | 1.328937000 |
| C | 1.959469000 | 2.150878000 | -1.527769000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.939649000 | 2.347278000 | -2.521174000 |
| H | 3.777263000 | 1.657330000 | -2.568621000 |
| C | 2.844918000 | 3.382630000 | -3.441184000 |
| H | 3.616147000 | 3.495896000 | -4.198847000 |
| C | 1.757714000 | 4.258456000 | -3.411089000 |
| H | 1.674030000 | 5.062807000 | -4.135956000 |
| C | 0.774533000 | 4.083080000 | -2.444453000 |
| H | -0.081722000 | 4.750520000 | -2.428647000 |
| C | 0.867423000 | 3.056589000 | -1.495684000 |
| C | -1.973801000 | 3.628280000 | -0.825182000 |
| C | -2.077036000 | 5.027598000 | -0.801776000 |
| H | -1.249719000 | 5.628846000 | -0.434345000 |
| C | -3.243665000 | 5.654876000 | -1.233227000 |
| H | -3.309555000 | 6.739390000 | -1.215355000 |
| C | -4.324719000 | 4.894970000 | -1.680852000 |
| H | -5.234420000 | 5.386684000 | -2.014402000 |
| C | -4.238838000 | 3.503981000 | -1.690121000 |
| H | -5.082148000 | 2.907371000 | -2.027702000 |
| C | -3.070642000 | 2.874478000 | -1.261661000 |
| H | -3.011793000 | 1.789317000 | -1.268019000 |
| C | 0.025801000 | 3.799883000 | 1.220948000 |
| C | 1.300657000 | 4.359898000 | 1.353186000 |
| H | 2.033854000 | 4.226266000 | 0.563460000 |
| C | 1.626315000 | 5.112512000 | 2.482990000 |
| H | 2.617763000 | 5.549245000 | 2.569861000 |
| C | 0.680632000 | 5.320725000 | 3.485244000 |
| H | 0.931854000 | 5.918297000 | 4.357309000 |
| C | -0.596536000 | 4.770367000 | 3.357510000 |
| H | -1.344525000 | 4.943275000 | 4.127133000 |
| C | -0.919729000 | 4.008192000 | 2.236861000 |
| H | -1.924840000 | 3.603400000 | 2.136148000 |
| C | -0.768158000 | 0.523339000 | -2.654235000 |
| C | -1.335484000 | -0.747157000 | -2.469259000 |
| H | -2.423749000 | -0.787403000 | -2.357519000 |
| C | -0.637096000 | -1.901561000 | -2.128635000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.365279000 | -3.184575000 | -1.803924000 |
| H | -0.933549000 | -4.022703000 | -2.365905000 |
| H | -2.401094000 | -3.093808000 | -2.154309000 |
| Y | 0.051540000 | -0.088521000 | -0.335679000 |
| H | 0.403165000 | -1.984604000 | -2.454404000 |
| O | 0.101132000 | 0.102133000 | 2.134722000 |
| C | -0.961739000 | 0.092869000 | 3.124890000 |
| C | 1.318274000 | 0.665171000 | 2.737255000 |
| C | -0.261262000 | 0.217971000 | 4.467238000 |
| H | -1.624656000 | 0.944706000 | 2.931376000 |
| H | -1.520221000 | -0.838716000 | 3.011196000 |
| C | 0.915278000 | 1.133766000 | 4.127837000 |
| H | 2.062206000 | -0.135603000 | 2.761659000 |
| H | 1.671686000 | 1.469423000 | 2.091201000 |
| H | 0.090510000 | -0.762527000 | 4.808101000 |
| H | -0.921118000 | 0.629500000 | 5.236188000 |
| H | 1.743078000 | 1.046437000 | 4.837057000 |
| H | 0.594226000 | 2.179588000 | 4.101635000 |
| H | -1.389612000 | 1.353260000 | -2.972911000 |
| H | 0.269737000 | 0.584708000 | -2.998920000 |
| C | -4.183994000 | -2.074560000 | -0.032627000 |
| C | -2.914028000 | -1.781550000 | 0.711817000 |
| H | -4.046173000 | -2.932408000 | -0.698647000 |
| H | -4.431726000 | -1.216052000 | -0.675505000 |
| H | -3.011929000 | -0.993703000 | 1.462468000 |
| C | -1.735480000 | -2.428899000 | 0.619635000 |
| C | -1.384158000 | -3.569871000 | -0.306229000 |
| H | -0.959269000 | -2.155023000 | 1.343417000 |
| H | -0.397941000 | -3.950199000 | -0.015963000 |
| H | -2.085754000 | -4.403223000 | -0.158920000 |

117

theta3_thf_C2_trans_1,2 E = -2200.650324 a.u.

| | | | |
|---|--------------|--------------|--------------|
| N | 1.160915000 | -1.201328000 | 1.025690000 |
| P | 2.791532000 | 1.000624000 | -0.170698000 |
| P | -1.651549000 | -2.052597000 | 0.258224000 |

| | | | |
|----|--------------|-------------|--------------|
| Si | -5.050793000 | 4.535713000 | -0.797759000 |
| C | -4.001400000 | 3.248153000 | -1.733530000 |
| H | -3.480512000 | 3.766679000 | -2.551562000 |
| H | -4.681839000 | 2.533821000 | -2.221163000 |
| C | -3.915747000 | 5.846973000 | -0.046533000 |
| H | -3.243873000 | 5.425991000 | 0.711796000 |
| H | -4.499286000 | 6.636984000 | 0.441565000 |
| H | -3.295849000 | 6.324730000 | -0.815029000 |
| C | -6.231177000 | 5.338578000 | -2.031318000 |
| H | -5.688682000 | 5.829066000 | -2.848495000 |
| H | -6.852536000 | 6.100770000 | -1.545665000 |
| H | -6.907630000 | 4.600318000 | -2.478667000 |
| C | -6.040882000 | 3.693684000 | 0.575558000 |
| H | -6.715224000 | 2.927637000 | 0.172782000 |
| H | -6.661052000 | 4.422771000 | 1.111072000 |
| H | -5.391052000 | 3.214260000 | 1.317955000 |
| C | 3.860913000 | 1.561847000 | -1.565772000 |
| C | 3.445389000 | 1.311098000 | -2.880651000 |
| H | 2.493702000 | 0.816837000 | -3.062113000 |
| C | 4.235541000 | 1.705254000 | -3.959151000 |
| H | 3.902462000 | 1.509775000 | -4.975146000 |
| C | 5.443989000 | 2.363744000 | -3.734400000 |
| H | 6.057022000 | 2.678015000 | -4.574598000 |
| C | 5.858577000 | 2.628599000 | -2.429542000 |
| H | 6.795871000 | 3.148442000 | -2.250405000 |
| C | 5.072130000 | 2.232558000 | -1.348811000 |
| H | 5.398033000 | 2.455088000 | -0.336431000 |
| C | 3.193603000 | 2.203127000 | 1.175461000 |
| C | 2.775690000 | 3.534824000 | 1.025264000 |
| H | 2.237617000 | 3.839781000 | 0.131005000 |
| C | 3.070436000 | 4.478968000 | 2.006317000 |
| H | 2.753571000 | 5.510405000 | 1.875503000 |
| C | 3.779931000 | 4.102126000 | 3.148834000 |
| H | 4.015519000 | 4.840378000 | 3.910732000 |
| C | 4.194684000 | 2.780413000 | 3.303114000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.756778000 | 2.484847000 | 4.185229000 |
| C | 3.902746000 | 1.831282000 | 2.322348000 |
| H | 4.237423000 | 0.805148000 | 2.444340000 |
| C | 3.461292000 | -0.610454000 | 0.380366000 |
| C | 2.528591000 | -1.512723000 | 0.958186000 |
| C | 3.040245000 | -2.762209000 | 1.378147000 |
| H | 2.366068000 | -3.483058000 | 1.830226000 |
| C | 4.380231000 | -3.094347000 | 1.225598000 |
| H | 4.722731000 | -4.072039000 | 1.556226000 |
| C | 5.281080000 | -2.199463000 | 0.644072000 |
| H | 6.326944000 | -2.462812000 | 0.518594000 |
| C | 4.807992000 | -0.961376000 | 0.225269000 |
| H | 5.490431000 | -0.252569000 | -0.236740000 |
| C | 0.437433000 | -1.741958000 | 2.099912000 |
| C | 0.991568000 | -1.826089000 | 3.398118000 |
| H | 2.020444000 | -1.512095000 | 3.544707000 |
| C | 0.250833000 | -2.274890000 | 4.482154000 |
| H | 0.718382000 | -2.321633000 | 5.463023000 |
| C | -1.087732000 | -2.645212000 | 4.326562000 |
| H | -1.674550000 | -2.984839000 | 5.174813000 |
| C | -1.657072000 | -2.578651000 | 3.060246000 |
| H | -2.696155000 | -2.864046000 | 2.928767000 |
| C | -0.914978000 | -2.154508000 | 1.948724000 |
| C | -3.476768000 | -2.178587000 | 0.490666000 |
| C | -4.100356000 | -3.378663000 | 0.867644000 |
| H | -3.508899000 | -4.278389000 | 1.014939000 |
| C | -5.481313000 | -3.425936000 | 1.041704000 |
| H | -5.955204000 | -4.359043000 | 1.334344000 |
| C | -6.254809000 | -2.281953000 | 0.837206000 |
| H | -7.332183000 | -2.323425000 | 0.972139000 |
| C | -5.645333000 | -1.091047000 | 0.447988000 |
| H | -6.244398000 | -0.201459000 | 0.274159000 |
| C | -4.262627000 | -1.042312000 | 0.270296000 |
| H | -3.791064000 | -0.122544000 | -0.063063000 |
| C | -1.256912000 | -3.680521000 | -0.539455000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.220556000 | -4.500896000 | -0.083225000 |
| H | 0.352458000 | -4.211483000 | 0.791992000 |
| C | 0.060598000 | -5.705956000 | -0.729355000 |
| H | 0.861710000 | -6.339730000 | -0.358100000 |
| C | -0.692372000 | -6.105146000 | -1.832794000 |
| H | -0.479606000 | -7.049565000 | -2.326251000 |
| C | -1.731300000 | -5.293214000 | -2.291381000 |
| H | -2.334433000 | -5.605154000 | -3.140131000 |
| C | -2.009390000 | -4.086260000 | -1.652727000 |
| H | -2.840233000 | -3.476627000 | -2.001672000 |
| C | -1.208250000 | 1.635530000 | 1.806457000 |
| C | -0.637680000 | 1.262785000 | 2.976287000 |
| H | -0.961073000 | 0.333543000 | 3.444307000 |
| C | 0.356615000 | 2.033068000 | 3.695309000 |
| C | 0.789994000 | 1.673639000 | 4.913506000 |
| H | 1.509672000 | 2.274962000 | 5.460353000 |
| H | 0.429309000 | 0.769981000 | 5.398849000 |
| Y | 0.025645000 | 0.296507000 | -0.417134000 |
| H | 0.730264000 | 2.942170000 | 3.227173000 |
| O | 0.572232000 | -1.068736000 | -2.325948000 |
| C | -0.298535000 | -1.355570000 | -3.461091000 |
| C | 1.688814000 | -2.026595000 | -2.321857000 |
| C | 0.549975000 | -2.181500000 | -4.410476000 |
| H | -1.160857000 | -1.918887000 | -3.091844000 |
| H | -0.634607000 | -0.406326000 | -3.879260000 |
| C | 1.390013000 | -3.012904000 | -3.440587000 |
| H | 2.603627000 | -1.455072000 | -2.502072000 |
| H | 1.731228000 | -2.482950000 | -1.333343000 |
| H | 1.184407000 | -1.531985000 | -5.024706000 |
| H | -0.064444000 | -2.791018000 | -5.078992000 |
| H | 2.308566000 | -3.399852000 | -3.890757000 |
| H | 0.809487000 | -3.858956000 | -3.060019000 |
| H | -2.070254000 | 1.090795000 | 1.421649000 |
| H | -0.994829000 | 2.608576000 | 1.366510000 |
| C | -2.964962000 | 2.475881000 | -0.892076000 |

| | | | |
|---|--------------|-------------|--------------|
| C | -2.131235000 | 1.556754000 | -1.770404000 |
| H | -2.315183000 | 3.196708000 | -0.382020000 |
| H | -3.495690000 | 1.932033000 | -0.099446000 |
| H | -2.723895000 | 0.913470000 | -2.423186000 |
| C | -0.879144000 | 1.926073000 | -2.262556000 |
| C | 0.154044000 | 2.599769000 | -1.584970000 |
| H | -0.572249000 | 1.456971000 | -3.200676000 |
| H | 1.038454000 | 2.893273000 | -2.143139000 |
| H | -0.092426000 | 3.261610000 | -0.750278000 |

117

theta3_thf_TS2_trans_1,2 E = -2200.624523 a.u. Imaginary frequency=294i

| | | | |
|----|--------------|--------------|--------------|
| N | -2.129692000 | 0.756274000 | -0.697989000 |
| P | 0.004012000 | 2.832979000 | -0.097630000 |
| P | -2.050268000 | -2.211730000 | -0.120012000 |
| Si | 7.545232000 | -1.892208000 | 0.316709000 |
| C | 5.748328000 | -2.264881000 | 0.833944000 |
| H | 5.479926000 | -1.592293000 | 1.661331000 |
| H | 5.715518000 | -3.281313000 | 1.254003000 |
| C | 7.665211000 | -0.113381000 | -0.312894000 |
| H | 7.065679000 | 0.043346000 | -1.218140000 |
| H | 8.701955000 | 0.142659000 | -0.562852000 |
| H | 7.323906000 | 0.604026000 | 0.443688000 |
| C | 8.648767000 | -2.107800000 | 1.832351000 |
| H | 8.360219000 | -1.425821000 | 2.641368000 |
| H | 9.698453000 | -1.903536000 | 1.588756000 |
| H | 8.596262000 | -3.130230000 | 2.225614000 |
| C | 8.085077000 | -3.085775000 | -1.044561000 |
| H | 8.015140000 | -4.129587000 | -0.714954000 |
| H | 9.127995000 | -2.902850000 | -1.330666000 |
| H | 7.477191000 | -2.981294000 | -1.951574000 |
| C | 0.733223000 | 3.822341000 | 1.285281000 |
| C | 1.022178000 | 3.183711000 | 2.498484000 |
| H | 0.825342000 | 2.120515000 | 2.605836000 |
| C | 1.563564000 | 3.899056000 | 3.565222000 |
| H | 1.789511000 | 3.391544000 | 4.499570000 |

| | | | |
|---|--------------|--------------|---------------|
| C | 1.828233000 | 5.261127000 | 3.429317000 |
| H | 2.255873000 | 5.818602000 | 4.258094000 |
| C | 1.552270000 | 5.903566000 | 2.222904000 |
| H | 1.762546000 | 6.963646000 | 2.109262000 |
| C | 1.010893000 | 5.190347000 | 1.154564000 |
| H | 0.815837000 | 5.698534000 | 0.214430000 |
| C | 0.549031000 | 3.775066000 | -1.591092000 |
| C | 1.923823000 | 3.836906000 | -1.867035000 |
| H | 2.638969000 | 3.380962000 | -1.185280000 |
| C | 2.382850000 | 4.494793000 | -3.005014000 |
| H | 3.449755000 | 4.544677000 | -3.205932000 |
| C | 1.475145000 | 5.089172000 | -3.884173000 |
| H | 1.833878000 | 5.600072000 | -4.773431000 |
| C | 0.109375000 | 5.028824000 | -3.615307000 |
| H | -0.600807000 | 5.495615000 | -4.292704000 |
| C | -0.355627000 | 4.375130000 | -2.472530000 |
| H | -1.421332000 | 4.339164000 | -2.265967000 |
| C | -1.814976000 | 3.086948000 | 0.012491000 |
| C | -2.658595000 | 2.008883000 | -0.364515000 |
| C | -4.051693000 | 2.234928000 | -0.3111545000 |
| H | -4.723890000 | 1.430379000 | -0.594350000 |
| C | -4.577543000 | 3.450647000 | 0.103269000 |
| H | -5.656781000 | 3.578537000 | 0.136276000 |
| C | -3.737770000 | 4.497712000 | 0.491225000 |
| H | -4.148595000 | 5.445958000 | 0.824549000 |
| C | -2.362701000 | 4.303398000 | 0.443040000 |
| H | -1.696746000 | 5.107944000 | 0.743933000 |
| C | -2.765920000 | 0.001123000 | -1.692069000 |
| C | -3.329119000 | 0.599393000 | -2.842396000 |
| H | -3.338363000 | 1.683008000 | -2.912667000 |
| C | -3.840743000 | -0.163265000 | -3.882199000 |
| H | -4.257510000 | 0.336354000 | -4.753131000 |
| C | -3.800718000 | -1.559325000 | -3.829139000 |
| H | -4.187392000 | -2.156976000 | -4.649074000 |
| C | -3.261794000 | -2.175592000 | -2.707134000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.231262000 | -3.259691000 | -2.657793000 |
| C | -2.767562000 | -1.422988000 | -1.630493000 |
| C | -1.867577000 | -4.008155000 | -0.494456000 |
| C | -2.982319000 | -4.845160000 | -0.659560000 |
| H | -3.986694000 | -4.438309000 | -0.575971000 |
| C | -2.807630000 | -6.202582000 | -0.916180000 |
| H | -3.676247000 | -6.842425000 | -1.045778000 |
| C | -1.522645000 | -6.741736000 | -0.998400000 |
| H | -1.390077000 | -7.802207000 | -1.194247000 |
| C | -0.411087000 | -5.922184000 | -0.813925000 |
| H | 0.589842000 | -6.343283000 | -0.858567000 |
| C | -0.582984000 | -4.561323000 | -0.559345000 |
| H | 0.286556000 | -3.930377000 | -0.393049000 |
| C | -3.416240000 | -2.220844000 | 1.129020000 |
| C | -4.610409000 | -1.518340000 | 0.942270000 |
| H | -4.770694000 | -0.956217000 | 0.027368000 |
| C | -5.608565000 | -1.560050000 | 1.917015000 |
| H | -6.535892000 | -1.015732000 | 1.759387000 |
| C | -5.426661000 | -2.308865000 | 3.078156000 |
| H | -6.209819000 | -2.348023000 | 3.830247000 |
| C | -4.240188000 | -3.020578000 | 3.265663000 |
| H | -4.099226000 | -3.620976000 | 4.160684000 |
| C | -3.236641000 | -2.971804000 | 2.300508000 |
| H | -2.324586000 | -3.546961000 | 2.447031000 |
| C | 2.226762000 | -2.508188000 | -1.929306000 |
| C | 1.176855000 | -1.653789000 | -2.221353000 |
| H | 0.171713000 | -2.077124000 | -2.324098000 |
| C | 1.374857000 | -0.281481000 | -2.590539000 |
| C | 0.376405000 | 0.604045000 | -2.890781000 |
| H | 0.603794000 | 1.625374000 | -3.171622000 |
| H | -0.641688000 | 0.263377000 | -3.080311000 |
| Y | -0.018310000 | -0.088184000 | -0.248767000 |
| H | 2.401134000 | 0.084346000 | -2.546732000 |
| O | -0.579815000 | 0.047431000 | 2.152184000 |
| C | 0.001831000 | -0.722550000 | 3.240642000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.779741000 | 0.740766000 | 2.639004000 |
| C | -0.599272000 | -0.143498000 | 4.510059000 |
| H | -0.277341000 | -1.774830000 | 3.105101000 |
| H | 1.088079000 | -0.625705000 | 3.182896000 |
| C | -2.010338000 | 0.226583000 | 4.051977000 |
| H | -1.563930000 | 1.812679000 | 2.618901000 |
| H | -2.592371000 | 0.518934000 | 1.948108000 |
| H | -0.044490000 | 0.747393000 | 4.825464000 |
| H | -0.585237000 | -0.862821000 | 5.333794000 |
| H | -2.480509000 | 0.985046000 | 4.684171000 |
| H | -2.655196000 | -0.657461000 | 4.038176000 |
| H | 2.058084000 | -3.576669000 | -1.852638000 |
| H | 3.234383000 | -2.205198000 | -2.187327000 |
| C | 4.690727000 | -2.141515000 | -0.281045000 |
| C | 3.303961000 | -2.471486000 | 0.213700000 |
| H | 4.714624000 | -1.127350000 | -0.700603000 |
| H | 4.962509000 | -2.821408000 | -1.101380000 |
| H | 3.153598000 | -3.517177000 | 0.483908000 |
| C | 2.467332000 | -1.554765000 | 0.836919000 |
| C | 2.392943000 | -0.153410000 | 0.664048000 |
| H | 1.696038000 | -2.007286000 | 1.474472000 |
| H | 2.031370000 | 0.427694000 | 1.518885000 |
| H | 3.196545000 | 0.353785000 | 0.132103000 |

117

theta3_thf_P2_trans_1,2 E = -2200.68143 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 2.041952000 | 1.191247000 | -0.414270000 |
| P | 2.632043000 | -1.800326000 | -0.096145000 |
| P | -0.585531000 | 2.643486000 | -0.155887000 |
| Si | -7.302708000 | -2.941035000 | 0.201347000 |
| C | -5.584016000 | -2.122564000 | 0.357128000 |
| H | -5.056321000 | -2.636047000 | 1.174240000 |
| H | -5.736974000 | -1.085875000 | 0.696034000 |
| C | -7.096124000 | -4.745610000 | -0.313246000 |
| H | -6.629225000 | -4.841892000 | -1.300800000 |
| H | -8.069619000 | -5.248106000 | -0.365096000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -6.479648000 | -5.302035000 | 0.403500000 |
| C | -8.144737000 | -2.847267000 | 1.887947000 |
| H | -7.570676000 | -3.379595000 | 2.656162000 |
| H | -9.142935000 | -3.300247000 | 1.853794000 |
| H | -8.268331000 | -1.810170000 | 2.222779000 |
| C | -8.332655000 | -2.016844000 | -1.083508000 |
| H | -8.456426000 | -0.959772000 | -0.817961000 |
| H | -9.335818000 | -2.453416000 | -1.160739000 |
| H | -7.883669000 | -2.060692000 | -2.083099000 |
| C | 2.879697000 | -3.141417000 | 1.156048000 |
| C | 1.994558000 | -3.227861000 | 2.239400000 |
| H | 1.182428000 | -2.510488000 | 2.326049000 |
| C | 2.149277000 | -4.221278000 | 3.204640000 |
| H | 1.455788000 | -4.280022000 | 4.039818000 |
| C | 3.186822000 | -5.146424000 | 3.093466000 |
| H | 3.304953000 | -5.925297000 | 3.841735000 |
| C | 4.067591000 | -5.073063000 | 2.015234000 |
| H | 4.875564000 | -5.793690000 | 1.921679000 |
| C | 3.916128000 | -4.078684000 | 1.049596000 |
| H | 4.601000000 | -4.039049000 | 0.207327000 |
| C | 3.452304000 | -2.491969000 | -1.599576000 |
| C | 2.874181000 | -3.616311000 | -2.207524000 |
| H | 1.993565000 | -4.082022000 | -1.769009000 |
| C | 3.431294000 | -4.155027000 | -3.363973000 |
| H | 2.980875000 | -5.030837000 | -3.823481000 |
| C | 4.565001000 | -3.569907000 | -3.931464000 |
| H | 4.997424000 | -3.987626000 | -4.836450000 |
| C | 5.141212000 | -2.451526000 | -3.332955000 |
| H | 6.026798000 | -1.995963000 | -3.768009000 |
| C | 4.589780000 | -1.912543000 | -2.169045000 |
| H | 5.048567000 | -1.045669000 | -1.702654000 |
| C | 3.697407000 | -0.406230000 | 0.463020000 |
| C | 3.279625000 | 0.922932000 | 0.180579000 |
| C | 4.142124000 | 1.964577000 | 0.591191000 |
| H | 3.853022000 | 2.990998000 | 0.387515000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.332295000 | 1.709141000 | 1.256838000 |
| H | 5.959573000 | 2.543310000 | 1.561662000 |
| C | 5.719585000 | 0.399099000 | 1.551128000 |
| H | 6.647786000 | 0.197880000 | 2.077494000 |
| C | 4.895261000 | -0.645342000 | 1.151951000 |
| H | 5.184764000 | -1.669845000 | 1.370499000 |
| C | 1.948769000 | 2.277891000 | -1.297321000 |
| C | 2.975671000 | 2.587808000 | -2.214108000 |
| H | 3.891409000 | 2.004683000 | -2.187795000 |
| C | 2.825757000 | 3.597273000 | -3.154756000 |
| H | 3.635582000 | 3.800781000 | -3.850881000 |
| C | 1.639660000 | 4.332227000 | -3.227749000 |
| H | 1.517274000 | 5.114219000 | -3.971213000 |
| C | 0.613523000 | 4.049720000 | -2.334390000 |
| H | -0.310810000 | 4.617161000 | -2.385260000 |
| C | 0.756386000 | 3.050378000 | -1.361094000 |
| C | -2.085471000 | 3.543006000 | -0.751732000 |
| C | -2.204365000 | 4.934945000 | -0.617948000 |
| H | -1.406191000 | 5.507402000 | -0.153159000 |
| C | -3.348282000 | 5.588452000 | -1.070107000 |
| H | -3.429548000 | 6.666805000 | -0.963264000 |
| C | -4.386915000 | 4.862667000 | -1.654902000 |
| H | -5.278673000 | 5.375390000 | -2.004902000 |
| C | -4.281827000 | 3.479009000 | -1.781474000 |
| H | -5.091667000 | 2.908342000 | -2.228152000 |
| C | -3.138143000 | 2.822431000 | -1.327800000 |
| H | -3.066974000 | 1.742804000 | -1.416373000 |
| C | -0.167456000 | 3.601538000 | 1.373756000 |
| C | 1.028800000 | 4.310967000 | 1.516921000 |
| H | 1.751377000 | 4.322287000 | 0.706410000 |
| C | 1.284353000 | 5.029373000 | 2.686385000 |
| H | 2.214832000 | 5.582329000 | 2.784505000 |
| C | 0.344731000 | 5.055130000 | 3.715009000 |
| H | 0.540597000 | 5.625294000 | 4.618986000 |
| C | -0.856646000 | 4.357313000 | 3.574227000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.601458000 | 4.387875000 | 4.365403000 |
| C | -1.108449000 | 3.627775000 | 2.414262000 |
| H | -2.056026000 | 3.103290000 | 2.306252000 |
| C | -2.739629000 | -1.292306000 | -2.253444000 |
| C | -1.456286000 | -0.487840000 | -2.333057000 |
| H | -1.575693000 | 0.578302000 | -2.556352000 |
| C | -0.282193000 | -1.080869000 | -2.853863000 |
| C | 0.949459000 | -0.464701000 | -2.971200000 |
| H | 1.817367000 | -1.020482000 | -3.306992000 |
| H | 1.020857000 | 0.621413000 | -3.054164000 |
| Y | 0.218535000 | -0.205363000 | -0.433699000 |
| H | -0.288183000 | -2.171109000 | -2.959288000 |
| O | 0.190176000 | -0.208275000 | 2.045542000 |
| C | -0.906969000 | -0.537996000 | 2.939623000 |
| C | 1.258470000 | 0.447240000 | 2.811791000 |
| C | -0.355462000 | -0.381513000 | 4.348329000 |
| H | -1.730364000 | 0.158434000 | 2.740816000 |
| H | -1.232599000 | -1.555746000 | 2.714884000 |
| C | 0.658445000 | 0.749023000 | 4.174639000 |
| H | 2.094821000 | -0.255090000 | 2.872991000 |
| H | 1.565308000 | 1.332696000 | 2.255807000 |
| H | 0.142315000 | -1.303472000 | 4.669975000 |
| H | -1.142839000 | -0.151115000 | 5.071657000 |
| H | 1.422063000 | 0.762075000 | 4.957361000 |
| H | 0.157250000 | 1.721670000 | 4.165846000 |
| H | -3.487473000 | -0.891904000 | -2.952809000 |
| H | -2.546266000 | -2.318490000 | -2.600503000 |
| C | -4.741885000 | -2.133854000 | -0.923010000 |
| C | -3.395487000 | -1.361059000 | -0.866305000 |
| H | -4.525627000 | -3.168087000 | -1.224003000 |
| H | -5.318805000 | -1.689683000 | -1.745500000 |
| H | -3.640421000 | -0.334427000 | -0.545302000 |
| C | -2.512806000 | -1.945337000 | 0.198996000 |
| C | -1.394911000 | -2.680486000 | 0.043689000 |
| H | -2.871491000 | -1.789890000 | 1.216726000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.897510000 | -3.141848000 | 0.894539000 |
| H | -1.017300000 | -2.956552000 | -0.939240000 |

117

theta1_thf_C2_cis_1,4 E = -2200.634694 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 1.425823000 | 0.418655000 | 1.325245000 |
| P | -0.091540000 | 2.779006000 | 0.246947000 |
| P | 1.869771000 | -2.330964000 | 0.155244000 |
| Si | -7.419621000 | -1.696926000 | -0.477403000 |
| C | -5.827557000 | -2.427897000 | 0.262510000 |
| H | -5.934027000 | -3.522723000 | 0.295572000 |
| H | -5.753741000 | -2.107957000 | 1.312157000 |
| C | -7.649701000 | -2.301418000 | -2.253962000 |
| H | -6.821002000 | -1.993878000 | -2.903479000 |
| H | -8.572211000 | -1.897464000 | -2.688615000 |
| H | -7.718301000 | -3.395216000 | -2.298835000 |
| C | -8.881821000 | -2.250416000 | 0.580003000 |
| H | -8.973750000 | -3.343180000 | 0.594209000 |
| H | -9.826601000 | -1.845854000 | 0.197222000 |
| H | -8.775398000 | -1.914275000 | 1.618521000 |
| C | -7.313171000 | 0.193306000 | -0.469060000 |
| H | -7.159705000 | 0.578393000 | 0.546684000 |
| H | -8.237263000 | 0.640488000 | -0.855032000 |
| H | -6.488889000 | 0.558299000 | -1.094609000 |
| C | -0.121137000 | 4.272138000 | -0.836521000 |
| C | 0.440818000 | 4.179670000 | -2.117675000 |
| H | 0.875847000 | 3.238930000 | -2.448634000 |
| C | 0.453067000 | 5.284749000 | -2.965963000 |
| H | 0.891602000 | 5.204214000 | -3.957373000 |
| C | -0.106348000 | 6.491905000 | -2.546341000 |
| H | -0.103506000 | 7.352513000 | -3.209517000 |
| C | -0.673939000 | 6.589866000 | -1.276773000 |
| H | -1.112245000 | 7.527842000 | -0.946837000 |
| C | -0.682682000 | 5.487091000 | -0.423052000 |
| H | -1.131581000 | 5.571337000 | 0.562543000 |
| C | -1.412800000 | 3.089012000 | 1.497427000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.749882000 | 3.096222000 | 1.074313000 |
| H | -2.991833000 | 2.951822000 | 0.023925000 |
| C | -3.776414000 | 3.303949000 | 1.991162000 |
| H | -4.808831000 | 3.314080000 | 1.652393000 |
| C | -3.478837000 | 3.493333000 | 3.341753000 |
| H | -4.280584000 | 3.649978000 | 4.058101000 |
| C | -2.152526000 | 3.483789000 | 3.768190000 |
| H | -1.916127000 | 3.637310000 | 4.817717000 |
| C | -1.119994000 | 3.284598000 | 2.851126000 |
| H | -0.087793000 | 3.289748000 | 3.188764000 |
| C | 1.488821000 | 2.869950000 | 1.177049000 |
| C | 2.025926000 | 1.644346000 | 1.650753000 |
| C | 3.218053000 | 1.715134000 | 2.402652000 |
| H | 3.650999000 | 0.795713000 | 2.784797000 |
| C | 3.848669000 | 2.927466000 | 2.651148000 |
| H | 4.770295000 | 2.937037000 | 3.228013000 |
| C | 3.321489000 | 4.124437000 | 2.159325000 |
| H | 3.818558000 | 5.070690000 | 2.350762000 |
| C | 2.141521000 | 4.084392000 | 1.424999000 |
| H | 1.712556000 | 5.006783000 | 1.041746000 |
| C | 1.449508000 | -0.595474000 | 2.302508000 |
| C | 1.225032000 | -0.313546000 | 3.665005000 |
| H | 1.061089000 | 0.717290000 | 3.964431000 |
| C | 1.192880000 | -1.323237000 | 4.617925000 |
| H | 1.007751000 | -1.066634000 | 5.657953000 |
| C | 1.376125000 | -2.658046000 | 4.249872000 |
| H | 1.345366000 | -3.447785000 | 4.994493000 |
| C | 1.591862000 | -2.964560000 | 2.911470000 |
| H | 1.729195000 | -3.999341000 | 2.610387000 |
| C | 1.640241000 | -1.954932000 | 1.940882000 |
| C | 1.577381000 | -4.146752000 | -0.018043000 |
| C | 2.621610000 | -5.072207000 | 0.119672000 |
| H | 3.631408000 | -4.731261000 | 0.328061000 |
| C | 2.371276000 | -6.437267000 | -0.011405000 |
| H | 3.188281000 | -7.145392000 | 0.097943000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.080774000 | -6.892388000 | -0.278665000 |
| H | 0.889039000 | -7.956940000 | -0.381614000 |
| C | 0.037012000 | -5.977630000 | -0.412254000 |
| H | -0.971875000 | -6.325831000 | -0.616958000 |
| C | 0.282234000 | -4.611317000 | -0.287183000 |
| H | -0.544728000 | -3.912746000 | -0.382055000 |
| C | 3.681875000 | -2.167775000 | -0.174775000 |
| C | 4.598062000 | -1.812400000 | 0.820233000 |
| H | 4.250556000 | -1.630779000 | 1.833279000 |
| C | 5.957709000 | -1.713570000 | 0.519272000 |
| H | 6.662875000 | -1.442674000 | 1.300573000 |
| C | 6.412947000 | -1.979959000 | -0.770891000 |
| H | 7.473415000 | -1.915892000 | -0.998864000 |
| C | 5.503811000 | -2.341760000 | -1.767550000 |
| H | 5.855835000 | -2.567050000 | -2.771107000 |
| C | 4.144287000 | -2.425317000 | -1.474376000 |
| H | 3.444110000 | -2.723675000 | -2.252726000 |
| C | -1.842180000 | -0.591026000 | 0.538497000 |
| C | -2.220824000 | -2.008592000 | 0.674707000 |
| H | -1.499166000 | -2.623268000 | 1.219251000 |
| C | -3.310800000 | -2.661425000 | 0.209916000 |
| C | -4.516646000 | -2.066496000 | -0.463580000 |
| H | -4.582957000 | -2.415371000 | -1.506554000 |
| H | -4.418210000 | -0.973544000 | -0.509701000 |
| Y | 0.232516000 | -0.002094000 | -0.585303000 |
| H | -3.380004000 | -3.731915000 | 0.411633000 |
| O | 2.050855000 | 0.792453000 | -2.150784000 |
| C | 2.330902000 | 0.650143000 | -3.569772000 |
| C | 3.234241000 | 1.364670000 | -1.489103000 |
| C | 3.550090000 | 1.516261000 | -3.839725000 |
| H | 2.533224000 | -0.407375000 | -3.775426000 |
| H | 1.445402000 | 0.964187000 | -4.126223000 |
| C | 4.335090000 | 1.367661000 | -2.537368000 |
| H | 2.969235000 | 2.374643000 | -1.164446000 |
| H | 3.461264000 | 0.749945000 | -0.617308000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.253965000 | 2.559441000 | -3.999128000 |
| H | 4.103221000 | 1.180543000 | -4.721537000 |
| H | 5.048149000 | 2.179709000 | -2.370024000 |
| H | 4.882673000 | 0.420124000 | -2.520741000 |
| H | -2.696039000 | 0.064664000 | 0.336142000 |
| H | -1.397317000 | -0.236274000 | 1.488596000 |
| C | -0.892009000 | -2.027088000 | -2.566689000 |
| C | -0.620856000 | -0.931924000 | -3.311742000 |
| H | -1.624272000 | -2.042108000 | -1.756675000 |
| H | -0.414020000 | -2.974189000 | -2.799258000 |
| H | 0.100550000 | -1.027225000 | -4.120993000 |
| C | -1.171034000 | 0.407973000 | -3.099861000 |
| C | -2.268203000 | 0.692226000 | -2.363439000 |
| H | -0.653855000 | 1.233878000 | -3.587005000 |
| H | -2.596376000 | 1.719880000 | -2.238455000 |
| H | -2.902468000 | -0.083068000 | -1.948581000 |

117

theta1_thf_TS2_cis_1,4 E = -2200.62655 a.u. Imaginary frequency=96i

| | | | |
|----|--------------|--------------|--------------|
| N | 1.276098000 | 0.542370000 | 1.338510000 |
| P | -0.627593000 | 2.628583000 | 0.244220000 |
| P | 2.289255000 | -2.026958000 | 0.087874000 |
| Si | -7.176795000 | -2.327214000 | -0.604726000 |
| C | -5.609164000 | -2.836316000 | 0.346551000 |
| H | -5.750258000 | -3.866907000 | 0.705521000 |
| H | -5.529704000 | -2.217806000 | 1.252387000 |
| C | -7.404498000 | -3.435201000 | -2.118103000 |
| H | -6.574880000 | -3.337774000 | -2.828834000 |
| H | -8.325065000 | -3.175733000 | -2.654976000 |
| H | -7.477728000 | -4.492400000 | -1.835318000 |
| C | -8.658092000 | -2.503898000 | 0.550595000 |
| H | -8.775873000 | -3.538390000 | 0.894914000 |
| H | -9.589443000 | -2.217375000 | 0.047262000 |
| H | -8.554552000 | -1.869553000 | 1.439288000 |
| C | -7.024145000 | -0.526020000 | -1.166794000 |
| H | -6.869067000 | 0.145672000 | -0.313332000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -7.935444000 | -0.198079000 | -1.681325000 |
| H | -6.188695000 | -0.384694000 | -1.863872000 |
| C | -0.846136000 | 4.153770000 | -0.769273000 |
| C | -0.173421000 | 4.245112000 | -1.996039000 |
| H | 0.439025000 | 3.414431000 | -2.341175000 |
| C | -0.288381000 | 5.389918000 | -2.781803000 |
| H | 0.237151000 | 5.451336000 | -3.731308000 |
| C | -1.087516000 | 6.450914000 | -2.355289000 |
| H | -1.184388000 | 7.340982000 | -2.970782000 |
| C | -1.766963000 | 6.363835000 | -1.141110000 |
| H | -2.392991000 | 7.186696000 | -0.806793000 |
| C | -1.648420000 | 5.222181000 | -0.348754000 |
| H | -2.185371000 | 5.162167000 | 0.593667000 |
| C | -2.100800000 | 2.596115000 | 1.354300000 |
| C | -3.365527000 | 2.392933000 | 0.782148000 |
| H | -3.469979000 | 2.293678000 | -0.296485000 |
| C | -4.499598000 | 2.342348000 | 1.588029000 |
| H | -5.476492000 | 2.196689000 | 1.135148000 |
| C | -4.380452000 | 2.479053000 | 2.972201000 |
| H | -5.265523000 | 2.435389000 | 3.600903000 |
| C | -3.125768000 | 2.676460000 | 3.544983000 |
| H | -3.029611000 | 2.790016000 | 4.621456000 |
| C | -1.987055000 | 2.738070000 | 2.740961000 |
| H | -1.013471000 | 2.908106000 | 3.191516000 |
| C | 0.817353000 | 2.961583000 | 1.325701000 |
| C | 1.569650000 | 1.843349000 | 1.773509000 |
| C | 2.669107000 | 2.114984000 | 2.619390000 |
| H | 3.264659000 | 1.283773000 | 2.984494000 |
| C | 3.007096000 | 3.410698000 | 2.984456000 |
| H | 3.866973000 | 3.572015000 | 3.630168000 |
| C | 2.266807000 | 4.502486000 | 2.522045000 |
| H | 2.533924000 | 5.516190000 | 2.805021000 |
| C | 1.177187000 | 4.265952000 | 1.693329000 |
| H | 0.589295000 | 5.102659000 | 1.324836000 |
| C | 1.458817000 | -0.493433000 | 2.273200000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.119145000 | -0.329355000 | 3.632770000 |
| H | 0.731232000 | 0.630095000 | 3.961711000 |
| C | 1.262316000 | -1.363323000 | 4.548425000 |
| H | 0.982502000 | -1.196701000 | 5.585679000 |
| C | 1.744332000 | -2.610462000 | 4.145836000 |
| H | 1.856610000 | -3.420120000 | 4.860672000 |
| C | 2.069759000 | -2.804572000 | 2.808477000 |
| H | 2.434393000 | -3.773439000 | 2.479097000 |
| C | 1.935637000 | -1.768542000 | 1.874438000 |
| C | 2.270429000 | -3.866752000 | -0.122241000 |
| C | 3.442642000 | -4.633238000 | -0.166408000 |
| H | 4.414051000 | -4.157292000 | -0.078695000 |
| C | 3.373450000 | -6.018487000 | -0.316682000 |
| H | 4.291541000 | -6.599058000 | -0.349194000 |
| C | 2.138462000 | -6.655589000 | -0.416512000 |
| H | 2.088319000 | -7.734575000 | -0.533960000 |
| C | 0.966709000 | -5.901659000 | -0.357412000 |
| H | -0.001959000 | -6.389911000 | -0.423422000 |
| C | 1.031645000 | -4.517738000 | -0.214221000 |
| H | 0.108646000 | -3.950303000 | -0.145067000 |
| C | 4.072950000 | -1.585875000 | -0.140692000 |
| C | 4.825347000 | -0.987201000 | 0.874741000 |
| H | 4.373643000 | -0.808549000 | 1.846039000 |
| C | 6.160430000 | -0.644235000 | 0.653779000 |
| H | 6.736620000 | -0.186452000 | 1.453593000 |
| C | 6.760201000 | -0.906598000 | -0.577068000 |
| H | 7.804038000 | -0.653035000 | -0.740937000 |
| C | 6.018454000 | -1.512062000 | -1.593709000 |
| H | 6.484374000 | -1.737636000 | -2.549576000 |
| C | 4.680991000 | -1.840302000 | -1.380428000 |
| H | 4.119144000 | -2.335371000 | -2.170544000 |
| C | -1.572399000 | -1.188754000 | 0.198387000 |
| C | -1.983537000 | -2.510174000 | 0.671743000 |
| H | -1.275011000 | -2.997028000 | 1.342759000 |
| C | -3.110953000 | -3.195063000 | 0.380066000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.286469000 | -2.750930000 | -0.440952000 |
| H | -4.363898000 | -3.386045000 | -1.336600000 |
| H | -4.139086000 | -1.725729000 | -0.806060000 |
| Y | 0.353453000 | 0.091971000 | -0.755221000 |
| H | -3.221365000 | -4.181623000 | 0.832814000 |
| O | 2.239277000 | 1.106274000 | -1.944505000 |
| C | 2.853509000 | 0.766709000 | -3.218382000 |
| C | 3.122254000 | 2.034320000 | -1.221479000 |
| C | 3.855203000 | 1.875390000 | -3.484847000 |
| H | 3.347688000 | -0.204428000 | -3.112306000 |
| H | 2.061941000 | 0.695384000 | -3.964701000 |
| C | 4.374542000 | 2.167403000 | -2.076456000 |
| H | 2.582724000 | 2.980536000 | -1.120617000 |
| H | 3.308630000 | 1.616029000 | -0.232264000 |
| H | 3.354765000 | 2.753383000 | -3.909526000 |
| H | 4.640333000 | 1.560043000 | -4.177742000 |
| H | 4.824192000 | 3.159624000 | -1.980797000 |
| H | 5.119484000 | 1.421493000 | -1.781897000 |
| H | -2.407990000 | -0.561809000 | -0.136106000 |
| H | -1.057242000 | -0.657226000 | 1.027081000 |
| C | -1.016689000 | -1.940682000 | -2.105584000 |
| C | -0.212938000 | -1.195278000 | -2.955576000 |
| H | -2.085170000 | -1.766495000 | -2.062873000 |
| H | -0.698876000 | -2.925365000 | -1.785589000 |
| H | 0.728961000 | -1.613733000 | -3.306105000 |
| C | -0.589172000 | 0.127692000 | -3.394649000 |
| C | -1.564948000 | 0.896888000 | -2.831362000 |
| H | 0.020711000 | 0.587229000 | -4.170321000 |
| H | -1.753910000 | 1.905170000 | -3.184166000 |
| H | -2.282191000 | 0.496240000 | -2.117320000 |

117

theta1_thf_P2_cis_1,4 E = -2200.678069 a.u.

| | | | |
|---|--------------|--------------|-------------|
| N | -1.569273000 | -1.255644000 | 0.947001000 |
| P | 1.331235000 | -1.556273000 | 0.627929000 |
| P | -2.829726000 | 1.335565000 | 0.140503000 |

| | | | |
|----|-------------|--------------|--------------|
| Si | 6.825114000 | 1.921427000 | -0.985405000 |
| C | 5.334531000 | 2.527557000 | 0.036089000 |
| H | 5.681622000 | 3.362602000 | 0.663410000 |
| H | 5.028546000 | 1.737858000 | 0.737419000 |
| C | 7.569663000 | 3.381778000 | -1.924274000 |
| H | 6.852582000 | 3.835817000 | -2.619032000 |
| H | 8.437655000 | 3.064909000 | -2.515163000 |
| H | 7.909768000 | 4.167483000 | -1.238765000 |
| C | 8.106007000 | 1.200006000 | 0.198095000 |
| H | 8.438255000 | 1.944781000 | 0.931314000 |
| H | 8.994395000 | 0.854571000 | -0.344332000 |
| H | 7.704095000 | 0.343846000 | 0.753370000 |
| C | 6.268430000 | 0.598718000 | -2.215748000 |
| H | 5.811105000 | -0.259241000 | -1.708328000 |
| H | 7.120317000 | 0.222883000 | -2.795750000 |
| H | 5.537974000 | 0.995054000 | -2.931825000 |
| C | 2.928998000 | -2.332634000 | 0.133826000 |
| C | 3.146344000 | -2.613749000 | -1.222415000 |
| H | 2.387161000 | -2.355719000 | -1.956440000 |
| C | 4.331430000 | -3.218253000 | -1.635831000 |
| H | 4.490074000 | -3.432732000 | -2.689308000 |
| C | 5.317030000 | -3.534196000 | -0.699840000 |
| H | 6.244727000 | -3.998689000 | -1.022630000 |
| C | 5.111407000 | -3.247581000 | 0.648930000 |
| H | 5.877117000 | -3.490305000 | 1.380811000 |
| C | 3.922443000 | -2.651229000 | 1.068155000 |
| H | 3.770680000 | -2.435149000 | 2.121551000 |
| C | 1.585744000 | -0.988921000 | 2.363129000 |
| C | 2.080901000 | 0.304688000 | 2.576098000 |
| H | 2.296012000 | 0.960482000 | 1.735569000 |
| C | 2.309713000 | 0.761965000 | 3.873012000 |
| H | 2.697848000 | 1.764953000 | 4.028726000 |
| C | 2.040564000 | -0.064535000 | 4.963584000 |
| H | 2.216744000 | 0.293565000 | 5.974280000 |
| C | 1.546209000 | -1.352141000 | 4.755906000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.338958000 | -1.999702000 | 5.603728000 |
| C | 1.318398000 | -1.815656000 | 3.461050000 |
| H | 0.935248000 | -2.820269000 | 3.304705000 |
| C | 0.147844000 | -2.967834000 | 0.756057000 |
| C | -1.209395000 | -2.611678000 | 0.973916000 |
| C | -2.144535000 | -3.657760000 | 1.122530000 |
| H | -3.184297000 | -3.407917000 | 1.317995000 |
| C | -1.752913000 | -4.988340000 | 1.032477000 |
| H | -2.496365000 | -5.772358000 | 1.155317000 |
| C | -0.419096000 | -5.325970000 | 0.782330000 |
| H | -0.117488000 | -6.367131000 | 0.713193000 |
| C | 0.525134000 | -4.313080000 | 0.646607000 |
| H | 1.568744000 | -4.563725000 | 0.476973000 |
| C | -2.413631000 | -0.749656000 | 1.935351000 |
| C | -2.603344000 | -1.385413000 | 3.182335000 |
| H | -2.089567000 | -2.319801000 | 3.383374000 |
| C | -3.409251000 | -0.828148000 | 4.165942000 |
| H | -3.519822000 | -1.349440000 | 5.113774000 |
| C | -4.057290000 | 0.392836000 | 3.963796000 |
| H | -4.679953000 | 0.829117000 | 4.738787000 |
| C | -3.874795000 | 1.046909000 | 2.751550000 |
| H | -4.351197000 | 2.009480000 | 2.580924000 |
| C | -3.075836000 | 0.491508000 | 1.742718000 |
| C | -2.720207000 | 3.129667000 | 0.571224000 |
| C | -3.420423000 | 4.114412000 | -0.133691000 |
| H | -4.111381000 | 3.838311000 | -0.924668000 |
| C | -3.255153000 | 5.461258000 | 0.191346000 |
| H | -3.811653000 | 6.216302000 | -0.357393000 |
| C | -2.393543000 | 5.836518000 | 1.219809000 |
| H | -2.271683000 | 6.885692000 | 1.474268000 |
| C | -1.697194000 | 4.857879000 | 1.930354000 |
| H | -1.036895000 | 5.140972000 | 2.745946000 |
| C | -1.854573000 | 3.511902000 | 1.607606000 |
| H | -1.324747000 | 2.757495000 | 2.184823000 |
| C | -4.417229000 | 1.146163000 | -0.794361000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -5.569943000 | 0.615817000 | -0.201478000 |
| H | -5.558126000 | 0.324581000 | 0.844470000 |
| C | -6.735761000 | 0.459340000 | -0.950994000 |
| H | -7.625362000 | 0.050987000 | -0.478772000 |
| C | -6.765949000 | 0.830279000 | -2.295084000 |
| H | -7.678256000 | 0.711635000 | -2.873239000 |
| C | -5.621395000 | 1.356229000 | -2.894683000 |
| H | -5.637625000 | 1.650430000 | -3.940892000 |
| C | -4.450836000 | 1.504894000 | -2.151698000 |
| H | -3.560788000 | 1.906249000 | -2.628970000 |
| C | 1.022982000 | 2.255328000 | -0.580103000 |
| C | 1.757118000 | 3.354798000 | 0.141469000 |
| H | 1.130392000 | 3.993343000 | 0.762959000 |
| C | 3.058941000 | 3.653965000 | 0.037026000 |
| C | 4.115610000 | 2.981072000 | -0.790153000 |
| H | 4.444890000 | 3.702594000 | -1.553807000 |
| H | 3.701387000 | 2.129491000 | -1.343963000 |
| Y | -0.714133000 | -0.288155000 | -0.974768000 |
| H | 3.414883000 | 4.512504000 | 0.609804000 |
| O | -1.901666000 | -1.886542000 | -2.227267000 |
| C | -1.295141000 | -2.888486000 | -3.101963000 |
| C | -3.323093000 | -2.182847000 | -2.045362000 |
| C | -2.350695000 | -3.972381000 | -3.260138000 |
| H | -1.057532000 | -2.396358000 | -4.050472000 |
| H | -0.374538000 | -3.238139000 | -2.629769000 |
| C | -3.654807000 | -3.180665000 | -3.141304000 |
| H | -3.443792000 | -2.610249000 | -1.045815000 |
| H | -3.867848000 | -1.239985000 | -2.116297000 |
| H | -2.269851000 | -4.704233000 | -2.449402000 |
| H | -2.250952000 | -4.499755000 | -4.212855000 |
| H | -4.512986000 | -3.804644000 | -2.877021000 |
| H | -3.883673000 | -2.663373000 | -4.080044000 |
| H | 1.709882000 | 1.423624000 | -0.783118000 |
| H | 0.240610000 | 1.892279000 | 0.118924000 |
| C | 0.358830000 | 2.751592000 | -1.882583000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.543172000 | 1.796419000 | -2.654325000 |
| H | 1.168512000 | 3.098668000 | -2.541937000 |
| H | -0.229599000 | 3.640181000 | -1.629273000 |
| H | -1.435496000 | 2.270176000 | -3.057778000 |
| C | -0.121872000 | 0.652742000 | -3.334770000 |
| C | 0.929311000 | -0.214264000 | -2.987109000 |
| H | -0.837109000 | 0.263064000 | -4.065552000 |
| H | 1.134092000 | -1.058224000 | -3.641920000 |
| H | 1.814466000 | 0.176734000 | -2.484084000 |

117

theta1_thf_C2_trans_1,4 E = -2200.65354 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.769215000 | -1.277829000 | 1.218021000 |
| P | 2.925110000 | 0.604647000 | 0.254181000 |
| P | -1.971454000 | -1.828902000 | 0.074504000 |
| Si | -4.884372000 | 4.592286000 | -0.198387000 |
| C | -4.059457000 | 3.151669000 | 0.735721000 |
| H | -4.805888000 | 2.356931000 | 0.883023000 |
| H | -3.801466000 | 3.504799000 | 1.744718000 |
| C | -5.464944000 | 4.017814000 | -1.905138000 |
| H | -4.630862000 | 3.693012000 | -2.539562000 |
| H | -5.975781000 | 4.831114000 | -2.434826000 |
| H | -6.173603000 | 3.183771000 | -1.830282000 |
| C | -6.365668000 | 5.179019000 | 0.811776000 |
| H | -7.100263000 | 4.377211000 | 0.953897000 |
| H | -6.878875000 | 6.011191000 | 0.314887000 |
| H | -6.059853000 | 5.527394000 | 1.805573000 |
| C | -3.647566000 | 6.007428000 | -0.404331000 |
| H | -3.246790000 | 6.333399000 | 0.563229000 |
| H | -4.124348000 | 6.877289000 | -0.872044000 |
| H | -2.798642000 | 5.724538000 | -1.039264000 |
| C | 4.248097000 | 0.876353000 | -1.016703000 |
| C | 3.981576000 | 0.540472000 | -2.351779000 |
| H | 3.009688000 | 0.133715000 | -2.618667000 |
| C | 4.950160000 | 0.718125000 | -3.338348000 |
| H | 4.731003000 | 0.450491000 | -4.369110000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 6.198574000 | 1.243995000 | -3.004331000 |
| H | 6.953518000 | 1.387594000 | -3.772432000 |
| C | 6.472017000 | 1.584305000 | -1.680639000 |
| H | 7.443045000 | 1.991987000 | -1.412400000 |
| C | 5.505260000 | 1.402336000 | -0.691302000 |
| H | 5.731809000 | 1.674904000 | 0.335091000 |
| C | 3.513609000 | 1.627636000 | 1.679649000 |
| C | 3.523268000 | 3.024311000 | 1.542529000 |
| H | 3.203997000 | 3.481445000 | 0.608601000 |
| C | 3.940241000 | 3.832009000 | 2.597033000 |
| H | 3.949842000 | 4.912309000 | 2.478092000 |
| C | 4.337750000 | 3.256976000 | 3.805590000 |
| H | 4.657825000 | 3.888400000 | 4.629899000 |
| C | 4.322552000 | 1.871730000 | 3.950093000 |
| H | 4.634481000 | 1.417550000 | 4.886901000 |
| C | 3.915783000 | 1.057223000 | 2.891624000 |
| H | 3.921653000 | -0.022163000 | 3.009947000 |
| C | 3.183223000 | -1.130206000 | 0.811829000 |
| C | 2.052744000 | -1.834652000 | 1.299543000 |
| C | 2.271234000 | -3.133957000 | 1.804216000 |
| H | 1.428599000 | -3.693734000 | 2.197103000 |
| C | 3.533687000 | -3.712980000 | 1.795765000 |
| H | 3.657198000 | -4.720634000 | 2.185076000 |
| C | 4.633960000 | -3.022955000 | 1.282389000 |
| H | 5.619582000 | -3.478565000 | 1.269677000 |
| C | 4.447160000 | -1.733428000 | 0.796949000 |
| H | 5.296054000 | -1.177224000 | 0.407729000 |
| C | -0.172115000 | -1.609015000 | 2.212832000 |
| C | 0.176305000 | -1.619295000 | 3.579119000 |
| H | 1.210959000 | -1.434247000 | 3.853183000 |
| C | -0.776004000 | -1.836098000 | 4.565142000 |
| H | -0.474597000 | -1.830797000 | 5.609553000 |
| C | -2.116382000 | -2.034614000 | 4.223650000 |
| H | -2.866162000 | -2.189357000 | 4.993954000 |
| C | -2.483018000 | -2.034522000 | 2.882854000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.523970000 | -2.186897000 | 2.614818000 |
| C | -1.529502000 | -1.850924000 | 1.871661000 |
| C | -3.817619000 | -1.812704000 | -0.018642000 |
| C | -4.580549000 | -2.920904000 | 0.381676000 |
| H | -4.090071000 | -3.806154000 | 0.777530000 |
| C | -5.967529000 | -2.900848000 | 0.258548000 |
| H | -6.548539000 | -3.762789000 | 0.575354000 |
| C | -6.608143000 | -1.783709000 | -0.279479000 |
| H | -7.689965000 | -1.773706000 | -0.380859000 |
| C | -5.857132000 | -0.687137000 | -0.697391000 |
| H | -6.349594000 | 0.179428000 | -1.130140000 |
| C | -4.468269000 | -0.702495000 | -0.568086000 |
| H | -3.886515000 | 0.151962000 | -0.899583000 |
| C | -1.630006000 | -3.558817000 | -0.508885000 |
| C | -1.012352000 | -4.523995000 | 0.292259000 |
| H | -0.719544000 | -4.276132000 | 1.307751000 |
| C | -0.796131000 | -5.813292000 | -0.197859000 |
| H | -0.320384000 | -6.556153000 | 0.437024000 |
| C | -1.203548000 | -6.153425000 | -1.486053000 |
| H | -1.044191000 | -7.160635000 | -1.861185000 |
| C | -1.831603000 | -5.198493000 | -2.288104000 |
| H | -2.169911000 | -5.462100000 | -3.287019000 |
| C | -2.036915000 | -3.907737000 | -1.805985000 |
| H | -2.547187000 | -3.177756000 | -2.431671000 |
| C | 0.118050000 | 2.410468000 | 1.345567000 |
| C | -1.030746000 | 1.717147000 | 1.749673000 |
| H | -0.914190000 | 1.087182000 | 2.635701000 |
| C | -2.180370000 | 1.486706000 | 0.984901000 |
| C | -2.796873000 | 2.549122000 | 0.087375000 |
| H | -3.065872000 | 2.161481000 | -0.906967000 |
| H | -2.068395000 | 3.351984000 | -0.081419000 |
| Y | 0.004793000 | 0.341145000 | -0.164689000 |
| H | -2.907544000 | 0.809070000 | 1.430836000 |
| O | 0.716342000 | -0.917754000 | -2.238179000 |
| C | 0.242403000 | -0.845066000 | -3.607341000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.411184000 | -2.198189000 | -2.039013000 |
| C | 1.069243000 | -1.860307000 | -4.377978000 |
| H | -0.826501000 | -1.094915000 | -3.624082000 |
| H | 0.380125000 | 0.178720000 | -3.962064000 |
| C | 1.254367000 | -2.969601000 | -3.342476000 |
| H | 2.455618000 | -1.967746000 | -1.813886000 |
| H | 0.957724000 | -2.695439000 | -1.181001000 |
| H | 2.034136000 | -1.427478000 | -4.666120000 |
| H | 0.562743000 | -2.196411000 | -5.287173000 |
| H | 2.124404000 | -3.600781000 | -3.543620000 |
| H | 0.369010000 | -3.610927000 | -3.302081000 |
| H | 0.050157000 | 3.182737000 | 0.574231000 |
| H | 0.933055000 | 2.540082000 | 2.048751000 |
| C | -0.471149000 | 2.402076000 | -2.455201000 |
| C | 0.843800000 | 2.700090000 | -2.535690000 |
| H | -1.178988000 | 3.108179000 | -2.032136000 |
| H | -0.898095000 | 1.524969000 | -2.936703000 |
| H | 1.531992000 | 2.002915000 | -3.014549000 |
| C | 1.426719000 | 3.946863000 | -2.065989000 |
| C | 2.718871000 | 4.262479000 | -2.242855000 |
| H | 0.752744000 | 4.657996000 | -1.589426000 |
| H | 3.116405000 | 5.220424000 | -1.920441000 |
| H | 3.413959000 | 3.578652000 | -2.724298000 |

117

theta1_thf_TS2_trans_1,4 E = -2200.61775 a.u. Imaginary frequency=266i

| | | | |
|----|--------------|--------------|--------------|
| N | -1.177435000 | -0.837123000 | 1.230818000 |
| P | 1.393675000 | -2.118401000 | 0.312209000 |
| P | -2.829475000 | 1.433623000 | 0.089396000 |
| Si | 6.567825000 | 2.948226000 | -0.754012000 |
| C | 5.017927000 | 3.468726000 | 0.223177000 |
| H | 5.159840000 | 4.512182000 | 0.542230000 |
| H | 4.963767000 | 2.884160000 | 1.152991000 |
| C | 6.753516000 | 4.035174000 | -2.287096000 |
| H | 5.908580000 | 3.924472000 | -2.977514000 |
| H | 7.662634000 | 3.772146000 | -2.841382000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 6.828456000 | 5.096426000 | -2.020752000 |
| C | 8.071722000 | 3.150056000 | 0.367234000 |
| H | 8.187591000 | 4.188770000 | 0.699153000 |
| H | 8.994159000 | 2.867572000 | -0.154376000 |
| H | 7.995882000 | 2.523133000 | 1.263980000 |
| C | 6.416224000 | 1.138089000 | -1.288292000 |
| H | 6.319278000 | 0.465056000 | -0.427195000 |
| H | 7.306968000 | 0.823611000 | -1.845683000 |
| H | 5.551820000 | 0.975030000 | -1.944393000 |
| C | 2.328311000 | -3.432556000 | -0.587050000 |
| C | 1.790463000 | -3.945520000 | -1.776298000 |
| H | 0.842665000 | -3.566061000 | -2.151525000 |
| C | 2.457161000 | -4.943963000 | -2.481057000 |
| H | 2.027312000 | -5.338054000 | -3.398277000 |
| C | 3.677707000 | -5.433225000 | -2.012588000 |
| H | 4.201760000 | -6.208108000 | -2.565163000 |
| C | 4.220495000 | -4.925058000 | -0.834662000 |
| H | 5.168692000 | -5.303907000 | -0.462946000 |
| C | 3.549645000 | -3.931462000 | -0.120437000 |
| H | 3.978897000 | -3.550143000 | 0.800955000 |
| C | 2.489122000 | -1.645890000 | 1.722611000 |
| C | 3.548097000 | -0.758757000 | 1.484808000 |
| H | 3.718842000 | -0.363395000 | 0.485679000 |
| C | 4.401736000 | -0.390574000 | 2.522349000 |
| H | 5.223811000 | 0.292732000 | 2.328693000 |
| C | 4.199089000 | -0.895502000 | 3.806947000 |
| H | 4.861954000 | -0.603163000 | 4.616718000 |
| C | 3.146646000 | -1.776829000 | 4.048841000 |
| H | 2.988909000 | -2.176945000 | 5.046841000 |
| C | 2.294495000 | -2.154737000 | 3.011628000 |
| H | 1.482210000 | -2.849560000 | 3.204134000 |
| C | -0.019565000 | -3.000132000 | 1.091734000 |
| C | -1.114087000 | -2.207516000 | 1.526790000 |
| C | -2.159161000 | -2.875932000 | 2.202296000 |
| H | -3.003599000 | -2.295788000 | 2.562138000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.133019000 | -4.249434000 | 2.405844000 |
| H | -2.962576000 | -4.725116000 | 2.923414000 |
| C | -1.063539000 | -5.021513000 | 1.943835000 |
| H | -1.045146000 | -6.095830000 | 2.100920000 |
| C | -0.011953000 | -4.387477000 | 1.291929000 |
| H | 0.837846000 | -4.969329000 | 0.944729000 |
| C | -1.715200000 | 0.003112000 | 2.220832000 |
| C | -1.440112000 | -0.200566000 | 3.589483000 |
| H | -0.816772000 | -1.042010000 | 3.876512000 |
| C | -1.932269000 | 0.657414000 | 4.563550000 |
| H | -1.690205000 | 0.471340000 | 5.606989000 |
| C | -2.716008000 | 1.759279000 | 4.213502000 |
| H | -3.099669000 | 2.432166000 | 4.974581000 |
| C | -2.991789000 | 1.988433000 | 2.870800000 |
| H | -3.593209000 | 2.846393000 | 2.583541000 |
| C | -2.507070000 | 1.127395000 | 1.876923000 |
| C | -3.290670000 | 3.227492000 | 0.026075000 |
| C | -4.620612000 | 3.668778000 | 0.018501000 |
| H | -5.436688000 | 2.953693000 | 0.040489000 |
| C | -4.910124000 | 5.033065000 | -0.011252000 |
| H | -5.946680000 | 5.359497000 | -0.017626000 |
| C | -3.880859000 | 5.972224000 | -0.025886000 |
| H | -4.110482000 | 7.033884000 | -0.050865000 |
| C | -2.554578000 | 5.542338000 | -0.001618000 |
| H | -1.744377000 | 6.266621000 | -0.003294000 |
| C | -2.262649000 | 4.180506000 | 0.021993000 |
| H | -1.226656000 | 3.860048000 | 0.058510000 |
| C | -4.433779000 | 0.576265000 | -0.266415000 |
| C | -5.003093000 | -0.326297000 | 0.637573000 |
| H | -4.526159000 | -0.499169000 | 1.597692000 |
| C | -6.196841000 | -0.979692000 | 0.326221000 |
| H | -6.633159000 | -1.671381000 | 1.042147000 |
| C | -6.840125000 | -0.730203000 | -0.885196000 |
| H | -7.777201000 | -1.228114000 | -1.119129000 |
| C | -6.284277000 | 0.177116000 | -1.789455000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -6.790181000 | 0.393064000 | -2.727035000 |
| C | -5.085522000 | 0.820047000 | -1.486069000 |
| H | -4.676873000 | 1.546121000 | -2.186598000 |
| C | 0.928179000 | 1.872312000 | 0.157757000 |
| C | 1.372895000 | 3.204045000 | 0.595680000 |
| H | 0.671602000 | 3.732717000 | 1.240683000 |
| C | 2.516540000 | 3.845530000 | 0.284218000 |
| C | 3.677866000 | 3.349522000 | -0.528893000 |
| H | 3.739442000 | 3.939238000 | -1.456781000 |
| H | 3.519074000 | 2.308185000 | -0.841112000 |
| Y | -0.337762000 | -0.049470000 | -0.793375000 |
| H | 2.648550000 | 4.846007000 | 0.698105000 |
| O | -1.945436000 | -1.320056000 | -2.098536000 |
| C | -2.635013000 | -0.986514000 | -3.338683000 |
| C | -2.463008000 | -2.592798000 | -1.584853000 |
| C | -3.298188000 | -2.276606000 | -3.789026000 |
| H | -3.372827000 | -0.211330000 | -3.114611000 |
| H | -1.899396000 | -0.598634000 | -4.045928000 |
| C | -3.664861000 | -2.925906000 | -2.454197000 |
| H | -1.663614000 | -3.335485000 | -1.679641000 |
| H | -2.705838000 | -2.454842000 | -0.531199000 |
| H | -2.592494000 | -2.901935000 | -4.348485000 |
| H | -4.165055000 | -2.086153000 | -4.427810000 |
| H | -3.823731000 | -4.005309000 | -2.529024000 |
| H | -4.571089000 | -2.470390000 | -2.041744000 |
| H | 1.780039000 | 1.194912000 | -0.041204000 |
| H | 0.319164000 | 1.442496000 | 0.976619000 |
| C | 0.396164000 | 2.384460000 | -1.905432000 |
| C | 0.090990000 | 1.350045000 | -2.814931000 |
| H | 1.414890000 | 2.758464000 | -1.874679000 |
| H | -0.349497000 | 3.147963000 | -1.710159000 |
| H | -0.906766000 | 1.263752000 | -3.242414000 |
| C | 1.118388000 | 0.377857000 | -3.089758000 |
| C | 0.989778000 | -0.919833000 | -3.481493000 |
| H | 2.127877000 | 0.696972000 | -2.812735000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 1.866376000 | -1.549132000 | -3.593538000 |
| H | 0.045639000 | -1.342116000 | -3.812299000 |

117

theta1_thf_P2_trans_1,2 E = -2200.676618 a.u.

| | | | |
|----|---------------|--------------|--------------|
| N | 2.431630000 | 0.704774000 | 0.757573000 |
| P | 0.146632000 | 2.482899000 | 0.424373000 |
| P | 1.656243000 | -2.163104000 | 0.396371000 |
| Si | -8.210875000 | -0.355080000 | -0.615102000 |
| C | -6.898116000 | -1.600050000 | -0.026297000 |
| H | -7.417471000 | -2.461965000 | 0.418968000 |
| H | -6.331220000 | -1.142491000 | 0.798134000 |
| C | -9.292124000 | -1.134377000 | -1.953731000 |
| H | -8.710671000 | -1.418756000 | -2.839069000 |
| H | -10.069219000 | -0.434419000 | -2.284218000 |
| H | -9.798163000 | -2.035253000 | -1.585651000 |
| C | -9.278249000 | 0.125612000 | 0.867111000 |
| H | -9.782382000 | -0.748417000 | 1.296963000 |
| H | -10.055753000 | 0.844120000 | 0.580318000 |
| H | -8.679999000 | 0.587169000 | 1.662217000 |
| C | -7.358393000 | 1.185545000 | -1.307747000 |
| H | -6.710698000 | 1.658071000 | -0.558550000 |
| H | -8.096360000 | 1.933662000 | -1.622016000 |
| H | -6.741168000 | 0.950029000 | -2.183422000 |
| C | -0.837645000 | 3.941326000 | -0.130399000 |
| C | -0.606868000 | 4.482677000 | -1.404703000 |
| H | 0.182744000 | 4.078560000 | -2.032977000 |
| C | -1.374185000 | 5.547935000 | -1.868817000 |
| H | -1.179890000 | 5.963185000 | -2.854206000 |
| C | -2.390903000 | 6.077128000 | -1.072925000 |
| H | -2.993090000 | 6.904603000 | -1.437642000 |
| C | -2.628937000 | 5.541565000 | 0.190810000 |
| H | -3.416179000 | 5.951466000 | 0.817689000 |
| C | -1.856355000 | 4.480798000 | 0.664056000 |
| H | -2.048820000 | 4.079087000 | 1.654179000 |
| C | -0.333176000 | 2.218422000 | 2.182011000 |

| | | | |
|---|--------------|--------------|-------------|
| C | -1.388547000 | 1.336082000 | 2.451578000 |
| H | -1.896110000 | 0.824972000 | 1.635442000 |
| C | -1.805920000 | 1.121997000 | 3.764530000 |
| H | -2.631239000 | 0.444223000 | 3.965862000 |
| C | -1.164885000 | 1.778438000 | 4.815016000 |
| H | -1.487102000 | 1.609146000 | 5.838804000 |
| C | -0.112134000 | 2.654649000 | 4.551125000 |
| H | 0.385490000 | 3.169559000 | 5.368501000 |
| C | 0.303185000 | 2.878111000 | 3.239494000 |
| H | 1.119400000 | 3.566624000 | 3.039241000 |
| C | 1.903244000 | 3.058393000 | 0.455411000 |
| C | 2.868274000 | 2.036662000 | 0.661524000 |
| C | 4.228156000 | 2.408911000 | 0.685465000 |
| H | 4.978632000 | 1.640860000 | 0.854200000 |
| C | 4.610218000 | 3.734773000 | 0.517734000 |
| H | 5.665235000 | 3.995761000 | 0.551197000 |
| C | 3.652215000 | 4.731627000 | 0.307180000 |
| H | 3.954551000 | 5.767482000 | 0.183029000 |
| C | 2.304516000 | 4.389030000 | 0.272999000 |
| H | 1.553677000 | 5.159566000 | 0.122482000 |
| C | 2.831344000 | -0.082423000 | 1.834279000 |
| C | 3.471589000 | 0.438458000 | 2.980661000 |
| H | 3.675136000 | 1.502727000 | 3.038175000 |
| C | 3.822808000 | -0.377434000 | 4.047936000 |
| H | 4.309181000 | 0.068206000 | 4.912378000 |
| C | 3.545420000 | -1.746273000 | 4.034922000 |
| H | 3.817341000 | -2.378958000 | 4.874180000 |
| C | 2.894145000 | -2.279234000 | 2.929222000 |
| H | 2.639963000 | -3.336311000 | 2.909867000 |
| C | 2.545492000 | -1.474060000 | 1.836941000 |
| C | 0.515516000 | -3.419703000 | 1.122897000 |
| C | 0.545395000 | -4.770343000 | 0.760975000 |
| H | 1.271882000 | -5.130085000 | 0.038358000 |
| C | -0.349259000 | -5.669661000 | 1.343039000 |
| H | -0.314404000 | -6.718398000 | 1.060655000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.273070000 | -5.229143000 | 2.288153000 |
| H | -1.964360000 | -5.932582000 | 2.743975000 |
| C | -1.304462000 | -3.881830000 | 2.652860000 |
| H | -2.019770000 | -3.534175000 | 3.393196000 |
| C | -0.419119000 | -2.978590000 | 2.071561000 |
| H | -0.439073000 | -1.934592000 | 2.376434000 |
| C | 2.897985000 | -3.130861000 | -0.576446000 |
| C | 4.200865000 | -3.359460000 | -0.117047000 |
| H | 4.500978000 | -2.996682000 | 0.861749000 |
| C | 5.112169000 | -4.053678000 | -0.913289000 |
| H | 6.119415000 | -4.231384000 | -0.545706000 |
| C | 4.733662000 | -4.527369000 | -2.169779000 |
| H | 5.445448000 | -5.072678000 | -2.783524000 |
| C | 3.436343000 | -4.305692000 | -2.634335000 |
| H | 3.132526000 | -4.679763000 | -3.608487000 |
| C | 2.525378000 | -3.603736000 | -1.845808000 |
| H | 1.514364000 | -3.439390000 | -2.213269000 |
| C | -2.733427000 | -1.801931000 | -0.927333000 |
| C | -3.583274000 | -2.945700000 | -0.452244000 |
| H | -3.027817000 | -3.761303000 | 0.013212000 |
| C | -4.913415000 | -3.071441000 | -0.544237000 |
| C | -5.911460000 | -2.097754000 | -1.102334000 |
| H | -6.476875000 | -2.593846000 | -1.904674000 |
| H | -5.406300000 | -1.244133000 | -1.569048000 |
| Y | 1.158702000 | 0.259549000 | -1.099141000 |
| H | -5.354880000 | -3.983907000 | -0.138224000 |
| O | 3.036874000 | 0.495044000 | -2.516713000 |
| C | 3.228450000 | 1.585200000 | -3.471837000 |
| C | 4.317969000 | -0.168924000 | -2.260893000 |
| C | 4.730783000 | 1.803158000 | -3.522119000 |
| H | 2.824784000 | 1.258747000 | -4.436124000 |
| H | 2.661315000 | 2.447452000 | -3.114719000 |
| C | 5.267489000 | 0.385952000 | -3.311086000 |
| H | 4.622542000 | 0.092136000 | -1.242961000 |
| H | 4.153334000 | -1.245653000 | -2.331454000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 5.048036000 | 2.462954000 | -2.707372000 |
| H | 5.046391000 | 2.246661000 | -4.470487000 |
| H | 6.306401000 | 0.365574000 | -2.970843000 |
| H | 5.200055000 | -0.194779000 | -4.237874000 |
| H | -3.355220000 | -1.035350000 | -1.401674000 |
| H | -2.248247000 | -1.322291000 | -0.059959000 |
| C | -1.636337000 | -2.265997000 | -1.895067000 |
| C | -0.689704000 | -1.187452000 | -2.374523000 |
| H | -2.121293000 | -2.731422000 | -2.767456000 |
| H | -1.066526000 | -3.071906000 | -1.413731000 |
| H | 0.128470000 | -1.555692000 | -3.012939000 |
| C | -1.030110000 | 0.150038000 | -2.540203000 |
| C | -0.165803000 | 1.146493000 | -3.047675000 |
| H | -1.937788000 | 0.499125000 | -2.043524000 |
| H | -0.556239000 | 2.153232000 | -3.163328000 |
| H | 0.539968000 | 0.844476000 | -3.828529000 |

104

theta3_C2_cis_1,4 E = -1968.317881 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.736906000 | -1.852656000 | 0.584022000 |
| P | -2.693180000 | 0.409884000 | 0.176275000 |
| P | 2.096489000 | -1.213158000 | 0.185526000 |
| Si | 2.954158000 | 4.654095000 | -0.570898000 |
| C | 1.412983000 | 3.918976000 | -1.417025000 |
| H | 1.612484000 | 3.855606000 | -2.496267000 |
| H | 0.593254000 | 4.644665000 | -1.310991000 |
| C | 4.441608000 | 3.518120000 | -0.835124000 |
| H | 4.298698000 | 2.519190000 | -0.405256000 |
| H | 5.341078000 | 3.943163000 | -0.373241000 |
| H | 4.654616000 | 3.389689000 | -1.903621000 |
| C | 3.296674000 | 6.332615000 | -1.359449000 |
| H | 3.498951000 | 6.238626000 | -2.433136000 |
| H | 4.169832000 | 6.812937000 | -0.901503000 |
| H | 2.446343000 | 7.014787000 | -1.240842000 |
| C | 2.626958000 | 4.876192000 | 1.277747000 |
| H | 1.785509000 | 5.558134000 | 1.450600000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.502986000 | 5.303317000 | 1.780822000 |
| H | 2.391017000 | 3.927811000 | 1.775427000 |
| C | -2.829833000 | 2.085287000 | 0.947642000 |
| C | -1.796015000 | 2.477454000 | 1.812182000 |
| H | -0.979670000 | 1.793602000 | 2.036002000 |
| C | -1.824856000 | 3.728849000 | 2.420777000 |
| H | -1.024448000 | 4.017020000 | 3.096909000 |
| C | -2.881281000 | 4.606094000 | 2.169647000 |
| H | -2.903714000 | 5.582658000 | 2.645348000 |
| C | -3.912245000 | 4.219789000 | 1.316916000 |
| H | -4.745432000 | 4.891444000 | 1.128214000 |
| C | -3.891106000 | 2.963676000 | 0.707780000 |
| H | -4.713357000 | 2.671079000 | 0.062109000 |
| C | -4.293968000 | 0.127864000 | -0.700524000 |
| C | -4.594823000 | 0.902757000 | -1.833126000 |
| H | -3.916352000 | 1.691393000 | -2.152703000 |
| C | -5.767464000 | 0.676653000 | -2.551280000 |
| H | -5.997177000 | 1.291989000 | -3.417213000 |
| C | -6.642619000 | -0.338318000 | -2.159515000 |
| H | -7.555125000 | -0.516690000 | -2.721544000 |
| C | -6.343099000 | -1.118691000 | -1.044392000 |
| H | -7.022457000 | -1.907686000 | -0.733088000 |
| C | -5.176239000 | -0.887446000 | -0.314444000 |
| H | -4.956295000 | -1.493501000 | 0.559438000 |
| C | -2.652446000 | -0.718438000 | 1.609178000 |
| C | -1.647436000 | -1.719940000 | 1.639722000 |
| C | -1.587001000 | -2.513052000 | 2.808965000 |
| H | -0.816430000 | -3.271022000 | 2.897538000 |
| C | -2.478311000 | -2.336216000 | 3.858311000 |
| H | -2.387768000 | -2.970364000 | 4.736924000 |
| C | -3.468110000 | -1.352032000 | 3.809006000 |
| H | -4.160744000 | -1.213712000 | 4.633397000 |
| C | -3.532865000 | -0.539654000 | 2.685105000 |
| H | -4.273809000 | 0.254821000 | 2.634771000 |
| C | 0.037738000 | -3.028895000 | 0.533335000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.526602000 | -4.318695000 | 0.588323000 |
| H | -1.595895000 | -4.417467000 | 0.755918000 |
| C | 0.259445000 | -5.453513000 | 0.416728000 |
| H | -0.205437000 | -6.435383000 | 0.456648000 |
| C | 1.632264000 | -5.340564000 | 0.180574000 |
| H | 2.242827000 | -6.228036000 | 0.042781000 |
| C | 2.212891000 | -4.076469000 | 0.128777000 |
| H | 3.279961000 | -3.978129000 | -0.050859000 |
| C | 1.434349000 | -2.927841000 | 0.316176000 |
| C | 3.814066000 | -1.399403000 | -0.455398000 |
| C | 4.890752000 | -1.693048000 | 0.392898000 |
| H | 4.728441000 | -1.800709000 | 1.461823000 |
| C | 6.173594000 | -1.840568000 | -0.131360000 |
| H | 7.003089000 | -2.067077000 | 0.532996000 |
| C | 6.394102000 | -1.695201000 | -1.501151000 |
| H | 7.396465000 | -1.807086000 | -1.905175000 |
| C | 5.328953000 | -1.396853000 | -2.350119000 |
| H | 5.498804000 | -1.272110000 | -3.416248000 |
| C | 4.045383000 | -1.244309000 | -1.828773000 |
| H | 3.221242000 | -0.996474000 | -2.493658000 |
| C | 2.315299000 | -0.642788000 | 1.927460000 |
| C | 2.117832000 | -1.493496000 | 3.020193000 |
| H | 1.825795000 | -2.526706000 | 2.858553000 |
| C | 2.303308000 | -1.018765000 | 4.318601000 |
| H | 2.149742000 | -1.686825000 | 5.161760000 |
| C | 2.689334000 | 0.302823000 | 4.534675000 |
| H | 2.836430000 | 0.668708000 | 5.547131000 |
| C | 2.892833000 | 1.154108000 | 3.447934000 |
| H | 3.204277000 | 2.182368000 | 3.610563000 |
| C | 2.701924000 | 0.686455000 | 2.149816000 |
| H | 2.871572000 | 1.354829000 | 1.309378000 |
| C | 0.539114000 | -2.421252000 | -3.565815000 |
| C | -0.364503000 | -2.884380000 | -2.666566000 |
| H | -0.039209000 | -3.610876000 | -1.927476000 |
| C | -1.769086000 | -2.480715000 | -2.602555000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.322131000 | -1.453575000 | -3.290925000 |
| H | -3.366174000 | -1.191646000 | -3.156989000 |
| H | -1.771587000 | -0.902003000 | -4.050490000 |
| Y | -0.340407000 | -0.463329000 | -1.249037000 |
| H | -2.387993000 | -3.022255000 | -1.889434000 |
| H | 1.572943000 | -2.751815000 | -3.524829000 |
| H | 0.256939000 | -1.819342000 | -4.420834000 |
| C | 0.912687000 | 2.540037000 | -0.926242000 |
| C | -0.322116000 | 2.115164000 | -1.700510000 |
| H | 1.729624000 | 1.808886000 | -1.028868000 |
| H | 0.677092000 | 2.598381000 | 0.144213000 |
| H | -1.212020000 | 2.700328000 | -1.476489000 |
| C | -0.264558000 | 1.517818000 | -2.961679000 |
| C | 0.747247000 | 0.662885000 | -3.429776000 |
| H | -1.183582000 | 1.548242000 | -3.553472000 |
| H | 0.691627000 | 0.309056000 | -4.453839000 |
| H | 1.763620000 | 0.767405000 | -3.047678000 |

104

theta3_TS2_cis_1,4 E = -1968.309717 a.u. Imaginary frequency=185i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.671646000 | -1.869734000 | 0.595255000 |
| P | -2.743754000 | 0.293713000 | 0.131932000 |
| P | 2.153305000 | -1.199942000 | 0.155048000 |
| Si | 2.744431000 | 4.793215000 | -0.459962000 |
| C | 1.231447000 | 4.001400000 | -1.312588000 |
| H | 1.389872000 | 4.054386000 | -2.399072000 |
| H | 0.357922000 | 4.637345000 | -1.108004000 |
| C | 4.285460000 | 3.756131000 | -0.807081000 |
| H | 4.210653000 | 2.735362000 | -0.412465000 |
| H | 5.171629000 | 4.214167000 | -0.351197000 |
| H | 4.477114000 | 3.680525000 | -1.884601000 |
| C | 2.960919000 | 6.521039000 | -1.180646000 |
| H | 3.147272000 | 6.488915000 | -2.260735000 |
| H | 3.810060000 | 7.036615000 | -0.716011000 |
| H | 2.070791000 | 7.139875000 | -1.015550000 |
| C | 2.438602000 | 4.912296000 | 1.400371000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.581035000 | 5.560513000 | 1.617646000 |
| H | 3.309477000 | 5.339715000 | 1.912154000 |
| H | 2.236045000 | 3.934561000 | 1.853700000 |
| C | -2.840919000 | 1.985392000 | 0.885563000 |
| C | -1.823197000 | 2.349662000 | 1.781400000 |
| H | -1.050620000 | 1.632656000 | 2.052203000 |
| C | -1.817229000 | 3.613574000 | 2.365053000 |
| H | -1.031888000 | 3.877624000 | 3.068226000 |
| C | -2.822479000 | 4.532217000 | 2.058120000 |
| H | -2.820129000 | 5.517162000 | 2.516866000 |
| C | -3.836690000 | 4.175186000 | 1.172967000 |
| H | -4.631898000 | 4.878806000 | 0.941412000 |
| C | -3.849431000 | 2.907497000 | 0.587719000 |
| H | -4.660670000 | 2.638305000 | -0.081644000 |
| C | -4.390616000 | 0.017815000 | -0.654998000 |
| C | -4.702107000 | 0.735667000 | -1.820846000 |
| H | -3.999453000 | 1.466637000 | -2.216770000 |
| C | -5.910943000 | 0.523885000 | -2.479787000 |
| H | -6.145594000 | 1.093878000 | -3.374874000 |
| C | -6.814183000 | -0.422688000 | -1.993832000 |
| H | -7.754799000 | -0.592703000 | -2.510225000 |
| C | -6.503817000 | -1.150402000 | -0.846652000 |
| H | -7.202222000 | -1.890427000 | -0.465187000 |
| C | -5.299201000 | -0.932351000 | -0.176304000 |
| H | -5.068303000 | -1.504334000 | 0.717149000 |
| C | -2.632538000 | -0.794992000 | 1.594535000 |
| C | -1.590832000 | -1.757631000 | 1.642407000 |
| C | -1.501459000 | -2.533448000 | 2.821453000 |
| H | -0.708249000 | -3.267669000 | 2.913319000 |
| C | -2.391484000 | -2.367675000 | 3.872871000 |
| H | -2.278775000 | -2.985969000 | 4.760177000 |
| C | -3.407707000 | -1.410601000 | 3.815307000 |
| H | -4.097000000 | -1.277049000 | 4.643315000 |
| C | -3.506907000 | -0.621763000 | 2.677500000 |
| H | -4.272985000 | 0.148140000 | 2.620604000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.114944000 | -3.037413000 | 0.522041000 |
| C | -0.436080000 | -4.332864000 | 0.569678000 |
| H | -1.504467000 | -4.442431000 | 0.737120000 |
| C | 0.363608000 | -5.458879000 | 0.406756000 |
| H | -0.090573000 | -6.445765000 | 0.445466000 |
| C | 1.736898000 | -5.331137000 | 0.183389000 |
| H | 2.358943000 | -6.212068000 | 0.055178000 |
| C | 2.303688000 | -4.060975000 | 0.129724000 |
| H | 3.370726000 | -3.951607000 | -0.043275000 |
| C | 1.510779000 | -2.920641000 | 0.307988000 |
| C | 3.871154000 | -1.385496000 | -0.488906000 |
| C | 4.965690000 | -1.591209000 | 0.361937000 |
| H | 4.819611000 | -1.630454000 | 1.437716000 |
| C | 6.245840000 | -1.741728000 | -0.168812000 |
| H | 7.088783000 | -1.899697000 | 0.498442000 |
| C | 6.446218000 | -1.689433000 | -1.548034000 |
| H | 7.446040000 | -1.804781000 | -1.957279000 |
| C | 5.362565000 | -1.482572000 | -2.401094000 |
| H | 5.515077000 | -1.435325000 | -3.476056000 |
| C | 4.082924000 | -1.325748000 | -1.872676000 |
| H | 3.243097000 | -1.155452000 | -2.542322000 |
| C | 2.378895000 | -0.604426000 | 1.887822000 |
| C | 2.177067000 | -1.438782000 | 2.992183000 |
| H | 1.878436000 | -2.472091000 | 2.844251000 |
| C | 2.367413000 | -0.948401000 | 4.284084000 |
| H | 2.209627000 | -1.604221000 | 5.136017000 |
| C | 2.764672000 | 0.372567000 | 4.482428000 |
| H | 2.916789000 | 0.750433000 | 5.489730000 |
| C | 2.973537000 | 1.207646000 | 3.384143000 |
| H | 3.294696000 | 2.234978000 | 3.532903000 |
| C | 2.775658000 | 0.724620000 | 2.092661000 |
| H | 2.949410000 | 1.380601000 | 1.243163000 |
| C | 0.442103000 | -1.593839000 | -3.832318000 |
| C | -0.007210000 | -2.501281000 | -2.865935000 |
| H | 0.704495000 | -3.172036000 | -2.390600000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -1.404120000 | -2.644848000 | -2.541123000 |
| C | -2.370281000 | -1.726100000 | -2.838331000 |
| H | -3.394809000 | -1.866924000 | -2.515159000 |
| H | -2.200892000 | -0.910335000 | -3.543250000 |
| Y | -0.346680000 | -0.559744000 | -1.270636000 |
| H | -1.666218000 | -3.481168000 | -1.896233000 |
| H | 1.480337000 | -1.639850000 | -4.144639000 |
| H | -0.252537000 | -1.273617000 | -4.603049000 |
| C | 0.884636000 | 2.541571000 | -0.934263000 |
| C | -0.325961000 | 2.102519000 | -1.728659000 |
| H | 1.754599000 | 1.899240000 | -1.125650000 |
| H | 0.673976000 | 2.485773000 | 0.141270000 |
| H | -1.244641000 | 2.626383000 | -1.471242000 |
| C | -0.285596000 | 1.484758000 | -2.965112000 |
| C | 0.768579000 | 0.674282000 | -3.487917000 |
| H | -1.202577000 | 1.513929000 | -3.559179000 |
| H | 0.820467000 | 0.602399000 | -4.568466000 |
| H | 1.755215000 | 0.759200000 | -3.027606000 |

104

theta3_P2_cis_1,4 E = -1968.346385 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.189453000 | -1.761814000 | 0.495729000 |
| P | -2.749252000 | 0.766526000 | 0.179547000 |
| P | 1.749220000 | -1.647151000 | 0.195421000 |
| Si | 4.196110000 | 4.427317000 | 0.118209000 |
| C | 2.438308000 | 4.048803000 | -0.530305000 |
| H | 2.324080000 | 4.521787000 | -1.515890000 |
| H | 1.715936000 | 4.552012000 | 0.129097000 |
| C | 5.476338000 | 3.659951000 | -1.037259000 |
| H | 5.408456000 | 2.565380000 | -1.062437000 |
| H | 6.491964000 | 3.912075000 | -0.708990000 |
| H | 5.365518000 | 4.028184000 | -2.064423000 |
| C | 4.393588000 | 6.300609000 | 0.165904000 |
| H | 4.272835000 | 6.743835000 | -0.829752000 |
| H | 5.388883000 | 6.581177000 | 0.530944000 |
| H | 3.656431000 | 6.768350000 | 0.829484000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.387791000 | 3.704736000 | 1.852933000 |
| H | 3.613616000 | 4.077694000 | 2.534651000 |
| H | 5.359359000 | 3.979234000 | 2.281310000 |
| H | 4.338347000 | 2.608945000 | 1.848692000 |
| C | -2.740777000 | 2.397347000 | 1.050607000 |
| C | -1.725355000 | 2.620248000 | 1.994499000 |
| H | -1.011334000 | 1.831618000 | 2.226449000 |
| C | -1.649751000 | 3.834073000 | 2.672404000 |
| H | -0.869320000 | 3.990588000 | 3.412518000 |
| C | -2.579541000 | 4.841794000 | 2.410059000 |
| H | -2.520820000 | 5.788582000 | 2.939731000 |
| C | -3.588559000 | 4.625282000 | 1.474440000 |
| H | -4.322493000 | 5.401265000 | 1.274253000 |
| C | -3.673150000 | 3.408157000 | 0.796154000 |
| H | -4.474305000 | 3.247909000 | 0.080721000 |
| C | -4.282875000 | 0.743057000 | -0.845134000 |
| C | -4.325556000 | 1.548550000 | -1.994098000 |
| H | -3.488014000 | 2.200410000 | -2.238158000 |
| C | -5.445466000 | 1.537824000 | -2.822000000 |
| H | -5.473242000 | 2.174081000 | -3.702554000 |
| C | -6.525603000 | 0.706483000 | -2.522288000 |
| H | -7.396886000 | 0.692340000 | -3.171155000 |
| C | -6.483046000 | -0.105971000 | -1.390816000 |
| H | -7.321779000 | -0.755126000 | -1.154327000 |
| C | -5.368671000 | -0.089043000 | -0.551711000 |
| H | -5.345450000 | -0.723323000 | 0.329249000 |
| C | -2.967374000 | -0.460877000 | 1.520997000 |
| C | -2.160941000 | -1.626255000 | 1.483875000 |
| C | -2.344992000 | -2.576984000 | 2.507994000 |
| H | -1.732432000 | -3.473308000 | 2.514937000 |
| C | -3.276206000 | -2.371253000 | 3.517871000 |
| H | -3.386472000 | -3.122833000 | 4.295676000 |
| C | -4.051979000 | -1.209921000 | 3.558561000 |
| H | -4.770325000 | -1.049996000 | 4.356765000 |
| C | -3.884168000 | -0.257439000 | 2.559948000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.471377000 | 0.657639000 | 2.579649000 |
| C | -0.692769000 | -3.012430000 | 0.109402000 |
| C | -1.518519000 | -4.130394000 | -0.142549000 |
| H | -2.582051000 | -4.051709000 | 0.064583000 |
| C | -0.989409000 | -5.300758000 | -0.663125000 |
| H | -1.645715000 | -6.146618000 | -0.851029000 |
| C | 0.375483000 | -5.396106000 | -0.967077000 |
| H | 0.782084000 | -6.314206000 | -1.381071000 |
| C | 1.209574000 | -4.313808000 | -0.722371000 |
| H | 2.271474000 | -4.388488000 | -0.938400000 |
| C | 0.699256000 | -3.129425000 | -0.164343000 |
| C | 3.448582000 | -2.102999000 | -0.350345000 |
| C | 4.271942000 | -2.935761000 | 0.420546000 |
| H | 3.917534000 | -3.325531000 | 1.370837000 |
| C | 5.552169000 | -3.257736000 | -0.024394000 |
| H | 6.184823000 | -3.903507000 | 0.578454000 |
| C | 6.022511000 | -2.751071000 | -1.236567000 |
| H | 7.022462000 | -3.002776000 | -1.579093000 |
| C | 5.212682000 | -1.914548000 | -2.003308000 |
| H | 5.579431000 | -1.511290000 | -2.943485000 |
| C | 3.932546000 | -1.586724000 | -1.558998000 |
| H | 3.305904000 | -0.925386000 | -2.151820000 |
| C | 1.851406000 | -1.576481000 | 2.035389000 |
| C | 1.542751000 | -2.674918000 | 2.845779000 |
| H | 1.207886000 | -3.605218000 | 2.395366000 |
| C | 1.666281000 | -2.577484000 | 4.231337000 |
| H | 1.427322000 | -3.435309000 | 4.854261000 |
| C | 2.097719000 | -1.387684000 | 4.816358000 |
| H | 2.193710000 | -1.315907000 | 5.896231000 |
| C | 2.408058000 | -0.290215000 | 4.013274000 |
| H | 2.749334000 | 0.637729000 | 4.464205000 |
| C | 2.282398000 | -0.382951000 | 2.628807000 |
| H | 2.533379000 | 0.474406000 | 2.008347000 |
| C | 0.542738000 | 0.395419000 | -4.312745000 |
| C | 0.635569000 | -0.955281000 | -3.621337000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.600403000 | -1.453374000 | -3.699086000 |
| C | -0.464282000 | -1.777989000 | -3.387828000 |
| C | -1.780228000 | -1.354796000 | -3.093429000 |
| H | -2.550383000 | -2.105613000 | -2.937714000 |
| H | -2.153177000 | -0.413161000 | -3.509557000 |
| Y | -0.477201000 | -0.465364000 | -1.178237000 |
| H | -0.236827000 | -2.823121000 | -3.161380000 |
| H | 1.084771000 | 0.320041000 | -5.265796000 |
| H | -0.499643000 | 0.606380000 | -4.588588000 |
| C | 2.080024000 | 2.550712000 | -0.641192000 |
| C | 0.671526000 | 2.385051000 | -1.130573000 |
| H | 2.790081000 | 2.041188000 | -1.300887000 |
| H | 2.171562000 | 2.083496000 | 0.348540000 |
| H | -0.099588000 | 2.728015000 | -0.435006000 |
| C | 0.264299000 | 1.993007000 | -2.360023000 |
| C | 1.107635000 | 1.603693000 | -3.545081000 |
| H | -0.810089000 | 2.078901000 | -2.573061000 |
| H | 1.142011000 | 2.467944000 | -4.226210000 |
| H | 2.142351000 | 1.408458000 | -3.242846000 |

104

theta3_C2_cis_1,2 E = -1968.312843 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.736906000 | -1.852656000 | 0.584022000 |
| P | -2.693180000 | 0.409884000 | 0.176275000 |
| P | 2.096489000 | -1.213158000 | 0.185526000 |
| Si | 2.954158000 | 4.654095000 | -0.570898000 |
| C | 1.412983000 | 3.918976000 | -1.417025000 |
| H | 1.612484000 | 3.855606000 | -2.496267000 |
| H | 0.593254000 | 4.644665000 | -1.310991000 |
| C | 4.441608000 | 3.518120000 | -0.835124000 |
| H | 4.298698000 | 2.519190000 | -0.405256000 |
| H | 5.341078000 | 3.943163000 | -0.373241000 |
| H | 4.654616000 | 3.389689000 | -1.903621000 |
| C | 3.296674000 | 6.332615000 | -1.359449000 |
| H | 3.498951000 | 6.238626000 | -2.433136000 |
| H | 4.169832000 | 6.812937000 | -0.901503000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.446343000 | 7.014787000 | -1.240842000 |
| C | 2.626958000 | 4.876192000 | 1.277747000 |
| H | 1.785509000 | 5.558134000 | 1.450600000 |
| H | 3.502986000 | 5.303317000 | 1.780822000 |
| H | 2.391017000 | 3.927811000 | 1.775427000 |
| C | -2.829833000 | 2.085287000 | 0.947642000 |
| C | -1.796015000 | 2.477454000 | 1.812182000 |
| H | -0.979670000 | 1.793602000 | 2.036002000 |
| C | -1.824856000 | 3.728849000 | 2.420777000 |
| H | -1.024448000 | 4.017020000 | 3.096909000 |
| C | -2.881281000 | 4.606094000 | 2.169647000 |
| H | -2.903714000 | 5.582658000 | 2.645348000 |
| C | -3.912245000 | 4.219789000 | 1.316916000 |
| H | -4.745432000 | 4.891444000 | 1.128214000 |
| C | -3.891106000 | 2.963676000 | 0.707780000 |
| H | -4.713357000 | 2.671079000 | 0.062109000 |
| C | -4.293968000 | 0.127864000 | -0.700524000 |
| C | -4.594823000 | 0.902757000 | -1.833126000 |
| H | -3.916352000 | 1.691393000 | -2.152703000 |
| C | -5.767464000 | 0.676653000 | -2.551280000 |
| H | -5.997177000 | 1.291989000 | -3.417213000 |
| C | -6.642619000 | -0.338318000 | -2.159515000 |
| H | -7.555125000 | -0.516690000 | -2.721544000 |
| C | -6.343099000 | -1.118691000 | -1.044392000 |
| H | -7.022457000 | -1.907686000 | -0.733088000 |
| C | -5.176239000 | -0.887446000 | -0.314444000 |
| H | -4.956295000 | -1.493501000 | 0.559438000 |
| C | -2.652446000 | -0.718438000 | 1.609178000 |
| C | -1.647436000 | -1.719940000 | 1.639722000 |
| C | -1.587001000 | -2.513052000 | 2.808965000 |
| H | -0.816430000 | -3.271022000 | 2.897538000 |
| C | -2.478311000 | -2.336216000 | 3.858311000 |
| H | -2.387768000 | -2.970364000 | 4.736924000 |
| C | -3.468110000 | -1.352032000 | 3.809006000 |
| H | -4.160744000 | -1.213712000 | 4.633397000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -3.532865000 | -0.539654000 | 2.685105000 |
| H | -4.273809000 | 0.254821000 | 2.634771000 |
| C | 0.037738000 | -3.028895000 | 0.533335000 |
| C | -0.526602000 | -4.318695000 | 0.588323000 |
| H | -1.595895000 | -4.417467000 | 0.755918000 |
| C | 0.259445000 | -5.453513000 | 0.416728000 |
| H | -0.205437000 | -6.435383000 | 0.456648000 |
| C | 1.632264000 | -5.340564000 | 0.180574000 |
| H | 2.242827000 | -6.228036000 | 0.042781000 |
| C | 2.212891000 | -4.076469000 | 0.128777000 |
| H | 3.279961000 | -3.978129000 | -0.050859000 |
| C | 1.434349000 | -2.927841000 | 0.316176000 |
| C | 3.814066000 | -1.399403000 | -0.455398000 |
| C | 4.890752000 | -1.693048000 | 0.392898000 |
| H | 4.728441000 | -1.800709000 | 1.461823000 |
| C | 6.173594000 | -1.840568000 | -0.131360000 |
| H | 7.003089000 | -2.067077000 | 0.532996000 |
| C | 6.394102000 | -1.695201000 | -1.501151000 |
| H | 7.396465000 | -1.807086000 | -1.905175000 |
| C | 5.328953000 | -1.396853000 | -2.350119000 |
| H | 5.498804000 | -1.272110000 | -3.416248000 |
| C | 4.045383000 | -1.244309000 | -1.828773000 |
| H | 3.221242000 | -0.996474000 | -2.493658000 |
| C | 2.315299000 | -0.642788000 | 1.927460000 |
| C | 2.117832000 | -1.493496000 | 3.020193000 |
| H | 1.825795000 | -2.526706000 | 2.858553000 |
| C | 2.303308000 | -1.018765000 | 4.318601000 |
| H | 2.149742000 | -1.686825000 | 5.161760000 |
| C | 2.689334000 | 0.302823000 | 4.534675000 |
| H | 2.836430000 | 0.668708000 | 5.547131000 |
| C | 2.892833000 | 1.154108000 | 3.447934000 |
| H | 3.204277000 | 2.182368000 | 3.610563000 |
| C | 2.701924000 | 0.686455000 | 2.149816000 |
| H | 2.871572000 | 1.354829000 | 1.309378000 |
| C | 0.539114000 | -2.421252000 | -3.565815000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.364503000 | -2.884380000 | -2.666566000 |
| H | -0.039209000 | -3.610876000 | -1.927476000 |
| C | -1.769086000 | -2.480715000 | -2.602555000 |
| C | -2.322131000 | -1.453575000 | -3.290925000 |
| H | -3.366174000 | -1.191646000 | -3.156989000 |
| H | -1.771587000 | -0.902003000 | -4.050490000 |
| Y | -0.340407000 | -0.463329000 | -1.249037000 |
| H | -2.387993000 | -3.022255000 | -1.889434000 |
| H | 1.572943000 | -2.751815000 | -3.524829000 |
| H | 0.256939000 | -1.819342000 | -4.420834000 |
| C | 0.912687000 | 2.540037000 | -0.926242000 |
| C | -0.322116000 | 2.115164000 | -1.700510000 |
| H | 1.729624000 | 1.808886000 | -1.028868000 |
| H | 0.677092000 | 2.598381000 | 0.144213000 |
| H | -1.212020000 | 2.700328000 | -1.476489000 |
| C | -0.264558000 | 1.517818000 | -2.961679000 |
| C | 0.747247000 | 0.662885000 | -3.429776000 |
| H | -1.183582000 | 1.548242000 | -3.553472000 |
| H | 0.691627000 | 0.309056000 | -4.453839000 |
| H | 1.763620000 | 0.767405000 | -3.047678000 |

104

theta3_TS2_cis_1,2 E = -1968.304219 a.u. Imaginary frequency=241i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.671646000 | -1.869734000 | 0.595255000 |
| P | -2.743754000 | 0.293713000 | 0.131932000 |
| P | 2.153305000 | -1.199942000 | 0.155048000 |
| Si | 2.744431000 | 4.793215000 | -0.459962000 |
| C | 1.231447000 | 4.001400000 | -1.312588000 |
| H | 1.389872000 | 4.054386000 | -2.399072000 |
| H | 0.357922000 | 4.637345000 | -1.108004000 |
| C | 4.285460000 | 3.756131000 | -0.807081000 |
| H | 4.210653000 | 2.735362000 | -0.412465000 |
| H | 5.171629000 | 4.214167000 | -0.351197000 |
| H | 4.477114000 | 3.680525000 | -1.884601000 |
| C | 2.960919000 | 6.521039000 | -1.180646000 |
| H | 3.147272000 | 6.488915000 | -2.260735000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.810060000 | 7.036615000 | -0.716011000 |
| H | 2.070791000 | 7.139875000 | -1.015550000 |
| C | 2.438602000 | 4.912296000 | 1.400371000 |
| H | 1.581035000 | 5.560513000 | 1.617646000 |
| H | 3.309477000 | 5.339715000 | 1.912154000 |
| H | 2.236045000 | 3.934561000 | 1.853700000 |
| C | -2.840919000 | 1.985392000 | 0.885563000 |
| C | -1.823197000 | 2.349662000 | 1.781400000 |
| H | -1.050620000 | 1.632656000 | 2.052203000 |
| C | -1.817229000 | 3.613574000 | 2.365053000 |
| H | -1.031888000 | 3.877624000 | 3.068226000 |
| C | -2.822479000 | 4.532217000 | 2.058120000 |
| H | -2.820129000 | 5.517162000 | 2.516866000 |
| C | -3.836690000 | 4.175186000 | 1.172967000 |
| H | -4.631898000 | 4.878806000 | 0.941412000 |
| C | -3.849431000 | 2.907497000 | 0.587719000 |
| H | -4.660670000 | 2.638305000 | -0.081644000 |
| C | -4.390616000 | 0.017815000 | -0.654998000 |
| C | -4.702107000 | 0.735667000 | -1.820846000 |
| H | -3.999453000 | 1.466637000 | -2.216770000 |
| C | -5.910943000 | 0.523885000 | -2.479787000 |
| H | -6.145594000 | 1.093878000 | -3.374874000 |
| C | -6.814183000 | -0.422688000 | -1.993832000 |
| H | -7.754799000 | -0.592703000 | -2.510225000 |
| C | -6.503817000 | -1.150402000 | -0.846652000 |
| H | -7.202222000 | -1.890427000 | -0.465187000 |
| C | -5.299201000 | -0.932351000 | -0.176304000 |
| H | -5.068303000 | -1.504334000 | 0.717149000 |
| C | -2.632538000 | -0.794992000 | 1.594535000 |
| C | -1.590832000 | -1.757631000 | 1.642407000 |
| C | -1.501459000 | -2.533448000 | 2.821453000 |
| H | -0.708249000 | -3.267669000 | 2.913319000 |
| C | -2.391484000 | -2.367675000 | 3.872871000 |
| H | -2.278775000 | -2.985969000 | 4.760177000 |
| C | -3.407707000 | -1.410601000 | 3.815307000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.097000000 | -1.277049000 | 4.643315000 |
| C | -3.506907000 | -0.621763000 | 2.677500000 |
| H | -4.272985000 | 0.148140000 | 2.620604000 |
| C | 0.114944000 | -3.037413000 | 0.522041000 |
| C | -0.436080000 | -4.332864000 | 0.569678000 |
| H | -1.504467000 | -4.442431000 | 0.737120000 |
| C | 0.363608000 | -5.458879000 | 0.406756000 |
| H | -0.090573000 | -6.445765000 | 0.445466000 |
| C | 1.736898000 | -5.331137000 | 0.183389000 |
| H | 2.358943000 | -6.212068000 | 0.055178000 |
| C | 2.303688000 | -4.060975000 | 0.129724000 |
| H | 3.370726000 | -3.951607000 | -0.043275000 |
| C | 1.510779000 | -2.920641000 | 0.307988000 |
| C | 3.871154000 | -1.385496000 | -0.488906000 |
| C | 4.965690000 | -1.591209000 | 0.361937000 |
| H | 4.819611000 | -1.630454000 | 1.437716000 |
| C | 6.245840000 | -1.741728000 | -0.168812000 |
| H | 7.088783000 | -1.899697000 | 0.498442000 |
| C | 6.446218000 | -1.689433000 | -1.548034000 |
| H | 7.446040000 | -1.804781000 | -1.957279000 |
| C | 5.362565000 | -1.482572000 | -2.401094000 |
| H | 5.515077000 | -1.435325000 | -3.476056000 |
| C | 4.082924000 | -1.325748000 | -1.872676000 |
| H | 3.243097000 | -1.155452000 | -2.542322000 |
| C | 2.378895000 | -0.604426000 | 1.887822000 |
| C | 2.177067000 | -1.438782000 | 2.992183000 |
| H | 1.878436000 | -2.472091000 | 2.844251000 |
| C | 2.367413000 | -0.948401000 | 4.284084000 |
| H | 2.209627000 | -1.604221000 | 5.136017000 |
| C | 2.764672000 | 0.372567000 | 4.482428000 |
| H | 2.916789000 | 0.750433000 | 5.489730000 |
| C | 2.973537000 | 1.207646000 | 3.384143000 |
| H | 3.294696000 | 2.234978000 | 3.532903000 |
| C | 2.775658000 | 0.724620000 | 2.092661000 |
| H | 2.949410000 | 1.380601000 | 1.243163000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.442103000 | -1.593839000 | -3.832318000 |
| C | -0.007210000 | -2.501281000 | -2.865935000 |
| H | 0.704495000 | -3.172036000 | -2.390600000 |
| C | -1.404120000 | -2.644848000 | -2.541123000 |
| C | -2.370281000 | -1.726100000 | -2.838331000 |
| H | -3.394809000 | -1.866924000 | -2.515159000 |
| H | -2.200892000 | -0.910335000 | -3.543250000 |
| Y | -0.346680000 | -0.559744000 | -1.270636000 |
| H | -1.666218000 | -3.481168000 | -1.896233000 |
| H | 1.480337000 | -1.639850000 | -4.144639000 |
| H | -0.252537000 | -1.273617000 | -4.603049000 |
| C | 0.884636000 | 2.541571000 | -0.934263000 |
| C | -0.325961000 | 2.102519000 | -1.728659000 |
| H | 1.754599000 | 1.899240000 | -1.125650000 |
| H | 0.673976000 | 2.485773000 | 0.141270000 |
| H | -1.244641000 | 2.626383000 | -1.471242000 |
| C | -0.285596000 | 1.484758000 | -2.965112000 |
| C | 0.768579000 | 0.674282000 | -3.487917000 |
| H | -1.202577000 | 1.513929000 | -3.559179000 |
| H | 0.820467000 | 0.602399000 | -4.568466000 |
| H | 1.755215000 | 0.759200000 | -3.027606000 |

104

theta3_P2_cis_1,2 E = -1968.334975 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.189453000 | -1.761814000 | 0.495729000 |
| P | -2.749252000 | 0.766526000 | 0.179547000 |
| P | 1.749220000 | -1.647151000 | 0.195421000 |
| Si | 4.196110000 | 4.427317000 | 0.118209000 |
| C | 2.438308000 | 4.048803000 | -0.530305000 |
| H | 2.324080000 | 4.521787000 | -1.515890000 |
| H | 1.715936000 | 4.552012000 | 0.129097000 |
| C | 5.476338000 | 3.659951000 | -1.037259000 |
| H | 5.408456000 | 2.565380000 | -1.062437000 |
| H | 6.491964000 | 3.912075000 | -0.708990000 |
| H | 5.365518000 | 4.028184000 | -2.064423000 |
| C | 4.393588000 | 6.300609000 | 0.165904000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.272835000 | 6.743835000 | -0.829752000 |
| H | 5.388883000 | 6.581177000 | 0.530944000 |
| H | 3.656431000 | 6.768350000 | 0.829484000 |
| C | 4.387791000 | 3.704736000 | 1.852933000 |
| H | 3.613616000 | 4.077694000 | 2.534651000 |
| H | 5.359359000 | 3.979234000 | 2.281310000 |
| H | 4.338347000 | 2.608945000 | 1.848692000 |
| C | -2.740777000 | 2.397347000 | 1.050607000 |
| C | -1.725355000 | 2.620248000 | 1.994499000 |
| H | -1.011334000 | 1.831618000 | 2.226449000 |
| C | -1.649751000 | 3.834073000 | 2.672404000 |
| H | -0.869320000 | 3.990588000 | 3.412518000 |
| C | -2.579541000 | 4.841794000 | 2.410059000 |
| H | -2.520820000 | 5.788582000 | 2.939731000 |
| C | -3.588559000 | 4.625282000 | 1.474440000 |
| H | -4.322493000 | 5.401265000 | 1.274253000 |
| C | -3.673150000 | 3.408157000 | 0.796154000 |
| H | -4.474305000 | 3.247909000 | 0.080721000 |
| C | -4.282875000 | 0.743057000 | -0.845134000 |
| C | -4.325556000 | 1.548550000 | -1.994098000 |
| H | -3.488014000 | 2.200410000 | -2.238158000 |
| C | -5.445466000 | 1.537824000 | -2.822000000 |
| H | -5.473242000 | 2.174081000 | -3.702554000 |
| C | -6.525603000 | 0.706483000 | -2.522288000 |
| H | -7.396886000 | 0.692340000 | -3.171155000 |
| C | -6.483046000 | -0.105971000 | -1.390816000 |
| H | -7.321779000 | -0.755126000 | -1.154327000 |
| C | -5.368671000 | -0.089043000 | -0.551711000 |
| H | -5.345450000 | -0.723323000 | 0.329249000 |
| C | -2.967374000 | -0.460877000 | 1.520997000 |
| C | -2.160941000 | -1.626255000 | 1.483875000 |
| C | -2.344992000 | -2.576984000 | 2.507994000 |
| H | -1.732432000 | -3.473308000 | 2.514937000 |
| C | -3.276206000 | -2.371253000 | 3.517871000 |
| H | -3.386472000 | -3.122833000 | 4.295676000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.051979000 | -1.209921000 | 3.558561000 |
| H | -4.770325000 | -1.049996000 | 4.356765000 |
| C | -3.884168000 | -0.257439000 | 2.559948000 |
| H | -4.471377000 | 0.657639000 | 2.579649000 |
| C | -0.692769000 | -3.012430000 | 0.109402000 |
| C | -1.518519000 | -4.130394000 | -0.142549000 |
| H | -2.582051000 | -4.051709000 | 0.064583000 |
| C | -0.989409000 | -5.300758000 | -0.663125000 |
| H | -1.645715000 | -6.146618000 | -0.851029000 |
| C | 0.375483000 | -5.396106000 | -0.967077000 |
| H | 0.782084000 | -6.314206000 | -1.381071000 |
| C | 1.209574000 | -4.313808000 | -0.722371000 |
| H | 2.271474000 | -4.388488000 | -0.938400000 |
| C | 0.699256000 | -3.129425000 | -0.164343000 |
| C | 3.448582000 | -2.102999000 | -0.350345000 |
| C | 4.271942000 | -2.935761000 | 0.420546000 |
| H | 3.917534000 | -3.325531000 | 1.370837000 |
| C | 5.552169000 | -3.257736000 | -0.024394000 |
| H | 6.184823000 | -3.903507000 | 0.578454000 |
| C | 6.022511000 | -2.751071000 | -1.236567000 |
| H | 7.022462000 | -3.002776000 | -1.579093000 |
| C | 5.212682000 | -1.914548000 | -2.003308000 |
| H | 5.579431000 | -1.511290000 | -2.943485000 |
| C | 3.932546000 | -1.586724000 | -1.558998000 |
| H | 3.305904000 | -0.925386000 | -2.151820000 |
| C | 1.851406000 | -1.576481000 | 2.035389000 |
| C | 1.542751000 | -2.674918000 | 2.845779000 |
| H | 1.207886000 | -3.605218000 | 2.395366000 |
| C | 1.666281000 | -2.577484000 | 4.231337000 |
| H | 1.427322000 | -3.435309000 | 4.854261000 |
| C | 2.097719000 | -1.387684000 | 4.816358000 |
| H | 2.193710000 | -1.315907000 | 5.896231000 |
| C | 2.408058000 | -0.290215000 | 4.013274000 |
| H | 2.749334000 | 0.637729000 | 4.464205000 |
| C | 2.282398000 | -0.382951000 | 2.628807000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.533379000 | 0.474406000 | 2.008347000 |
| C | 0.542738000 | 0.395419000 | -4.312745000 |
| C | 0.635569000 | -0.955281000 | -3.621337000 |
| H | 1.600403000 | -1.453374000 | -3.699086000 |
| C | -0.464282000 | -1.777989000 | -3.387828000 |
| C | -1.780228000 | -1.354796000 | -3.093429000 |
| H | -2.550383000 | -2.105613000 | -2.937714000 |
| H | -2.153177000 | -0.413161000 | -3.509557000 |
| Y | -0.477201000 | -0.465364000 | -1.178237000 |
| H | -0.236827000 | -2.823121000 | -3.161380000 |
| H | 1.084771000 | 0.320041000 | -5.265796000 |
| H | -0.499643000 | 0.606380000 | -4.588588000 |
| C | 2.080024000 | 2.550712000 | -0.641192000 |
| C | 0.671526000 | 2.385051000 | -1.130573000 |
| H | 2.790081000 | 2.041188000 | -1.300887000 |
| H | 2.171562000 | 2.083496000 | 0.348540000 |
| H | -0.099588000 | 2.728015000 | -0.435006000 |
| C | 0.264299000 | 1.993007000 | -2.360023000 |
| C | 1.107635000 | 1.603693000 | -3.545081000 |
| H | -0.810089000 | 2.078901000 | -2.573061000 |
| H | 1.142011000 | 2.467944000 | -4.226210000 |
| H | 2.142351000 | 1.408458000 | -3.242846000 |

104

theta3_C2_trans_1,4 E = -1968.326074 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.049410000 | -1.547282000 | -0.680684000 |
| P | -2.837129000 | 0.601404000 | 0.267351000 |
| P | 1.757851000 | -1.512506000 | 0.164996000 |
| Si | 4.659535000 | 3.844223000 | 0.456510000 |
| C | 2.834655000 | 3.566829000 | 0.926295000 |
| H | 2.227464000 | 4.321603000 | 0.406822000 |
| H | 2.727811000 | 3.799146000 | 1.996241000 |
| C | 4.901118000 | 3.521123000 | -1.394942000 |
| H | 4.671457000 | 2.482375000 | -1.664536000 |
| H | 5.940261000 | 3.709545000 | -1.690659000 |
| H | 4.266952000 | 4.177502000 | -2.004271000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 5.079487000 | 5.641549000 | 0.840491000 |
| H | 4.446347000 | 6.333764000 | 0.272554000 |
| H | 6.122878000 | 5.867730000 | 0.589935000 |
| H | 4.941399000 | 5.864539000 | 1.905235000 |
| C | 5.776384000 | 2.691011000 | 1.449535000 |
| H | 5.641679000 | 2.837736000 | 2.528124000 |
| H | 6.832428000 | 2.884823000 | 1.224820000 |
| H | 5.584569000 | 1.633871000 | 1.230501000 |
| C | -3.279570000 | 1.286914000 | 1.925331000 |
| C | -2.467888000 | 0.919395000 | 3.010164000 |
| H | -1.630017000 | 0.240922000 | 2.861785000 |
| C | -2.743613000 | 1.397261000 | 4.287972000 |
| H | -2.114023000 | 1.099917000 | 5.122457000 |
| C | -3.825096000 | 2.254646000 | 4.497379000 |
| H | -4.037039000 | 2.630712000 | 5.494419000 |
| C | -4.634154000 | 2.621975000 | 3.424879000 |
| H | -5.483166000 | 3.281717000 | 3.582446000 |
| C | -4.366547000 | 2.140450000 | 2.142286000 |
| H | -5.012870000 | 2.427033000 | 1.318136000 |
| C | -4.084649000 | 1.300425000 | -0.903939000 |
| C | -4.063982000 | 2.678671000 | -1.172695000 |
| H | -3.367526000 | 3.327091000 | -0.646775000 |
| C | -4.946869000 | 3.231634000 | -2.097863000 |
| H | -4.930083000 | 4.301890000 | -2.286333000 |
| C | -5.850680000 | 2.413382000 | -2.778086000 |
| H | -6.537573000 | 2.844295000 | -3.501278000 |
| C | -5.873177000 | 1.043744000 | -2.520124000 |
| H | -6.580378000 | 0.402773000 | -3.039881000 |
| C | -4.997311000 | 0.487247000 | -1.586710000 |
| H | -5.029465000 | -0.579595000 | -1.386226000 |
| C | -3.199714000 | -1.180429000 | 0.397622000 |
| C | -2.230460000 | -2.060866000 | -0.140886000 |
| C | -2.495700000 | -3.443568000 | -0.042631000 |
| H | -1.771711000 | -4.154699000 | -0.427224000 |
| C | -3.656926000 | -3.912633000 | 0.558810000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -3.820273000 | -4.985790000 | 0.621717000 |
| C | -4.600543000 | -3.033800000 | 1.095738000 |
| H | -5.500807000 | -3.407518000 | 1.573738000 |
| C | -4.357453000 | -1.667598000 | 1.015037000 |
| H | -5.070214000 | -0.963507000 | 1.437937000 |
| C | -0.274020000 | -2.372691000 | -1.512943000 |
| C | -0.804631000 | -3.044875000 | -2.634581000 |
| H | -1.875856000 | -2.998913000 | -2.814607000 |
| C | 0.018105000 | -3.763649000 | -3.493785000 |
| H | -0.416641000 | -4.271507000 | -4.351008000 |
| C | 1.396628000 | -3.832890000 | -3.266655000 |
| H | 2.036576000 | -4.396943000 | -3.938931000 |
| C | 1.941574000 | -3.188681000 | -2.160050000 |
| H | 3.008605000 | -3.255436000 | -1.966643000 |
| C | 1.121140000 | -2.476063000 | -1.274861000 |
| C | 3.587781000 | -1.735226000 | 0.090967000 |
| C | 4.219906000 | -2.830371000 | 0.695142000 |
| H | 3.636118000 | -3.559489000 | 1.249590000 |
| C | 5.601295000 | -2.986317000 | 0.592391000 |
| H | 6.082119000 | -3.837909000 | 1.065953000 |
| C | 6.363507000 | -2.055769000 | -0.113135000 |
| H | 7.440100000 | -2.180013000 | -0.190099000 |
| C | 5.742853000 | -0.959699000 | -0.711808000 |
| H | 6.333483000 | -0.225406000 | -1.252729000 |
| C | 4.362741000 | -0.796801000 | -0.603060000 |
| H | 3.888584000 | 0.072340000 | -1.051669000 |
| C | 1.235807000 | -2.429986000 | 1.672742000 |
| C | 0.860306000 | -3.777477000 | 1.642231000 |
| H | 0.846554000 | -4.317318000 | 0.699422000 |
| C | 0.506078000 | -4.428890000 | 2.823181000 |
| H | 0.215828000 | -5.475671000 | 2.794472000 |
| C | 0.526421000 | -3.742415000 | 4.036610000 |
| H | 0.251383000 | -4.253835000 | 4.954925000 |
| C | 0.900769000 | -2.398870000 | 4.071586000 |
| H | 0.921652000 | -1.862620000 | 5.016566000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.250386000 | -1.741813000 | 2.893534000 |
| H | 1.544149000 | -0.694768000 | 2.924437000 |
| C | 1.932937000 | 0.980271000 | -3.247562000 |
| C | 0.723987000 | 0.418501000 | -3.467282000 |
| H | 0.651665000 | -0.662773000 | -3.597400000 |
| C | -0.522542000 | 1.178345000 | -3.523218000 |
| C | -1.737700000 | 0.593244000 | -3.474653000 |
| H | -2.649663000 | 1.181346000 | -3.494863000 |
| H | -1.844953000 | -0.489088000 | -3.445763000 |
| Y | -0.084000000 | 0.545953000 | -0.729857000 |
| H | -0.446756000 | 2.262466000 | -3.584250000 |
| H | 2.833887000 | 0.375060000 | -3.221978000 |
| H | 2.057040000 | 2.057910000 | -3.158943000 |
| C | 2.220891000 | 2.170190000 | 0.682886000 |
| C | 0.775894000 | 2.085255000 | 1.147838000 |
| H | 2.318594000 | 1.934894000 | -0.399071000 |
| H | 2.813879000 | 1.402522000 | 1.193341000 |
| H | 0.631244000 | 1.863866000 | 2.203769000 |
| C | -0.232410000 | 2.824471000 | 0.512945000 |
| C | -0.244601000 | 3.147628000 | -0.849590000 |
| H | -1.164749000 | 2.946458000 | 1.065102000 |
| H | -1.095094000 | 3.674457000 | -1.271507000 |
| H | 0.699246000 | 3.321974000 | -1.370109000 |

104

theta3_TS2_trans_1,4 E = -1968.304891 a.u. Imaginary frequency=286i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.665691000 | -1.872039000 | 0.645446000 |
| P | -2.657494000 | 0.345448000 | 0.161574000 |
| P | 2.114281000 | -1.177632000 | 0.170196000 |
| Si | 2.694258000 | 4.740102000 | -0.506742000 |
| C | 1.285762000 | 3.919877000 | -1.500259000 |
| H | 1.594636000 | 3.887315000 | -2.554782000 |
| H | 0.410874000 | 4.585154000 | -1.464370000 |
| C | 4.244187000 | 3.664392000 | -0.598671000 |
| H | 4.104221000 | 2.680066000 | -0.135709000 |
| H | 5.081791000 | 4.148425000 | -0.081883000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.553985000 | 3.501324000 | -1.638310000 |
| C | 3.031772000 | 6.421622000 | -1.288947000 |
| H | 3.341240000 | 6.322782000 | -2.336278000 |
| H | 3.833289000 | 6.949192000 | -0.757964000 |
| H | 2.142914000 | 7.063278000 | -1.263989000 |
| C | 2.163873000 | 4.964919000 | 1.292828000 |
| H | 1.276101000 | 5.604292000 | 1.366143000 |
| H | 2.961341000 | 5.439700000 | 1.877194000 |
| H | 1.923980000 | 4.010808000 | 1.777622000 |
| C | -2.673456000 | 2.067706000 | 0.849459000 |
| C | -1.728926000 | 2.397208000 | 1.833935000 |
| H | -1.054089000 | 1.636885000 | 2.220834000 |
| C | -1.674857000 | 3.689385000 | 2.351659000 |
| H | -0.950387000 | 3.928113000 | 3.125582000 |
| C | -2.554087000 | 4.669299000 | 1.888957000 |
| H | -2.514962000 | 5.675032000 | 2.298330000 |
| C | -3.492241000 | 4.347768000 | 0.910617000 |
| H | -4.191188000 | 5.100642000 | 0.555960000 |
| C | -3.554439000 | 3.053784000 | 0.391605000 |
| H | -4.308832000 | 2.814693000 | -0.351967000 |
| C | -4.320831000 | 0.134657000 | -0.611733000 |
| C | -4.528757000 | 0.705502000 | -1.877103000 |
| H | -3.732715000 | 1.273241000 | -2.356613000 |
| C | -5.750331000 | 0.553703000 | -2.530100000 |
| H | -5.903133000 | 1.008426000 | -3.505349000 |
| C | -6.771457000 | -0.186934000 | -1.933525000 |
| H | -7.722616000 | -0.311623000 | -2.443511000 |
| C | -6.565672000 | -0.769665000 | -0.683894000 |
| H | -7.356415000 | -1.351034000 | -0.217407000 |
| C | -5.347761000 | -0.610085000 | -0.022041000 |
| H | -5.197036000 | -1.075716000 | 0.947019000 |
| C | -2.562149000 | -0.707716000 | 1.652161000 |
| C | -1.558171000 | -1.712076000 | 1.703187000 |
| C | -1.475838000 | -2.471635000 | 2.892054000 |
| H | -0.703639000 | -3.228586000 | 2.982630000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.339213000 | -2.251319000 | 3.955772000 |
| H | -2.234370000 | -2.856128000 | 4.853210000 |
| C | -3.315919000 | -1.253510000 | 3.898873000 |
| H | -3.980172000 | -1.074628000 | 4.738736000 |
| C | -3.405684000 | -0.479692000 | 2.749391000 |
| H | -4.134366000 | 0.326119000 | 2.698760000 |
| C | 0.110970000 | -3.039646000 | 0.549114000 |
| C | -0.428300000 | -4.339038000 | 0.631411000 |
| H | -1.482560000 | -4.458342000 | 0.866982000 |
| C | 0.368826000 | -5.457774000 | 0.417213000 |
| H | -0.074044000 | -6.448205000 | 0.484778000 |
| C | 1.725011000 | -5.320364000 | 0.106984000 |
| H | 2.342979000 | -6.197636000 | -0.060119000 |
| C | 2.281681000 | -4.047418000 | 0.026204000 |
| H | 3.337872000 | -3.931283000 | -0.200853000 |
| C | 1.493834000 | -2.912467000 | 0.256513000 |
| C | 3.836544000 | -1.314154000 | -0.480872000 |
| C | 4.957157000 | -1.015870000 | 0.303573000 |
| H | 4.835326000 | -0.730878000 | 1.344119000 |
| C | 6.237310000 | -1.086732000 | -0.246462000 |
| H | 7.099393000 | -0.853431000 | 0.372479000 |
| C | 6.412806000 | -1.458679000 | -1.577622000 |
| H | 7.411577000 | -1.514589000 | -2.001482000 |
| C | 5.301334000 | -1.760779000 | -2.365368000 |
| H | 5.431274000 | -2.055958000 | -3.403221000 |
| C | 4.021739000 | -1.681174000 | -1.822519000 |
| H | 3.162493000 | -1.922745000 | -2.443697000 |
| C | 2.308435000 | -0.663272000 | 1.929709000 |
| C | 2.459597000 | -1.604206000 | 2.955182000 |
| H | 2.443065000 | -2.665929000 | 2.725990000 |
| C | 2.634214000 | -1.180584000 | 4.271595000 |
| H | 2.751832000 | -1.916696000 | 5.062268000 |
| C | 2.662203000 | 0.180663000 | 4.573652000 |
| H | 2.799921000 | 0.507253000 | 5.600759000 |
| C | 2.516303000 | 1.122339000 | 3.555498000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.545019000 | 2.184030000 | 3.785538000 |
| C | 2.336030000 | 0.702847000 | 2.238317000 |
| H | 2.226529000 | 1.442354000 | 1.449275000 |
| C | 0.397888000 | -1.719345000 | -3.827573000 |
| C | -0.437937000 | -2.468145000 | -2.969029000 |
| H | -0.026825000 | -3.272853000 | -2.358055000 |
| C | -1.863610000 | -2.220190000 | -2.961040000 |
| C | -2.736231000 | -2.578112000 | -1.983153000 |
| H | -3.786508000 | -2.317996000 | -2.050319000 |
| H | -2.434500000 | -3.218185000 | -1.157758000 |
| Y | -0.392080000 | -0.692259000 | -1.296601000 |
| H | -2.246373000 | -1.600530000 | -3.777909000 |
| H | 1.416242000 | -2.061768000 | -3.987764000 |
| H | -0.067057000 | -1.303541000 | -4.719308000 |
| C | 0.858705000 | 2.499126000 | -1.062705000 |
| C | -0.225104000 | 2.000303000 | -1.989774000 |
| H | 1.732027000 | 1.835618000 | -1.071939000 |
| H | 0.484430000 | 2.534852000 | -0.031874000 |
| H | -1.159596000 | 2.557393000 | -1.927306000 |
| C | -0.042502000 | 1.217748000 | -3.105957000 |
| C | 1.038783000 | 0.292527000 | -3.368489000 |
| H | -0.862561000 | 1.201062000 | -3.830431000 |
| H | 1.363122000 | 0.253426000 | -4.404433000 |
| H | 1.907058000 | 0.351740000 | -2.704238000 |

104

theta3_P2_trans_1,4 E = -1968.325647 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.621402000 | -2.003201000 | 0.431802000 |
| P | -2.557160000 | 0.299311000 | 0.238215000 |
| P | 2.132134000 | -1.060546000 | 0.227368000 |
| Si | 2.471480000 | 4.708577000 | -0.714243000 |
| C | 1.120728000 | 3.840559000 | -1.740333000 |
| H | 1.531490000 | 3.620319000 | -2.735806000 |
| H | 0.309955000 | 4.564070000 | -1.910325000 |
| C | 4.025550000 | 3.633878000 | -0.654174000 |
| H | 3.852461000 | 2.650922000 | -0.199359000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 4.815360000 | 4.124963000 | -0.072650000 |
| H | 4.422323000 | 3.463134000 | -1.662494000 |
| C | 2.873874000 | 6.346188000 | -1.558136000 |
| H | 3.224340000 | 6.194419000 | -2.586133000 |
| H | 3.661776000 | 6.885631000 | -1.018693000 |
| H | 1.996027000 | 7.002024000 | -1.600493000 |
| C | 1.838940000 | 5.034276000 | 1.037220000 |
| H | 0.957116000 | 5.686286000 | 1.024735000 |
| H | 2.606374000 | 5.530987000 | 1.643312000 |
| H | 1.553563000 | 4.110600000 | 1.555244000 |
| C | -2.629779000 | 1.897385000 | 1.167112000 |
| C | -1.598493000 | 2.154547000 | 2.083761000 |
| H | -0.814608000 | 1.418328000 | 2.249760000 |
| C | -1.589046000 | 3.338898000 | 2.815469000 |
| H | -0.793033000 | 3.521241000 | 3.532111000 |
| C | -2.600799000 | 4.283309000 | 2.635238000 |
| H | -2.593358000 | 5.206579000 | 3.207946000 |
| C | -3.625419000 | 4.032366000 | 1.725972000 |
| H | -4.423731000 | 4.756947000 | 1.589303000 |
| C | -3.644095000 | 2.843965000 | 0.993853000 |
| H | -4.462553000 | 2.655764000 | 0.305853000 |
| C | -4.186117000 | 0.156983000 | -0.623989000 |
| C | -4.454116000 | 1.009207000 | -1.707994000 |
| H | -3.721801000 | 1.754159000 | -2.009779000 |
| C | -5.660468000 | 0.915749000 | -2.399622000 |
| H | -5.862459000 | 1.592062000 | -3.226162000 |
| C | -6.604282000 | -0.044405000 | -2.031580000 |
| H | -7.543608000 | -0.120110000 | -2.572311000 |
| C | -6.338111000 | -0.904011000 | -0.967042000 |
| H | -7.069940000 | -1.652442000 | -0.675050000 |
| C | -5.137725000 | -0.804571000 | -0.262418000 |
| H | -4.944898000 | -1.474093000 | 0.570513000 |
| C | -2.532565000 | -0.964530000 | 1.554920000 |
| C | -1.534883000 | -1.973661000 | 1.492291000 |
| C | -1.484732000 | -2.875186000 | 2.580407000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.719032000 | -3.642597000 | 2.602009000 |
| C | -2.379091000 | -2.792786000 | 3.639211000 |
| H | -2.296172000 | -3.509394000 | 4.452853000 |
| C | -3.360822000 | -1.801006000 | 3.682819000 |
| H | -4.053134000 | -1.734743000 | 4.516352000 |
| C | -3.414745000 | -0.884108000 | 2.641404000 |
| H | -4.145458000 | -0.078946000 | 2.669831000 |
| C | 0.268260000 | -3.095018000 | 0.351714000 |
| C | -0.157471000 | -4.436360000 | 0.292547000 |
| H | -1.219342000 | -4.654809000 | 0.375908000 |
| C | 0.757330000 | -5.472741000 | 0.134323000 |
| H | 0.399763000 | -6.498439000 | 0.091481000 |
| C | 2.125303000 | -5.206115000 | 0.024375000 |
| H | 2.836516000 | -6.018301000 | -0.094670000 |
| C | 2.569752000 | -3.888011000 | 0.074241000 |
| H | 3.630487000 | -3.668133000 | -0.010634000 |
| C | 1.657086000 | -2.839284000 | 0.241655000 |
| C | 3.892332000 | -1.037046000 | -0.315919000 |
| C | 4.954364000 | -0.997899000 | 0.596432000 |
| H | 4.757262000 | -0.971024000 | 1.664204000 |
| C | 6.270569000 | -0.989772000 | 0.135997000 |
| H | 7.088750000 | -0.957095000 | 0.850293000 |
| C | 6.537324000 | -1.024163000 | -1.231906000 |
| H | 7.564352000 | -1.015949000 | -1.586358000 |
| C | 5.483842000 | -1.064232000 | -2.145773000 |
| H | 5.687215000 | -1.086391000 | -3.213084000 |
| C | 4.167424000 | -1.063998000 | -1.690875000 |
| H | 3.350565000 | -1.086344000 | -2.408787000 |
| C | 2.166382000 | -0.533793000 | 1.993073000 |
| C | 2.093056000 | -1.452109000 | 3.046097000 |
| H | 2.001881000 | -2.513902000 | 2.836959000 |
| C | 2.144291000 | -1.006006000 | 4.366474000 |
| H | 2.088416000 | -1.725314000 | 5.178972000 |
| C | 2.273353000 | 0.353961000 | 4.644499000 |
| H | 2.317882000 | 0.696865000 | 5.674556000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.350415000 | 1.273841000 | 3.598107000 |
| H | 2.461988000 | 2.334083000 | 3.808789000 |
| C | 2.290407000 | 0.833742000 | 2.277401000 |
| H | 2.357574000 | 1.556794000 | 1.468023000 |
| C | 0.637901000 | -3.045689000 | -3.160781000 |
| C | -0.670639000 | -2.919976000 | -2.856557000 |
| H | -1.090028000 | -3.534847000 | -2.060988000 |
| C | -1.579462000 | -1.989861000 | -3.517785000 |
| C | -2.832290000 | -1.756956000 | -3.076872000 |
| H | -3.493025000 | -1.054113000 | -3.573408000 |
| H | -3.244281000 | -2.293259000 | -2.224645000 |
| Y | -0.268498000 | -0.500582000 | -1.305505000 |
| H | -1.207896000 | -1.466898000 | -4.398163000 |
| H | 1.266938000 | -3.752318000 | -2.627745000 |
| H | 1.093324000 | -2.480053000 | -3.969153000 |
| C | 0.495551000 | 2.548951000 | -1.162170000 |
| C | -0.555096000 | 1.973827000 | -2.094778000 |
| H | 1.311992000 | 1.826379000 | -0.971953000 |
| H | 0.043013000 | 2.765510000 | -0.186651000 |
| H | -1.504952000 | 2.504341000 | -2.093782000 |
| C | -0.226610000 | 1.246995000 | -3.240002000 |
| C | 0.923144000 | 0.448978000 | -3.396002000 |
| H | -1.031090000 | 1.102880000 | -3.965512000 |
| H | 1.063637000 | -0.076826000 | -4.337054000 |
| H | 1.856025000 | 0.758720000 | -2.920868000 |

104

theta3_C2_trans_1,2 E = -1968.318039 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.878388000 | -1.343243000 | -1.118720000 |
| P | 2.954829000 | 0.547051000 | -0.002976000 |
| P | -1.977694000 | -1.540145000 | -0.095158000 |
| Si | -3.891414000 | 4.631130000 | 0.436648000 |
| C | -2.972520000 | 3.690004000 | -0.942160000 |
| H | -2.159284000 | 4.324372000 | -1.321546000 |
| H | -3.662294000 | 3.561086000 | -1.788446000 |
| C | -2.713421000 | 4.940773000 | 1.885049000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.376505000 | 4.006861000 | 2.353149000 |
| H | -3.206674000 | 5.529918000 | 2.667638000 |
| H | -1.825013000 | 5.501305000 | 1.568219000 |
| C | -4.482246000 | 6.274128000 | -0.271681000 |
| H | -3.642995000 | 6.884806000 | -0.625612000 |
| H | -5.021011000 | 6.859843000 | 0.482766000 |
| H | -5.162641000 | 6.123930000 | -1.118365000 |
| C | -5.364838000 | 3.609847000 | 1.034376000 |
| H | -6.054077000 | 3.383126000 | 0.212007000 |
| H | -5.933888000 | 4.154300000 | 1.797597000 |
| H | -5.054173000 | 2.656505000 | 1.480272000 |
| C | 4.123908000 | 1.970850000 | -0.010022000 |
| C | 3.625790000 | 3.263687000 | 0.191908000 |
| H | 2.559951000 | 3.413754000 | 0.338695000 |
| C | 4.487669000 | 4.360175000 | 0.203561000 |
| H | 4.089600000 | 5.358847000 | 0.361593000 |
| C | 5.855836000 | 4.172564000 | 0.017896000 |
| H | 6.528419000 | 5.025856000 | 0.028008000 |
| C | 6.363458000 | 2.886229000 | -0.172158000 |
| H | 7.430909000 | 2.736003000 | -0.308974000 |
| C | 5.505613000 | 1.789070000 | -0.181841000 |
| H | 5.912468000 | 0.789703000 | -0.312315000 |
| C | 3.850960000 | -0.717383000 | 1.009077000 |
| C | 4.509979000 | -0.310014000 | 2.179565000 |
| H | 4.568009000 | 0.744814000 | 2.437656000 |
| C | 5.130339000 | -1.249317000 | 3.002482000 |
| H | 5.654085000 | -0.918717000 | 3.895653000 |
| C | 5.090005000 | -2.604798000 | 2.673184000 |
| H | 5.579098000 | -3.335776000 | 3.311220000 |
| C | 4.429305000 | -3.014996000 | 1.515947000 |
| H | 4.399906000 | -4.068000000 | 1.248751000 |
| C | 3.811558000 | -2.078343000 | 0.687480000 |
| H | 3.305606000 | -2.409701000 | -0.212694000 |
| C | 2.894111000 | -0.087795000 | -1.741917000 |
| C | 1.836014000 | -0.972056000 | -2.085915000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.725283000 | -1.373995000 | -3.434432000 |
| H | 0.917717000 | -2.044652000 | -3.713807000 |
| C | 2.619493000 | -0.927903000 | -4.396337000 |
| H | 2.505950000 | -1.258449000 | -5.425620000 |
| C | 3.647094000 | -0.044851000 | -4.053103000 |
| H | 4.343991000 | 0.311438000 | -4.805975000 |
| C | 3.768348000 | 0.377627000 | -2.735461000 |
| H | 4.556212000 | 1.075481000 | -2.469944000 |
| C | 0.378181000 | -2.650371000 | -1.124349000 |
| C | 1.151650000 | -3.745437000 | -1.569492000 |
| H | 2.160995000 | -3.567621000 | -1.928696000 |
| C | 0.645038000 | -5.037517000 | -1.580630000 |
| H | 1.275907000 | -5.849809000 | -1.933021000 |
| C | -0.660608000 | -5.300262000 | -1.158643000 |
| H | -1.064159000 | -6.307677000 | -1.190277000 |
| C | -1.438659000 | -4.241853000 | -0.707960000 |
| H | -2.466157000 | -4.422240000 | -0.400424000 |
| C | -0.933242000 | -2.934168000 | -0.663419000 |
| C | -2.563531000 | -1.952625000 | 1.610216000 |
| C | -3.364113000 | -1.001607000 | 2.265825000 |
| H | -3.661047000 | -0.090733000 | 1.748737000 |
| C | -3.805045000 | -1.219196000 | 3.569774000 |
| H | -4.435333000 | -0.480533000 | 4.057860000 |
| C | -3.437541000 | -2.384778000 | 4.244372000 |
| H | -3.779190000 | -2.556535000 | 5.261310000 |
| C | -2.632814000 | -3.327492000 | 3.606190000 |
| H | -2.345763000 | -4.238309000 | 4.125140000 |
| C | -2.195996000 | -3.115739000 | 2.297344000 |
| H | -1.566213000 | -3.857472000 | 1.816466000 |
| C | -3.488910000 | -1.661814000 | -1.157954000 |
| C | -4.778241000 | -1.848548000 | -0.650170000 |
| H | -4.940396000 | -1.955359000 | 0.417981000 |
| C | -5.869167000 | -1.918638000 | -1.518298000 |
| H | -6.866066000 | -2.069911000 | -1.112977000 |
| C | -5.682890000 | -1.806339000 | -2.893839000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -6.534208000 | -1.863877000 | -3.566386000 |
| C | -4.396696000 | -1.629101000 | -3.406517000 |
| H | -4.242071000 | -1.552206000 | -4.479462000 |
| C | -3.306057000 | -1.553778000 | -2.544978000 |
| H | -2.305788000 | -1.431520000 | -2.954528000 |
| C | -2.400428000 | 2.301039000 | -0.579040000 |
| C | -1.695158000 | 1.623965000 | -1.736193000 |
| H | -3.210411000 | 1.650621000 | -0.226325000 |
| H | -1.727066000 | 2.443121000 | 0.294869000 |
| C | -0.448250000 | 2.025865000 | -2.206545000 |
| C | 0.534417000 | 2.687991000 | -1.439155000 |
| H | 1.489715000 | 2.909902000 | -1.904504000 |
| H | 0.220358000 | 3.417403000 | -0.687717000 |
| H | -2.329377000 | 1.042593000 | -2.400118000 |
| C | -0.260017000 | 1.414514000 | 2.516844000 |
| C | 0.645818000 | 0.497812000 | 2.941907000 |
| H | 0.054675000 | 2.416821000 | 2.227167000 |
| H | -1.328871000 | 1.243398000 | 2.642447000 |
| C | 0.316150000 | -0.797802000 | 3.504748000 |
| C | 1.260408000 | -1.679577000 | 3.872254000 |
| H | 0.994426000 | -2.636928000 | 4.310265000 |
| H | 2.320458000 | -1.472084000 | 3.746734000 |
| H | 1.707467000 | 0.739357000 | 2.881977000 |
| Y | 0.075764000 | 0.533719000 | -0.188226000 |
| H | -0.737318000 | -1.032241000 | 3.641876000 |
| H | -0.114899000 | 1.575129000 | -3.144288000 |

104

theta3_TS2_trans_1,2 E = -1968.292829 a.u. Imaginary frequency=291i

| | | | |
|----|--------------|--------------|--------------|
| N | 1.285701000 | -1.637231000 | -0.051905000 |
| P | -1.715627000 | -1.647628000 | 0.021332000 |
| P | 3.031258000 | 0.745191000 | 0.281146000 |
| Si | -5.301127000 | 3.550107000 | 0.345670000 |
| C | -3.399831000 | 3.481700000 | 0.515247000 |
| H | -3.128818000 | 3.239301000 | 1.551377000 |
| H | -3.045993000 | 4.511612000 | 0.353615000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -6.043483000 | 1.818369000 | 0.427756000 |
| H | -5.684483000 | 1.177689000 | -0.386687000 |
| H | -7.136481000 | 1.864508000 | 0.347329000 |
| H | -5.802564000 | 1.317277000 | 1.372019000 |
| C | -5.965210000 | 4.613097000 | 1.754328000 |
| H | -5.736497000 | 4.175051000 | 2.733397000 |
| H | -7.054724000 | 4.718892000 | 1.687705000 |
| H | -5.536363000 | 5.622224000 | 1.734057000 |
| C | -5.723814000 | 4.343853000 | -1.316100000 |
| H | -5.306504000 | 5.355032000 | -1.396051000 |
| H | -6.810269000 | 4.428946000 | -1.439669000 |
| H | -5.348677000 | 3.760237000 | -2.166012000 |
| C | -3.265810000 | -1.574345000 | 1.019792000 |
| C | -3.198238000 | -1.019158000 | 2.307005000 |
| H | -2.249877000 | -0.658366000 | 2.699408000 |
| C | -4.332470000 | -0.971273000 | 3.112871000 |
| H | -4.265675000 | -0.551569000 | 4.113070000 |
| C | -5.547526000 | -1.471143000 | 2.640816000 |
| H | -6.431655000 | -1.437506000 | 3.271338000 |
| C | -5.621165000 | -2.018595000 | 1.361924000 |
| H | -6.562611000 | -2.414737000 | 0.991364000 |
| C | -4.486360000 | -2.072262000 | 0.551506000 |
| H | -4.553810000 | -2.515234000 | -0.437595000 |
| C | -2.165618000 | -2.503625000 | -1.550504000 |
| C | -2.871232000 | -1.786322000 | -2.529369000 |
| H | -3.179139000 | -0.759300000 | -2.339039000 |
| C | -3.205423000 | -2.389826000 | -3.740015000 |
| H | -3.761829000 | -1.831313000 | -4.488030000 |
| C | -2.823955000 | -3.709072000 | -3.989309000 |
| H | -3.079728000 | -4.178590000 | -4.935119000 |
| C | -2.118021000 | -4.424001000 | -3.022547000 |
| H | -1.825269000 | -5.453172000 | -3.212222000 |
| C | -1.789594000 | -3.827181000 | -1.805216000 |
| H | -1.246104000 | -4.389618000 | -1.051308000 |
| C | -0.630644000 | -2.782128000 | 0.957307000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 0.771088000 | -2.620365000 | 0.800892000 |
| C | 1.598534000 | -3.464190000 | 1.575083000 |
| H | 2.675878000 | -3.351470000 | 1.509524000 |
| C | 1.064534000 | -4.424874000 | 2.423841000 |
| H | 1.740138000 | -5.049887000 | 3.002744000 |
| C | -0.316731000 | -4.586815000 | 2.551788000 |
| H | -0.731307000 | -5.341329000 | 3.213264000 |
| C | -1.154545000 | -3.752372000 | 1.821723000 |
| H | -2.232315000 | -3.850426000 | 1.920578000 |
| C | 2.593581000 | -1.854663000 | -0.541420000 |
| C | 2.954468000 | -3.074021000 | -1.147516000 |
| H | 2.205244000 | -3.856637000 | -1.228532000 |
| C | 4.239728000 | -3.288787000 | -1.627460000 |
| H | 4.484681000 | -4.241039000 | -2.090978000 |
| C | 5.216837000 | -2.295390000 | -1.514345000 |
| H | 6.227479000 | -2.471243000 | -1.871143000 |
| C | 4.880448000 | -1.077381000 | -0.934719000 |
| H | 5.635694000 | -0.302150000 | -0.836862000 |
| C | 3.581078000 | -0.842008000 | -0.467625000 |
| C | 4.005945000 | 2.117512000 | -0.471558000 |
| C | 4.104783000 | 3.329357000 | 0.232607000 |
| H | 3.729772000 | 3.401401000 | 1.250744000 |
| C | 4.703675000 | 4.442208000 | -0.353673000 |
| H | 4.784069000 | 5.367611000 | 0.210369000 |
| C | 5.203601000 | 4.368082000 | -1.654052000 |
| H | 5.674547000 | 5.235346000 | -2.108245000 |
| C | 5.100312000 | 3.173841000 | -2.364719000 |
| H | 5.492275000 | 3.104849000 | -3.376036000 |
| C | 4.502868000 | 2.056169000 | -1.781567000 |
| H | 4.437920000 | 1.132076000 | -2.347329000 |
| C | 3.584302000 | 0.652185000 | 2.042222000 |
| C | 4.874954000 | 1.026898000 | 2.438891000 |
| H | 5.573443000 | 1.438997000 | 1.716066000 |
| C | 5.269130000 | 0.876804000 | 3.766802000 |
| H | 6.271307000 | 1.171820000 | 4.065890000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.385317000 | 0.347230000 | 4.707197000 |
| H | 4.696724000 | 0.232292000 | 5.741779000 |
| C | 3.104376000 | -0.038919000 | 4.316162000 |
| H | 2.415079000 | -0.461093000 | 5.042541000 |
| C | 2.703533000 | 0.113525000 | 2.989604000 |
| H | 1.710619000 | -0.210915000 | 2.689565000 |
| C | -2.660824000 | 2.541475000 | -0.458175000 |
| C | -1.194441000 | 2.925483000 | -0.620082000 |
| H | -3.136603000 | 2.583913000 | -1.446811000 |
| H | -2.777514000 | 1.500236000 | -0.121292000 |
| C | -0.281979000 | 2.730162000 | 0.482306000 |
| C | -0.370211000 | 1.806750000 | 1.501551000 |
| H | 0.381569000 | 1.787128000 | 2.284403000 |
| H | -1.303947000 | 1.280847000 | 1.705291000 |
| H | -1.095433000 | 3.939348000 | -1.008327000 |
| C | -0.599121000 | 2.338228000 | -2.506810000 |
| C | -0.117600000 | 1.044241000 | -2.864277000 |
| H | -1.596622000 | 2.599347000 | -2.849366000 |
| H | 0.116702000 | 3.150757000 | -2.631124000 |
| C | 1.297105000 | 0.826652000 | -3.129659000 |
| C | 1.879684000 | -0.363562000 | -3.401441000 |
| H | 2.944878000 | -0.444544000 | -3.587841000 |
| H | 1.300179000 | -1.280239000 | -3.494261000 |
| H | -0.825327000 | 0.290384000 | -3.217038000 |
| Y | 0.293259000 | 0.371229000 | -0.578595000 |
| H | 1.939068000 | 1.709961000 | -3.070785000 |
| H | 0.636923000 | 3.321794000 | 0.439886000 |

104

theta3_P2_trans_1,2 E = -1968.342423 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.711610000 | 1.619725000 | -0.219095000 |
| P | 1.237059000 | 2.018867000 | 0.035845000 |
| P | -2.889070000 | -1.068571000 | 0.229275000 |
| Si | 5.833785000 | -3.144995000 | 0.486896000 |
| C | 3.952107000 | -3.461337000 | 0.440051000 |
| H | 3.507469000 | -3.051331000 | 1.357561000 |

| | | | |
|---|-------------|--------------|--------------|
| H | 3.809873000 | -4.551023000 | 0.508362000 |
| C | 6.189434000 | -1.302749000 | 0.258456000 |
| H | 5.857198000 | -0.941826000 | -0.722866000 |
| H | 7.266767000 | -1.107882000 | 0.326104000 |
| H | 5.696931000 | -0.693129000 | 1.025548000 |
| C | 6.476195000 | -3.720388000 | 2.164483000 |
| H | 6.016937000 | -3.158820000 | 2.987092000 |
| H | 7.561903000 | -3.585469000 | 2.239475000 |
| H | 6.265835000 | -4.783803000 | 2.330690000 |
| C | 6.665815000 | -4.126055000 | -0.895207000 |
| H | 6.477860000 | -5.201749000 | -0.792696000 |
| H | 7.752724000 | -3.981215000 | -0.875136000 |
| H | 6.317173000 | -3.820872000 | -1.889366000 |
| C | 2.612925000 | 1.961187000 | 1.264234000 |
| C | 2.348332000 | 1.388448000 | 2.518056000 |
| H | 1.349379000 | 1.028233000 | 2.755188000 |
| C | 3.350693000 | 1.313331000 | 3.481170000 |
| H | 3.132941000 | 0.878625000 | 4.453082000 |
| C | 4.627709000 | 1.803547000 | 3.201730000 |
| H | 5.409103000 | 1.747157000 | 3.954506000 |
| C | 4.894385000 | 2.373888000 | 1.958791000 |
| H | 5.883473000 | 2.766612000 | 1.739546000 |
| C | 3.892657000 | 2.454410000 | 0.990179000 |
| H | 4.109948000 | 2.912952000 | 0.030183000 |
| C | 1.886393000 | 2.949317000 | -1.419771000 |
| C | 2.772659000 | 2.293644000 | -2.289151000 |
| H | 3.098926000 | 1.277059000 | -2.074510000 |
| C | 3.261854000 | 2.944327000 | -3.419721000 |
| H | 3.954693000 | 2.431952000 | -4.081702000 |
| C | 2.856877000 | 4.249893000 | -3.700725000 |
| H | 3.232443000 | 4.756375000 | -4.585473000 |
| C | 1.970400000 | 4.902803000 | -2.845387000 |
| H | 1.655595000 | 5.920237000 | -3.061003000 |
| C | 1.485270000 | 4.259006000 | -1.707217000 |
| H | 0.797818000 | 4.774433000 | -1.043048000 |

| | | | |
|---|--------------|--------------|---------------|
| C | -0.044039000 | 3.068796000 | 0.806964000 |
| C | -1.400552000 | 2.745952000 | 0.541921000 |
| C | -2.380442000 | 3.577484000 | 1.124122000 |
| H | -3.429794000 | 3.360013000 | 0.952150000 |
| C | -2.029373000 | 4.657336000 | 1.924221000 |
| H | -2.816442000 | 5.268489000 | 2.359211000 |
| C | -0.690923000 | 4.956962000 | 2.187665000 |
| H | -0.422144000 | 5.799106000 | 2.817836000 |
| C | 0.294206000 | 4.151581000 | 1.627888000 |
| H | 1.342392000 | 4.362221000 | 1.825324000 |
| C | -2.982572000 | 1.513503000 | -0.814165000 |
| C | -3.550560000 | 2.548820000 | -1.583135000 |
| H | -3.009062000 | 3.485847000 | -1.677735000 |
| C | -4.770332000 | 2.377399000 | -2.222897000 |
| H | -5.182243000 | 3.192040000 | -2.813055000 |
| C | -5.462359000 | 1.165173000 | -2.129298000 |
| H | -6.415101000 | 1.035014000 | -2.634048000 |
| C | -4.921007000 | 0.126304000 | -1.382559000 |
| H | -5.452060000 | -0.818166000 | -1.304572000 |
| C | -3.700311000 | 0.292438000 | -0.7111373000 |
| C | -3.860327000 | -2.584847000 | -0.153033000 |
| C | -4.973540000 | -2.959395000 | 0.610746000 |
| H | -5.278535000 | -2.356745000 | 1.461640000 |
| C | -5.690377000 | -4.109173000 | 0.283253000 |
| H | -6.551973000 | -4.393717000 | 0.880989000 |
| C | -5.305723000 | -4.890655000 | -0.805894000 |
| H | -5.866450000 | -5.786638000 | -1.057294000 |
| C | -4.197839000 | -4.524194000 | -1.570047000 |
| H | -3.893553000 | -5.132470000 | -2.417571000 |
| C | -3.474646000 | -3.379694000 | -1.241202000 |
| H | -2.608222000 | -3.103864000 | -1.839121000 |
| C | -3.175457000 | -0.754861000 | 2.020436000 |
| C | -3.967928000 | 0.302102000 | 2.477758000 |
| H | -4.453031000 | 0.963434000 | 1.766051000 |
| C | -4.140469000 | 0.501496000 | 3.847615000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -4.759477000 | 1.323298000 | 4.197090000 |
| C | -3.527498000 | -0.350870000 | 4.764501000 |
| H | -3.666092000 | -0.193372000 | 5.830543000 |
| C | -2.740205000 | -1.411014000 | 4.312436000 |
| H | -2.268757000 | -2.083834000 | 5.023739000 |
| C | -2.560220000 | -1.611028000 | 2.946020000 |
| H | -1.958528000 | -2.450568000 | 2.602018000 |
| C | 3.218202000 | -2.937312000 | -0.802335000 |
| C | 1.754126000 | -3.393414000 | -0.922017000 |
| H | 3.736049000 | -3.293203000 | -1.703254000 |
| H | 3.280927000 | -1.840166000 | -0.841918000 |
| C | 0.784133000 | -2.747627000 | 0.039067000 |
| C | 0.996728000 | -1.726589000 | 0.897075000 |
| H | 0.234349000 | -1.442687000 | 1.624453000 |
| H | 1.968307000 | -1.248899000 | 1.003186000 |
| H | 1.734310000 | -4.471013000 | -0.691386000 |
| C | 1.176787000 | -3.217328000 | -2.346269000 |
| C | 0.866641000 | -1.770891000 | -2.629584000 |
| H | 1.888333000 | -3.633722000 | -3.074737000 |
| H | 0.256230000 | -3.809119000 | -2.444053000 |
| C | -0.255495000 | -1.295493000 | -3.281835000 |
| C | -0.607804000 | 0.077398000 | -3.380018000 |
| H | -1.516820000 | 0.351114000 | -3.909159000 |
| H | 0.203238000 | 0.809394000 | -3.484940000 |
| H | 1.709531000 | -1.074254000 | -2.512571000 |
| Y | -0.440413000 | -0.124387000 | -0.946624000 |
| H | -1.034338000 | -2.026224000 | -3.521524000 |
| H | -0.208657000 | -3.209095000 | 0.043844000 |

104

theta1_TS2_cis_1,4 E = -1968.283555 a.u. Imaginary frequency=58i

| | | | |
|----|--------------|--------------|--------------|
| N | 1.924490000 | 1.329744000 | -0.685782000 |
| P | -0.758435000 | 2.349862000 | 0.133366000 |
| P | 2.603824000 | -1.397492000 | 0.234854000 |
| Si | -6.753597000 | -2.542325000 | 0.343553000 |
| C | -5.095039000 | -3.298502000 | 0.892981000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -5.272792000 | -4.346573000 | 1.175298000 |
| H | -4.771349000 | -2.795450000 | 1.815897000 |
| C | -7.425240000 | -3.470769000 | -1.157744000 |
| H | -6.742423000 | -3.420457000 | -2.014700000 |
| H | -8.384625000 | -3.048384000 | -1.480418000 |
| H | -7.594828000 | -4.530396000 | -0.931169000 |
| C | -7.968210000 | -2.664844000 | 1.780938000 |
| H | -8.122248000 | -3.706657000 | 2.086486000 |
| H | -8.947648000 | -2.254762000 | 1.506397000 |
| H | -7.612896000 | -2.111521000 | 2.658650000 |
| C | -6.497658000 | -0.721321000 | -0.115397000 |
| H | -6.063721000 | -0.152096000 | 0.716214000 |
| H | -7.455280000 | -0.251896000 | -0.372057000 |
| H | -5.838144000 | -0.611803000 | -0.985867000 |
| C | -2.382392000 | 3.208618000 | 0.055908000 |
| C | -3.495814000 | 2.515193000 | -0.434212000 |
| H | -3.391807000 | 1.485428000 | -0.766883000 |
| C | -4.744837000 | 3.132315000 | -0.485281000 |
| H | -5.603933000 | 2.582569000 | -0.859737000 |
| C | -4.888385000 | 4.445723000 | -0.041016000 |
| H | -5.861847000 | 4.927159000 | -0.074770000 |
| C | -3.785237000 | 5.139699000 | 0.458711000 |
| H | -3.898982000 | 6.160233000 | 0.813904000 |
| C | -2.536410000 | 4.525258000 | 0.512766000 |
| H | -1.685924000 | 5.064245000 | 0.921512000 |
| C | -0.016194000 | 2.881691000 | 1.732170000 |
| C | -0.433569000 | 2.221180000 | 2.896538000 |
| H | -1.167280000 | 1.418847000 | 2.838542000 |
| C | 0.073574000 | 2.602303000 | 4.136913000 |
| H | -0.260705000 | 2.093299000 | 5.036968000 |
| C | 1.006951000 | 3.636110000 | 4.221548000 |
| H | 1.404191000 | 3.931394000 | 5.188733000 |
| C | 1.428641000 | 4.290606000 | 3.065059000 |
| H | 2.154403000 | 5.096768000 | 3.129361000 |
| C | 0.920328000 | 3.916901000 | 1.821321000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 1.252442000 | 4.429432000 | 0.922870000 |
| C | 0.287624000 | 3.071339000 | -1.208766000 |
| C | 1.539748000 | 2.446105000 | -1.456291000 |
| C | 2.312597000 | 2.920471000 | -2.535914000 |
| H | 3.271365000 | 2.449547000 | -2.736003000 |
| C | 1.865261000 | 3.963876000 | -3.335530000 |
| H | 2.483376000 | 4.308860000 | -4.160405000 |
| C | 0.623345000 | 4.560332000 | -3.095400000 |
| H | 0.273715000 | 5.374808000 | -3.723166000 |
| C | -0.162046000 | 4.105791000 | -2.042559000 |
| H | -1.128371000 | 4.564191000 | -1.852655000 |
| C | 3.200929000 | 1.286331000 | -0.120068000 |
| C | 4.022474000 | 2.422131000 | 0.028744000 |
| H | 3.672549000 | 3.384318000 | -0.331088000 |
| C | 5.266068000 | 2.334551000 | 0.643222000 |
| H | 5.867996000 | 3.234352000 | 0.744173000 |
| C | 5.742082000 | 1.120741000 | 1.142669000 |
| H | 6.712093000 | 1.060357000 | 1.626471000 |
| C | 4.943196000 | -0.010417000 | 1.018620000 |
| H | 5.286336000 | -0.962419000 | 1.416554000 |
| C | 3.695041000 | 0.059378000 | 0.390511000 |
| C | 2.774131000 | -2.314872000 | 1.825568000 |
| C | 3.578988000 | -3.451142000 | 1.966678000 |
| H | 4.130503000 | -3.839896000 | 1.115939000 |
| C | 3.680959000 | -4.085440000 | 3.205041000 |
| H | 4.309293000 | -4.966254000 | 3.306144000 |
| C | 2.987148000 | -3.590943000 | 4.307731000 |
| H | 3.068947000 | -4.088223000 | 5.270252000 |
| C | 2.190166000 | -2.453318000 | 4.174532000 |
| H | 1.652369000 | -2.059661000 | 5.032763000 |
| C | 2.080192000 | -1.820307000 | 2.939434000 |
| H | 1.467947000 | -0.924933000 | 2.850515000 |
| C | 3.353875000 | -2.485310000 | -1.055026000 |
| C | 4.400756000 | -2.044800000 | -1.873243000 |
| H | 4.849469000 | -1.070074000 | -1.703794000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.879907000 | -2.863058000 | -2.897548000 |
| H | 5.697001000 | -2.514929000 | -3.523739000 |
| C | 4.324449000 | -4.123516000 | -3.109933000 |
| H | 4.704269000 | -4.760032000 | -3.904290000 |
| C | 3.283411000 | -4.570610000 | -2.293718000 |
| H | 2.853742000 | -5.556870000 | -2.448099000 |
| C | 2.793781000 | -3.753909000 | -1.277336000 |
| H | 1.988611000 | -4.112435000 | -0.639085000 |
| C | -1.156290000 | -1.837901000 | 0.271957000 |
| C | -1.499349000 | -3.213902000 | 0.597850000 |
| H | -0.691564000 | -3.807020000 | 1.027743000 |
| C | -2.680650000 | -3.834902000 | 0.383713000 |
| C | -3.951996000 | -3.235628000 | -0.140973000 |
| H | -4.258838000 | -3.778581000 | -1.047174000 |
| H | -3.792614000 | -2.194395000 | -0.450051000 |
| Y | 0.213278000 | -0.146296000 | -0.842230000 |
| H | -2.748861000 | -4.886939000 | 0.662460000 |
| H | -2.037497000 | -1.183419000 | 0.168941000 |
| H | -0.468553000 | -1.419679000 | 1.044795000 |
| C | -0.616948000 | -2.423804000 | -2.132026000 |
| C | 0.105095000 | -1.568504000 | -2.952956000 |
| H | -1.700641000 | -2.394797000 | -2.083187000 |
| H | -0.171678000 | -3.348872000 | -1.786278000 |
| H | 1.128947000 | -1.834258000 | -3.212906000 |
| C | -0.409547000 | -0.314633000 | -3.460957000 |
| C | -1.547109000 | 0.307003000 | -3.031698000 |
| H | 0.239354000 | 0.231956000 | -4.145004000 |
| H | -1.832391000 | 1.279169000 | -3.418669000 |
| H | -2.288005000 | -0.206646000 | -2.417124000 |

104

theta1_P2_cis_1,4 E = -1968.323624 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 1.734753000 | 1.693432000 | -0.333688000 |
| P | -1.242003000 | 1.960977000 | 0.029373000 |
| P | 2.970288000 | -0.985217000 | 0.185259000 |
| Si | -6.433897000 | -2.693860000 | 0.314911000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.690479000 | -3.360726000 | 0.702109000 |
| H | -4.821889000 | -4.357257000 | 1.150845000 |
| H | -4.231424000 | -2.744960000 | 1.489287000 |
| C | -7.326267000 | -3.907692000 | -0.823271000 |
| H | -6.811712000 | -4.032671000 | -1.783772000 |
| H | -8.342340000 | -3.558335000 | -1.043612000 |
| H | -7.414620000 | -4.899038000 | -0.362536000 |
| C | -7.369613000 | -2.533311000 | 1.945248000 |
| H | -7.436080000 | -3.497199000 | 2.464096000 |
| H | -8.394034000 | -2.178875000 | 1.779263000 |
| H | -6.881545000 | -1.823833000 | 2.624499000 |
| C | -6.314307000 | -1.007626000 | -0.529776000 |
| H | -5.797489000 | -0.271596000 | 0.097775000 |
| H | -7.314010000 | -0.610566000 | -0.744296000 |
| H | -5.777585000 | -1.069421000 | -1.484301000 |
| C | -2.962930000 | 2.458987000 | -0.392069000 |
| C | -3.485739000 | 2.069597000 | -1.633500000 |
| H | -2.878819000 | 1.485059000 | -2.320232000 |
| C | -4.776472000 | 2.442811000 | -1.998862000 |
| H | -5.171899000 | 2.142614000 | -2.965348000 |
| C | -5.561515000 | 3.192467000 | -1.121837000 |
| H | -6.571013000 | 3.477690000 | -1.404607000 |
| C | -5.050524000 | 3.571511000 | 0.118207000 |
| H | -5.659226000 | 4.154043000 | 0.804363000 |
| C | -3.754110000 | 3.210449000 | 0.484997000 |
| H | -3.362850000 | 3.515636000 | 1.451031000 |
| C | -1.022337000 | 2.365670000 | 1.810158000 |
| C | -1.385731000 | 1.394726000 | 2.754458000 |
| H | -1.789024000 | 0.437457000 | 2.427300000 |
| C | -1.252887000 | 1.656458000 | 4.116647000 |
| H | -1.543205000 | 0.902812000 | 4.843665000 |
| C | -0.747574000 | 2.884691000 | 4.543524000 |
| H | -0.640026000 | 3.088007000 | 5.605375000 |
| C | -0.381977000 | 3.852081000 | 3.607792000 |
| H | 0.008597000 | 4.810216000 | 3.939675000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.518647000 | 3.597411000 | 2.243956000 |
| H | -0.235841000 | 4.355545000 | 1.518946000 |
| C | -0.159647000 | 3.131306000 | -0.914469000 |
| C | 1.231423000 | 2.849935000 | -0.966823000 |
| C | 2.054845000 | 3.698850000 | -1.731973000 |
| H | 3.118805000 | 3.483889000 | -1.783253000 |
| C | 1.524693000 | 4.786085000 | -2.412788000 |
| H | 2.182335000 | 5.425740000 | -2.995523000 |
| C | 0.152550000 | 5.051842000 | -2.365113000 |
| H | -0.261123000 | 5.902768000 | -2.898440000 |
| C | -0.682259000 | 4.220171000 | -1.628927000 |
| H | -1.748691000 | 4.422032000 | -1.591544000 |
| C | 2.839514000 | 1.783441000 | 0.519905000 |
| C | 3.272999000 | 3.000647000 | 1.081840000 |
| H | 2.753568000 | 3.918851000 | 0.827101000 |
| C | 4.339988000 | 3.041588000 | 1.971043000 |
| H | 4.641278000 | 3.998914000 | 2.389015000 |
| C | 5.014356000 | 1.876958000 | 2.343153000 |
| H | 5.843620000 | 1.913948000 | 3.042870000 |
| C | 4.598103000 | 0.664221000 | 1.805982000 |
| H | 5.101812000 | -0.255658000 | 2.093037000 |
| C | 3.534203000 | 0.606818000 | 0.898357000 |
| C | 2.977460000 | -2.168705000 | 1.602535000 |
| C | 3.987609000 | -3.114065000 | 1.812110000 |
| H | 4.822404000 | -3.185330000 | 1.121263000 |
| C | 3.927728000 | -3.969830000 | 2.912600000 |
| H | 4.717831000 | -4.699690000 | 3.067044000 |
| C | 2.866937000 | -3.886961000 | 3.812301000 |
| H | 2.824622000 | -4.554949000 | 4.668061000 |
| C | 1.860317000 | -2.941076000 | 3.613718000 |
| H | 1.034061000 | -2.867008000 | 4.315626000 |
| C | 1.912758000 | -2.090872000 | 2.512593000 |
| H | 1.130656000 | -1.344067000 | 2.379762000 |
| C | 4.310241000 | -1.544574000 | -0.950979000 |
| C | 5.352880000 | -0.691139000 | -1.329285000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 5.423948000 | 0.304607000 | -0.901813000 |
| C | 6.311400000 | -1.121494000 | -2.247812000 |
| H | 7.118693000 | -0.452088000 | -2.532425000 |
| C | 6.241565000 | -2.402956000 | -2.789774000 |
| H | 6.992642000 | -2.736398000 | -3.500452000 |
| C | 5.205594000 | -3.260140000 | -2.414079000 |
| H | 5.149157000 | -4.263153000 | -2.828502000 |
| C | 4.239546000 | -2.831629000 | -1.507508000 |
| H | 3.437297000 | -3.508151000 | -1.220673000 |
| C | -0.618179000 | -2.653758000 | -0.850244000 |
| C | -1.199884000 | -3.918267000 | -0.279887000 |
| H | -0.449915000 | -4.652287000 | 0.015396000 |
| C | -2.489717000 | -4.252396000 | -0.153723000 |
| C | -3.723268000 | -3.468827000 | -0.492868000 |
| H | -4.227346000 | -3.985422000 | -1.323833000 |
| H | -3.475016000 | -2.467647000 | -0.867541000 |
| Y | 0.517920000 | -0.022831000 | -1.025810000 |
| H | -2.693001000 | -5.244096000 | 0.254140000 |
| H | -1.401775000 | -1.874745000 | -0.877480000 |
| H | 0.182182000 | -2.347057000 | -0.139459000 |
| C | -0.000008000 | -2.887637000 | -2.260221000 |
| C | 0.991182000 | -1.872438000 | -2.820005000 |
| H | -0.840291000 | -3.016315000 | -2.957120000 |
| H | 0.510370000 | -3.856138000 | -2.216841000 |
| H | 1.997424000 | -2.241103000 | -2.998123000 |
| C | 0.619226000 | -0.710620000 | -3.487305000 |
| C | -0.587273000 | -0.005710000 | -3.278309000 |
| H | 1.415572000 | -0.182964000 | -4.019382000 |
| H | -0.775529000 | 0.894082000 | -3.858269000 |
| H | -1.486102000 | -0.579541000 | -3.026872000 |

104

theta1_C2_trans_1,4 E = -1968.321524 a.u.

| | | | |
|---|--------------|--------------|--------------|
| N | -1.013213000 | -1.502386000 | -0.858151000 |
| P | 1.758794000 | -1.701223000 | 0.179799000 |
| P | -2.889140000 | 0.585476000 | 0.156954000 |

| | | | |
|----|-------------|--------------|--------------|
| Si | 4.455038000 | 4.208928000 | 0.647803000 |
| C | 2.565063000 | 4.104094000 | 0.892948000 |
| H | 2.144888000 | 5.108985000 | 0.742107000 |
| H | 2.362878000 | 3.856438000 | 1.944154000 |
| C | 4.850717000 | 4.341573000 | -1.196798000 |
| H | 4.540635000 | 3.447945000 | -1.753449000 |
| H | 5.929312000 | 4.461708000 | -1.354879000 |
| H | 4.357402000 | 5.208394000 | -1.653607000 |
| C | 5.073042000 | 5.742846000 | 1.551318000 |
| H | 4.635432000 | 6.659361000 | 1.137955000 |
| H | 6.163143000 | 5.834042000 | 1.472966000 |
| H | 4.823071000 | 5.707850000 | 2.618528000 |
| C | 5.271924000 | 2.668865000 | 1.374288000 |
| H | 5.070088000 | 2.587883000 | 2.449587000 |
| H | 6.361132000 | 2.710297000 | 1.250885000 |
| H | 4.926930000 | 1.741200000 | 0.901736000 |
| C | 3.594884000 | -1.849779000 | 0.100061000 |
| C | 4.319428000 | -0.879593000 | -0.606043000 |
| H | 3.797453000 | -0.051826000 | -1.081343000 |
| C | 5.705854000 | -0.969098000 | -0.709627000 |
| H | 6.258289000 | -0.212025000 | -1.259641000 |
| C | 6.383383000 | -2.022329000 | -0.094786000 |
| H | 7.465380000 | -2.088790000 | -0.167573000 |
| C | 5.670892000 | -2.984524000 | 0.619228000 |
| H | 6.195688000 | -3.803904000 | 1.102844000 |
| C | 4.282156000 | -2.902437000 | 0.717505000 |
| H | 3.735405000 | -3.656222000 | 1.276604000 |
| C | 1.260117000 | -2.761635000 | 1.600141000 |
| C | 1.340880000 | -2.223248000 | 2.891924000 |
| H | 1.678185000 | -1.200087000 | 3.037378000 |
| C | 0.998133000 | -2.999725000 | 3.996516000 |
| H | 1.069757000 | -2.578098000 | 4.995567000 |
| C | 0.564254000 | -4.314048000 | 3.819369000 |
| H | 0.294294000 | -4.918204000 | 4.681200000 |
| C | 0.479990000 | -4.852332000 | 2.536110000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.145685000 | -5.876655000 | 2.395291000 |
| C | 0.827587000 | -4.081237000 | 1.427267000 |
| H | 0.765021000 | -4.507471000 | 0.430035000 |
| C | 1.152132000 | -2.549822000 | -1.339662000 |
| C | -0.196182000 | -2.293387000 | -1.694718000 |
| C | -0.661874000 | -2.809579000 | -2.921377000 |
| H | -1.691982000 | -2.617680000 | -3.210458000 |
| C | 0.164288000 | -3.568901000 | -3.742559000 |
| H | -0.225551000 | -3.959050000 | -4.679375000 |
| C | 1.487893000 | -3.828843000 | -3.373829000 |
| H | 2.129614000 | -4.429578000 | -4.011847000 |
| C | 1.977771000 | -3.307972000 | -2.179976000 |
| H | 3.008321000 | -3.494513000 | -1.890580000 |
| C | -2.262144000 | -2.030918000 | -0.507298000 |
| C | -2.555174000 | -3.410757000 | -0.576286000 |
| H | -1.796071000 | -4.099343000 | -0.932085000 |
| C | -3.789826000 | -3.909702000 | -0.182231000 |
| H | -3.969210000 | -4.980185000 | -0.246826000 |
| C | -4.788784000 | -3.065262000 | 0.307673000 |
| H | -5.750256000 | -3.461048000 | 0.620003000 |
| C | -4.518181000 | -1.706170000 | 0.402608000 |
| H | -5.269745000 | -1.030226000 | 0.803470000 |
| C | -3.281928000 | -1.187303000 | -0.003692000 |
| C | -3.568817000 | 1.036687000 | 1.818116000 |
| C | -4.508064000 | 2.054072000 | 2.016621000 |
| H | -4.913500000 | 2.601886000 | 1.171574000 |
| C | -4.950710000 | 2.358331000 | 3.305159000 |
| H | -5.685732000 | 3.146320000 | 3.445764000 |
| C | -4.464732000 | 1.650915000 | 4.401804000 |
| H | -4.813942000 | 1.888336000 | 5.402851000 |
| C | -3.534958000 | 0.627870000 | 4.208606000 |
| H | -3.161754000 | 0.061741000 | 5.057913000 |
| C | -3.085936000 | 0.323250000 | 2.926837000 |
| H | -2.376986000 | -0.489601000 | 2.786861000 |
| C | -3.943231000 | 1.478923000 | -1.070548000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.792464000 | 0.801063000 | -1.952785000 |
| H | -4.877853000 | -0.280208000 | -1.899569000 |
| C | -5.537541000 | 1.511701000 | -2.894719000 |
| H | -6.196638000 | 0.975049000 | -3.571883000 |
| C | -5.446773000 | 2.900695000 | -2.963207000 |
| H | -6.033823000 | 3.450494000 | -3.693611000 |
| C | -4.600082000 | 3.584608000 | -2.089311000 |
| H | -4.527005000 | 4.668052000 | -2.134974000 |
| C | -3.844394000 | 2.877912000 | -1.155566000 |
| H | -3.181435000 | 3.419007000 | -0.483005000 |
| C | 0.323495000 | 1.265212000 | 1.964269000 |
| C | -0.234752000 | 2.427548000 | 1.384951000 |
| H | -1.261598000 | 2.668280000 | 1.660915000 |
| C | 0.301564000 | 3.123120000 | 0.308862000 |
| C | 1.782214000 | 3.124066000 | -0.011841000 |
| H | 1.943470000 | 3.409395000 | -1.059455000 |
| H | 2.230440000 | 2.115812000 | 0.102484000 |
| Y | -0.020283000 | 0.515035000 | -0.400174000 |
| H | -0.261278000 | 3.974673000 | -0.068208000 |
| H | 1.410275000 | 1.169455000 | 2.016681000 |
| H | -0.202669000 | 0.803069000 | 2.794662000 |
| C | -0.615053000 | 2.428659000 | -2.649702000 |
| C | -0.043546000 | 1.267405000 | -3.054154000 |
| H | -0.014498000 | 3.311430000 | -2.450439000 |
| H | -1.693528000 | 2.547751000 | -2.610007000 |
| H | -0.677460000 | 0.426459000 | -3.345625000 |
| C | 1.399674000 | 1.082018000 | -3.179916000 |
| C | 1.973131000 | -0.075879000 | -3.556450000 |
| H | 2.023699000 | 1.953866000 | -2.981310000 |
| H | 3.049938000 | -0.162885000 | -3.664323000 |
| H | 1.382961000 | -0.957761000 | -3.793236000 |

104

theta1_TS2_trans_1,4 E = -1968.280142 a.u. Imaginary frequency=210i

| | | | |
|---|--------------|-------------|--------------|
| N | 1.847680000 | 1.518197000 | -0.113007000 |
| P | -1.044541000 | 2.246284000 | 0.133485000 |

| | | | |
|----|--------------|--------------|--------------|
| P | 2.789857000 | -1.284066000 | 0.145725000 |
| Si | -6.586038000 | -2.921844000 | 0.099766000 |
| C | -4.886624000 | -3.604136000 | 0.626001000 |
| H | -5.002859000 | -4.675070000 | 0.849177000 |
| H | -4.603350000 | -3.133963000 | 1.579101000 |
| C | -7.158163000 | -3.771501000 | -1.486698000 |
| H | -6.474516000 | -3.587517000 | -2.324382000 |
| H | -8.147361000 | -3.405978000 | -1.788107000 |
| H | -7.237555000 | -4.857384000 | -1.354837000 |
| C | -7.810924000 | -3.258764000 | 1.493823000 |
| H | -7.904997000 | -4.332866000 | 1.693797000 |
| H | -8.810204000 | -2.883312000 | 1.242489000 |
| H | -7.502148000 | -2.773645000 | 2.427735000 |
| C | -6.451858000 | -1.057296000 | -0.193016000 |
| H | -6.111189000 | -0.532888000 | 0.708516000 |
| H | -7.425896000 | -0.634835000 | -0.468160000 |
| H | -5.753786000 | -0.817229000 | -1.004796000 |
| C | -2.658225000 | 2.976913000 | -0.363333000 |
| C | -3.252659000 | 2.542383000 | -1.555954000 |
| H | -2.763265000 | 1.782829000 | -2.161743000 |
| C | -4.467141000 | 3.079863000 | -1.975248000 |
| H | -4.919563000 | 2.738733000 | -2.902475000 |
| C | -5.105050000 | 4.047069000 | -1.198254000 |
| H | -6.056185000 | 4.461913000 | -1.520194000 |
| C | -4.524726000 | 4.476178000 | -0.005361000 |
| H | -5.021546000 | 5.226604000 | 0.603436000 |
| C | -3.305115000 | 3.946048000 | 0.413912000 |
| H | -2.861264000 | 4.284003000 | 1.346054000 |
| C | -0.913431000 | 2.513058000 | 1.949047000 |
| C | -1.520951000 | 1.576197000 | 2.797280000 |
| H | -2.055450000 | 0.724740000 | 2.379268000 |
| C | -1.457981000 | 1.738070000 | 4.179563000 |
| H | -1.935759000 | 1.011642000 | 4.831381000 |
| C | -0.780940000 | 2.830195000 | 4.723347000 |
| H | -0.728171000 | 2.954429000 | 5.801427000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -0.172660000 | 3.762352000 | 3.883355000 |
| H | 0.352556000 | 4.614819000 | 4.305518000 |
| C | -0.236922000 | 3.607718000 | 2.498946000 |
| H | 0.236878000 | 4.337472000 | 1.848224000 |
| C | 0.248298000 | 3.298746000 | -0.655743000 |
| C | 1.568950000 | 2.780133000 | -0.679884000 |
| C | 2.557394000 | 3.532613000 | -1.344011000 |
| H | 3.572764000 | 3.146694000 | -1.373290000 |
| C | 2.251665000 | 4.741689000 | -1.955518000 |
| H | 3.036018000 | 5.297266000 | -2.463126000 |
| C | 0.945371000 | 5.238921000 | -1.933699000 |
| H | 0.707604000 | 6.184619000 | -2.411941000 |
| C | -0.050869000 | 4.511375000 | -1.292219000 |
| H | -1.069566000 | 4.888892000 | -1.274564000 |
| C | 2.942712000 | 1.413152000 | 0.753211000 |
| C | 3.492142000 | 2.518996000 | 1.434332000 |
| H | 3.068802000 | 3.505293000 | 1.274511000 |
| C | 4.553663000 | 2.367099000 | 2.318192000 |
| H | 4.943195000 | 3.244427000 | 2.828775000 |
| C | 5.112445000 | 1.112135000 | 2.567905000 |
| H | 5.939236000 | 0.998975000 | 3.262337000 |
| C | 4.582392000 | 0.005097000 | 1.915335000 |
| H | 4.993139000 | -0.983514000 | 2.104534000 |
| C | 3.519351000 | 0.144939000 | 1.016039000 |
| C | 2.969095000 | -2.710615000 | 1.300500000 |
| C | 3.953794000 | -3.692809000 | 1.144328000 |
| H | 4.650395000 | -3.641788000 | 0.312931000 |
| C | 4.047750000 | -4.741118000 | 2.060371000 |
| H | 4.816619000 | -5.498082000 | 1.931357000 |
| C | 3.166903000 | -4.815141000 | 3.137380000 |
| H | 3.243452000 | -5.632797000 | 3.848699000 |
| C | 2.188003000 | -3.834272000 | 3.303075000 |
| H | 1.502455000 | -3.882731000 | 4.144752000 |
| C | 2.086327000 | -2.789994000 | 2.387881000 |
| H | 1.328420000 | -2.023129000 | 2.536546000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.901926000 | -1.649547000 | -1.282892000 |
| C | 4.968437000 | -0.808782000 | -1.622043000 |
| H | 5.201320000 | 0.049687000 | -0.998465000 |
| C | 5.741304000 | -1.081310000 | -2.751711000 |
| H | 6.570756000 | -0.426281000 | -3.004496000 |
| C | 5.460641000 | -2.191413000 | -3.546397000 |
| H | 6.067934000 | -2.402097000 | -4.422297000 |
| C | 4.401407000 | -3.036646000 | -3.211099000 |
| H | 4.183660000 | -3.908944000 | -3.821522000 |
| C | 3.620897000 | -2.763499000 | -2.090447000 |
| H | 2.804732000 | -3.434606000 | -1.830198000 |
| C | -0.943031000 | -1.965473000 | -0.016051000 |
| C | -1.274918000 | -3.359790000 | 0.306828000 |
| H | -0.449216000 | -3.941243000 | 0.717193000 |
| C | -2.448343000 | -3.990527000 | 0.109862000 |
| C | -3.742145000 | -3.419270000 | -0.390791000 |
| H | -4.013703000 | -3.925005000 | -1.329558000 |
| H | -3.632511000 | -2.355088000 | -0.638147000 |
| Y | 0.354790000 | -0.042405000 | -0.843894000 |
| H | -2.492569000 | -5.045169000 | 0.384541000 |
| H | -1.835265000 | -1.324255000 | -0.127795000 |
| H | -0.316487000 | -1.569976000 | 0.816285000 |
| C | -0.350577000 | -2.356656000 | -2.118744000 |
| C | 0.274986000 | -1.361046000 | -2.895861000 |
| H | -1.418022000 | -2.527986000 | -2.239568000 |
| H | 0.203751000 | -3.252865000 | -1.860295000 |
| H | 1.353787000 | -1.402543000 | -3.066106000 |
| C | -0.456114000 | -0.203974000 | -3.349082000 |
| C | 0.072244000 | 1.045866000 | -3.501919000 |
| H | -1.543339000 | -0.308500000 | -3.415446000 |
| H | -0.540227000 | 1.890198000 | -3.800261000 |
| H | 1.150364000 | 1.217648000 | -3.486003000 |

104

theta1_P2_trans_1,4 E = -1968.321992 a.u.

| | | | |
|---|-------------|-------------|--------------|
| N | 2.222231000 | 1.424667000 | -0.407954000 |
|---|-------------|-------------|--------------|

| | | | |
|----|--------------|--------------|--------------|
| P | -0.581630000 | 2.331034000 | 0.107945000 |
| P | 2.735691000 | -1.413813000 | 0.206763000 |
| Si | -7.327965000 | -1.786730000 | 0.208395000 |
| C | -5.817906000 | -2.682518000 | 0.944310000 |
| H | -6.187547000 | -3.468050000 | 1.620415000 |
| H | -5.265823000 | -1.979632000 | 1.585509000 |
| C | -8.432124000 | -3.024409000 | -0.693777000 |
| H | -7.913363000 | -3.505140000 | -1.531810000 |
| H | -9.322403000 | -2.530735000 | -1.102024000 |
| H | -8.777226000 | -3.816606000 | -0.018438000 |
| C | -8.287525000 | -0.974541000 | 1.616226000 |
| H | -8.627195000 | -1.715065000 | 2.350361000 |
| H | -9.177102000 | -0.454794000 | 1.240206000 |
| H | -7.674937000 | -0.236984000 | 2.148885000 |
| C | -6.745960000 | -0.457465000 | -1.008023000 |
| H | -6.066893000 | 0.257231000 | -0.526158000 |
| H | -7.597879000 | 0.110196000 | -1.401939000 |
| H | -6.223180000 | -0.896474000 | -1.866884000 |
| C | -2.208103000 | 3.099570000 | -0.264920000 |
| C | -3.007369000 | 2.527040000 | -1.263889000 |
| H | -2.667882000 | 1.640534000 | -1.796583000 |
| C | -4.240880000 | 3.088983000 | -1.584848000 |
| H | -4.854527000 | 2.639885000 | -2.360617000 |
| C | -4.690330000 | 4.217961000 | -0.899355000 |
| H | -5.656078000 | 4.651721000 | -1.143357000 |
| C | -3.904366000 | 4.785413000 | 0.103123000 |
| H | -4.255389000 | 5.661881000 | 0.640758000 |
| C | -2.665500000 | 4.231610000 | 0.421825000 |
| H | -2.060261000 | 4.676439000 | 1.206691000 |
| C | -0.142483000 | 2.843775000 | 1.814951000 |
| C | -0.642788000 | 2.081603000 | 2.879671000 |
| H | -1.267748000 | 1.211960000 | 2.685437000 |
| C | -0.354078000 | 2.443884000 | 4.193346000 |
| H | -0.747857000 | 1.853101000 | 5.015805000 |
| C | 0.440426000 | 3.561647000 | 4.450051000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.668601000 | 3.841281000 | 5.474800000 |
| C | 0.940971000 | 4.320476000 | 3.392702000 |
| H | 1.557151000 | 5.192980000 | 3.591952000 |
| C | 0.651916000 | 3.966086000 | 2.075597000 |
| H | 1.042313000 | 4.561321000 | 1.254796000 |
| C | 0.625904000 | 3.154970000 | -1.031577000 |
| C | 1.937433000 | 2.606722000 | -1.113367000 |
| C | 2.858692000 | 3.214391000 | -1.991998000 |
| H | 3.860559000 | 2.800159000 | -2.064426000 |
| C | 2.495052000 | 4.310500000 | -2.760163000 |
| H | 3.223614000 | 4.759703000 | -3.429990000 |
| C | 1.195724000 | 4.827590000 | -2.694440000 |
| H | 0.914347000 | 5.682423000 | -3.302349000 |
| C | 0.267215000 | 4.244654000 | -1.842636000 |
| H | -0.740061000 | 4.646675000 | -1.783330000 |
| C | 3.381618000 | 1.285404000 | 0.355483000 |
| C | 4.166024000 | 2.374384000 | 0.780117000 |
| H | 3.886010000 | 3.381061000 | 0.485369000 |
| C | 5.278591000 | 2.178633000 | 1.590762000 |
| H | 5.858688000 | 3.041561000 | 1.908132000 |
| C | 5.648906000 | 0.899899000 | 2.010761000 |
| H | 6.515500000 | 0.754754000 | 2.648413000 |
| C | 4.883175000 | -0.188488000 | 1.604781000 |
| H | 5.150528000 | -1.189492000 | 1.933727000 |
| C | 3.767640000 | -0.009991000 | 0.781513000 |
| C | 2.631687000 | -2.587703000 | 1.621303000 |
| C | 3.554454000 | -3.624854000 | 1.806729000 |
| H | 4.351392000 | -3.783392000 | 1.085852000 |
| C | 3.449193000 | -4.463169000 | 2.915875000 |
| H | 4.168585000 | -5.266022000 | 3.052241000 |
| C | 2.428745000 | -4.272558000 | 3.846420000 |
| H | 2.349184000 | -4.928706000 | 4.708701000 |
| C | 1.508867000 | -3.238835000 | 3.669126000 |
| H | 0.712129000 | -3.086591000 | 4.392140000 |
| C | 1.607091000 | -2.402442000 | 2.559725000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.889199000 | -1.594239000 | 2.432934000 |
| C | 3.739821000 | -2.270344000 | -1.085215000 |
| C | 4.828528000 | -1.636101000 | -1.696507000 |
| H | 5.152868000 | -0.659394000 | -1.349053000 |
| C | 5.510577000 | -2.265626000 | -2.738214000 |
| H | 6.358699000 | -1.768617000 | -3.201442000 |
| C | 5.116454000 | -3.528950000 | -3.175177000 |
| H | 5.653458000 | -4.018316000 | -3.982942000 |
| C | 4.034669000 | -4.168159000 | -2.567427000 |
| H | 3.728749000 | -5.157297000 | -2.897265000 |
| C | 3.343700000 | -3.540841000 | -1.533602000 |
| H | 2.509355000 | -4.052685000 | -1.059141000 |
| C | -1.704325000 | -2.792477000 | -0.269938000 |
| C | -2.418442000 | -3.862278000 | 0.505006000 |
| H | -1.763672000 | -4.546324000 | 1.047170000 |
| C | -3.738729000 | -4.077692000 | 0.570934000 |
| C | -4.848522000 | -3.304254000 | -0.080648000 |
| H | -5.405633000 | -3.993330000 | -0.732925000 |
| H | -4.449553000 | -2.522456000 | -0.738239000 |
| Y | 0.600948000 | 0.061344000 | -1.085929000 |
| H | -4.074315000 | -4.918569000 | 1.180772000 |
| H | -2.408866000 | -2.022957000 | -0.611827000 |
| H | -0.987311000 | -2.291272000 | 0.408728000 |
| C | -0.913964000 | -3.335634000 | -1.478823000 |
| C | -0.101578000 | -2.277112000 | -2.194478000 |
| H | -1.620618000 | -3.819084000 | -2.167170000 |
| H | -0.244433000 | -4.131373000 | -1.130833000 |
| H | 0.959465000 | -2.493408000 | -2.359381000 |
| C | -0.660971000 | -1.257066000 | -2.944072000 |
| C | 0.057797000 | -0.142191000 | -3.460243000 |
| H | -1.752955000 | -1.168859000 | -2.928450000 |
| H | -0.470258000 | 0.586961000 | -4.070509000 |
| H | 1.089007000 | -0.322121000 | -3.795963000 |

97

P1_trans_1,4_isoprene E = -1851.721475 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 0.291849000 | -1.825031000 | -0.435253000 |
| P | 2.694031000 | -0.104714000 | 0.148901000 |
| P | -2.393250000 | -0.663717000 | 0.200968000 |
| Si | -0.793580000 | 4.675742000 | 0.480509000 |
| C | -0.634212000 | 2.975068000 | -0.417369000 |
| H | -1.166542000 | 2.270726000 | 0.253961000 |
| H | 0.455984000 | 2.779059000 | -0.379965000 |
| C | -2.619961000 | 5.060513000 | 0.717181000 |
| H | -3.146591000 | 5.182874000 | -0.236378000 |
| H | -2.739960000 | 5.998626000 | 1.272643000 |
| H | -3.128864000 | 4.274626000 | 1.288136000 |
| C | 0.069999000 | 4.483292000 | 2.144232000 |
| H | -0.394455000 | 3.696565000 | 2.751252000 |
| H | 0.014097000 | 5.414354000 | 2.721044000 |
| H | 1.133335000 | 4.240868000 | 2.024172000 |
| C | 0.054556000 | 5.988571000 | -0.567138000 |
| H | 1.110626000 | 5.750533000 | -0.743584000 |
| H | 0.020235000 | 6.960292000 | -0.059681000 |
| H | -0.430192000 | 6.114605000 | -1.542121000 |
| C | 4.309318000 | 0.723833000 | -0.149975000 |
| C | 4.395314000 | 1.676237000 | -1.175521000 |
| H | 3.521256000 | 1.905721000 | -1.780456000 |
| C | 5.601566000 | 2.323949000 | -1.431962000 |
| H | 5.661383000 | 3.057494000 | -2.231470000 |
| C | 6.726426000 | 2.036339000 | -0.658325000 |
| H | 7.665242000 | 2.547235000 | -0.853584000 |
| C | 6.644211000 | 1.095967000 | 0.367776000 |
| H | 7.518196000 | 0.871336000 | 0.973045000 |
| C | 5.441647000 | 0.438578000 | 0.623550000 |
| H | 5.386072000 | -0.290676000 | 1.426662000 |
| C | 2.800964000 | -0.796656000 | 1.851107000 |
| C | 2.496776000 | 0.051167000 | 2.925953000 |
| H | 2.212938000 | 1.086091000 | 2.742815000 |
| C | 2.577436000 | -0.419507000 | 4.234820000 |
| H | 2.349086000 | 0.244905000 | 5.063900000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 2.952085000 | -1.741208000 | 4.478378000 |
| H | 3.011396000 | -2.109648000 | 5.498775000 |
| C | 3.252998000 | -2.588244000 | 3.412452000 |
| H | 3.549269000 | -3.616556000 | 3.601018000 |
| C | 3.180027000 | -2.120227000 | 2.100893000 |
| H | 3.419820000 | -2.781759000 | 1.273264000 |
| C | 2.657029000 | -1.559550000 | -0.997364000 |
| C | 1.434671000 | -2.274167000 | -1.125691000 |
| C | 1.390355000 | -3.355731000 | -2.029104000 |
| H | 0.458994000 | -3.904894000 | -2.138365000 |
| C | 2.506090000 | -3.714029000 | -2.772853000 |
| H | 2.443493000 | -4.553063000 | -3.461009000 |
| C | 3.699706000 | -2.994443000 | -2.654617000 |
| H | 4.570829000 | -3.274546000 | -3.239673000 |
| C | 3.766334000 | -1.918130000 | -1.778654000 |
| H | 4.691349000 | -1.357121000 | -1.681676000 |
| C | -0.501017000 | -2.715663000 | 0.291039000 |
| C | -0.049843000 | -3.987117000 | 0.699083000 |
| H | 0.946378000 | -4.312818000 | 0.416932000 |
| C | -0.849301000 | -4.819671000 | 1.472457000 |
| H | -0.463584000 | -5.790953000 | 1.772271000 |
| C | -2.124301000 | -4.421666000 | 1.880682000 |
| H | -2.741694000 | -5.073490000 | 2.491096000 |
| C | -2.585590000 | -3.167895000 | 1.497166000 |
| H | -3.569961000 | -2.832752000 | 1.815439000 |
| C | -1.799884000 | -2.323224000 | 0.703900000 |
| C | -3.106706000 | 0.055962000 | 1.747674000 |
| C | -2.203800000 | 0.420852000 | 2.758794000 |
| H | -1.136155000 | 0.245118000 | 2.631138000 |
| C | -2.664799000 | 0.967457000 | 3.953480000 |
| H | -1.957587000 | 1.233343000 | 4.734719000 |
| C | -4.032671000 | 1.166475000 | 4.148586000 |
| H | -4.393332000 | 1.595398000 | 5.079361000 |
| C | -4.933722000 | 0.804790000 | 3.149694000 |
| H | -6.000553000 | 0.946344000 | 3.300609000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -4.476625000 | 0.248983000 | 1.953529000 |
| H | -5.191519000 | -0.038972000 | 1.188619000 |
| C | -3.816875000 | -0.936975000 | -0.939172000 |
| C | -4.549344000 | 0.173253000 | -1.389352000 |
| H | -4.310538000 | 1.169986000 | -1.024470000 |
| C | -5.597142000 | 0.006785000 | -2.291447000 |
| H | -6.166768000 | 0.871144000 | -2.622333000 |
| C | -5.911582000 | -1.265985000 | -2.770956000 |
| H | -6.726157000 | -1.394747000 | -3.478283000 |
| C | -5.179287000 | -2.369534000 | -2.338609000 |
| H | -5.421314000 | -3.362912000 | -2.706664000 |
| C | -4.137440000 | -2.210120000 | -1.423818000 |
| H | -3.580457000 | -3.077959000 | -1.083697000 |
| C | -1.213245000 | 2.953951000 | -1.860818000 |
| C | -1.395674000 | 1.624669000 | -2.596239000 |
| H | -0.588733000 | 3.620817000 | -2.472136000 |
| H | -2.202677000 | 3.422706000 | -1.814638000 |
| C | -0.395016000 | 1.028205000 | -3.365822000 |
| C | 0.977156000 | 1.253735000 | -3.086914000 |
| H | 1.727822000 | 0.771017000 | -3.708718000 |
| H | 1.269920000 | 2.243907000 | -2.721199000 |
| Y | 0.090474000 | 0.336736000 | -0.934472000 |
| H | -2.422945000 | 1.336644000 | -2.805868000 |
| C | -0.766481000 | -0.078117000 | -4.328427000 |
| H | -0.755543000 | 0.324328000 | -5.349304000 |
| H | -0.046846000 | -0.904706000 | -4.304994000 |
| H | -1.768653000 | -0.475093000 | -4.138300000 |

110

theta3_C2_trans_1,4_isoprene E = -2046.896924 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.662132000 | -1.622648000 | 0.789569000 |
| P | -2.715206000 | 0.556429000 | 0.275195000 |
| P | 2.179014000 | -1.260824000 | 0.157973000 |
| Si | 3.330448000 | 4.558116000 | -0.447869000 |
| C | 1.752037000 | 3.876354000 | -1.269518000 |
| H | 1.930399000 | 3.829234000 | -2.353771000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.955467000 | 4.622977000 | -1.133673000 |
| C | 4.774727000 | 3.368662000 | -0.716206000 |
| H | 4.613841000 | 2.386278000 | -0.256243000 |
| H | 5.697016000 | 3.778931000 | -0.286952000 |
| H | 4.958081000 | 3.206838000 | -1.785703000 |
| C | 3.730275000 | 6.215019000 | -1.256435000 |
| H | 3.917236000 | 6.102599000 | -2.331167000 |
| H | 4.627268000 | 6.663542000 | -0.812471000 |
| H | 2.910017000 | 6.932763000 | -1.135699000 |
| C | 3.032195000 | 4.815550000 | 1.401734000 |
| H | 2.241895000 | 5.556410000 | 1.574322000 |
| H | 3.938665000 | 5.185264000 | 1.896315000 |
| H | 2.733738000 | 3.890738000 | 1.910019000 |
| C | -2.977584000 | 2.317046000 | 0.785586000 |
| C | -1.913141000 | 2.966859000 | 1.428632000 |
| H | -0.989236000 | 2.430050000 | 1.631303000 |
| C | -2.039490000 | 4.289647000 | 1.841913000 |
| H | -1.210647000 | 4.777162000 | 2.348172000 |
| C | -3.228251000 | 4.984302000 | 1.611924000 |
| H | -3.327146000 | 6.017431000 | 1.933379000 |
| C | -4.290025000 | 4.343975000 | 0.978224000 |
| H | -5.223569000 | 4.873524000 | 0.807828000 |
| C | -4.169850000 | 3.014833000 | 0.568069000 |
| H | -5.015194000 | 2.525833000 | 0.094455000 |
| C | -4.371537000 | -0.012400000 | -0.322375000 |
| C | -4.881748000 | 0.515492000 | -1.519420000 |
| H | -4.322016000 | 1.273063000 | -2.064996000 |
| C | -6.114199000 | 0.090780000 | -2.011708000 |
| H | -6.505053000 | 0.518130000 | -2.931452000 |
| C | -6.844240000 | -0.879890000 | -1.323197000 |
| H | -7.804208000 | -1.213161000 | -1.707724000 |
| C | -6.340032000 | -1.414245000 | -0.138949000 |
| H | -6.906875000 | -2.165314000 | 0.404799000 |
| C | -5.111114000 | -0.982292000 | 0.363019000 |
| H | -4.731330000 | -1.396154000 | 1.292286000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -2.425690000 | -0.301742000 | 1.865349000 |
| C | -1.427778000 | -1.308520000 | 1.919355000 |
| C | -1.213749000 | -1.923153000 | 3.173571000 |
| H | -0.439421000 | -2.676952000 | 3.267131000 |
| C | -1.952086000 | -1.568710000 | 4.294073000 |
| H | -1.746482000 | -2.065182000 | 5.239289000 |
| C | -2.933248000 | -0.576849000 | 4.226660000 |
| H | -3.506141000 | -0.297439000 | 5.105536000 |
| C | -3.151370000 | 0.056327000 | 3.010184000 |
| H | -3.896198000 | 0.845127000 | 2.937994000 |
| C | 0.013580000 | -2.859354000 | 0.779254000 |
| C | -0.634296000 | -4.083146000 | 1.039278000 |
| H | -1.673503000 | -4.070238000 | 1.357443000 |
| C | 0.033787000 | -5.294632000 | 0.891642000 |
| H | -0.495339000 | -6.223112000 | 1.091276000 |
| C | 1.369072000 | -5.327335000 | 0.481378000 |
| H | 1.885899000 | -6.274874000 | 0.360751000 |
| C | 2.038579000 | -4.128781000 | 0.247141000 |
| H | 3.084679000 | -4.140632000 | -0.047061000 |
| C | 1.380825000 | -2.903741000 | 0.409443000 |
| C | 3.829623000 | -1.631156000 | -0.582868000 |
| C | 4.930173000 | -2.000858000 | 0.202766000 |
| H | 4.832721000 | -2.063635000 | 1.282913000 |
| C | 6.157235000 | -2.279289000 | -0.396803000 |
| H | 7.004702000 | -2.563443000 | 0.221138000 |
| C | 6.300106000 | -2.190186000 | -1.781427000 |
| H | 7.259441000 | -2.404309000 | -2.244388000 |
| C | 5.212748000 | -1.815351000 | -2.569372000 |
| H | 5.322081000 | -1.732273000 | -3.647465000 |
| C | 3.985924000 | -1.531550000 | -1.971888000 |
| H | 3.147688000 | -1.221154000 | -2.590111000 |
| C | 2.576755000 | -0.710693000 | 1.878159000 |
| C | 2.562694000 | -1.600042000 | 2.959440000 |
| H | 2.286959000 | -2.639123000 | 2.805305000 |
| C | 2.914043000 | -1.159276000 | 4.234927000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 2.903514000 | -1.858374000 | 5.066934000 |
| C | 3.282030000 | 0.169043000 | 4.441874000 |
| H | 3.556895000 | 0.509895000 | 5.436270000 |
| C | 3.301986000 | 1.058694000 | 3.368016000 |
| H | 3.597058000 | 2.092942000 | 3.522169000 |
| C | 2.948084000 | 0.623040000 | 2.092638000 |
| H | 2.973015000 | 1.322527000 | 1.261961000 |
| C | 0.442664000 | -2.431104000 | -3.382268000 |
| C | -0.502580000 | -2.851079000 | -2.508062000 |
| H | -0.220314000 | -3.567113000 | -1.738147000 |
| C | -1.917270000 | -2.440476000 | -2.530075000 |
| C | -2.297623000 | -1.274438000 | -3.108606000 |
| H | -3.336111000 | -0.960580000 | -3.106100000 |
| H | -1.602289000 | -0.665552000 | -3.684947000 |
| Y | -0.337558000 | -0.384340000 | -1.145778000 |
| H | 1.468339000 | -2.775340000 | -3.288994000 |
| H | 0.202066000 | -1.846018000 | -4.262666000 |
| C | 1.227504000 | 2.501333000 | -0.798685000 |
| C | -0.051846000 | 2.130497000 | -1.543103000 |
| H | 2.015716000 | 1.750266000 | -0.945886000 |
| H | 1.035146000 | 2.534465000 | 0.281853000 |
| H | -0.877499000 | 2.807588000 | -1.319357000 |
| C | -0.026044000 | 1.631429000 | -2.866861000 |
| C | 0.912416000 | 0.686210000 | -3.295493000 |
| H | 0.907611000 | 0.359787000 | -4.331591000 |
| H | 1.883901000 | 0.622098000 | -2.804367000 |
| C | -1.169885000 | 2.003598000 | -3.784987000 |
| H | -0.984005000 | 3.012611000 | -4.174249000 |
| H | -1.263502000 | 1.335334000 | -4.647102000 |
| H | -2.130261000 | 2.043465000 | -3.257862000 |
| C | -2.898130000 | -3.355573000 | -1.855978000 |
| H | -2.977427000 | -4.287203000 | -2.431658000 |
| H | -2.557135000 | -3.629632000 | -0.852563000 |
| H | -3.891385000 | -2.906918000 | -1.785258000 |

theta3_TS2_trans_1,4_isoprene E = -2046.887531 a.u. Imaginary frequency=154i

| | | | |
|----|--------------|--------------|--------------|
| N | -0.236484000 | -1.340820000 | 1.032706000 |
| P | -2.852619000 | -0.055299000 | 0.156456000 |
| P | 2.531037000 | -0.917888000 | 0.044521000 |
| Si | 1.703981000 | 5.244654000 | -0.224238000 |
| C | 0.441394000 | 4.113903000 | -1.102243000 |
| H | 0.533397000 | 4.296087000 | -2.182861000 |
| H | -0.562800000 | 4.470619000 | -0.830260000 |
| C | 3.444036000 | 4.879448000 | -0.864612000 |
| H | 3.757181000 | 3.846504000 | -0.673074000 |
| H | 4.182128000 | 5.537035000 | -0.389454000 |
| H | 3.508472000 | 5.047891000 | -1.946659000 |
| C | 1.241244000 | 7.019701000 | -0.663806000 |
| H | 1.271857000 | 7.188483000 | -1.746911000 |
| H | 1.935866000 | 7.731451000 | -0.201481000 |
| H | 0.232525000 | 7.273579000 | -0.316459000 |
| C | 1.612033000 | 5.003819000 | 1.645140000 |
| H | 0.604031000 | 5.213649000 | 2.023851000 |
| H | 2.298005000 | 5.690068000 | 2.156974000 |
| H | 1.879230000 | 3.985595000 | 1.950652000 |
| C | -3.681399000 | 1.609512000 | 0.181739000 |
| C | -2.989903000 | 2.690225000 | 0.752676000 |
| H | -2.024777000 | 2.529518000 | 1.226275000 |
| C | -3.546513000 | 3.966882000 | 0.756046000 |
| H | -3.005197000 | 4.787667000 | 1.219337000 |
| C | -4.798477000 | 4.188438000 | 0.181305000 |
| H | -5.234213000 | 5.183674000 | 0.186273000 |
| C | -5.492025000 | 3.121859000 | -0.384970000 |
| H | -6.475319000 | 3.279571000 | -0.820055000 |
| C | -4.940386000 | 1.839659000 | -0.384206000 |
| H | -5.513169000 | 1.019228000 | -0.804149000 |
| C | -4.258121000 | -1.254363000 | 0.000714000 |
| C | -4.912878000 | -1.382419000 | -1.234962000 |
| H | -4.601203000 | -0.778704000 | -2.085333000 |
| C | -5.968975000 | -2.278517000 | -1.389343000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -6.473958000 | -2.357617000 | -2.348465000 |
| C | -6.370950000 | -3.074770000 | -0.316480000 |
| H | -7.190850000 | -3.777406000 | -0.436838000 |
| C | -5.715923000 | -2.965092000 | 0.908411000 |
| H | -6.024232000 | -3.582054000 | 1.748295000 |
| C | -4.667230000 | -2.058767000 | 1.070089000 |
| H | -4.172560000 | -1.975399000 | 2.032832000 |
| C | -2.254474000 | -0.231439000 | 1.881759000 |
| C | -1.021298000 | -0.891803000 | 2.104066000 |
| C | -0.601815000 | -1.035810000 | 3.444851000 |
| H | 0.344397000 | -1.525343000 | 3.648471000 |
| C | -1.361454000 | -0.554190000 | 4.500911000 |
| H | -0.996157000 | -0.680059000 | 5.517161000 |
| C | -2.575496000 | 0.098126000 | 4.270488000 |
| H | -3.170909000 | 0.475309000 | 5.096443000 |
| C | -3.007516000 | 0.257286000 | 2.960487000 |
| H | -3.949442000 | 0.762189000 | 2.762835000 |
| C | 0.573114000 | -2.472580000 | 1.250691000 |
| C | 0.080374000 | -3.631980000 | 1.882911000 |
| H | -0.935376000 | -3.624923000 | 2.268111000 |
| C | 0.861634000 | -4.775127000 | 1.998019000 |
| H | 0.450074000 | -5.655584000 | 2.485153000 |
| C | 2.156520000 | -4.807886000 | 1.473238000 |
| H | 2.761580000 | -5.706502000 | 1.549941000 |
| C | 2.669992000 | -3.668861000 | 0.860427000 |
| H | 3.682156000 | -3.680810000 | 0.466560000 |
| C | 1.905157000 | -2.498650000 | 0.766502000 |
| C | 4.140271000 | -1.347460000 | -0.759293000 |
| C | 5.276737000 | -1.664069000 | 0.000354000 |
| H | 5.225349000 | -1.653980000 | 1.085685000 |
| C | 6.478395000 | -1.977018000 | -0.630394000 |
| H | 7.352009000 | -2.221882000 | -0.032359000 |
| C | 6.564486000 | -1.967898000 | -2.023312000 |
| H | 7.504832000 | -2.207835000 | -2.511853000 |
| C | 5.446381000 | -1.636377000 | -2.785737000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 5.512654000 | -1.611474000 | -3.870232000 |
| C | 4.242596000 | -1.323955000 | -2.154702000 |
| H | 3.380493000 | -1.042028000 | -2.751055000 |
| C | 3.100909000 | 0.044818000 | 1.519599000 |
| C | 3.092098000 | -0.480058000 | 2.815807000 |
| H | 2.713347000 | -1.482104000 | 2.993276000 |
| C | 3.593856000 | 0.270380000 | 3.879975000 |
| H | 3.586016000 | -0.148172000 | 4.882920000 |
| C | 4.115247000 | 1.543096000 | 3.657851000 |
| H | 4.511884000 | 2.122489000 | 4.486984000 |
| C | 4.135426000 | 2.068203000 | 2.365072000 |
| H | 4.552182000 | 3.054739000 | 2.182309000 |
| C | 3.625075000 | 1.325810000 | 1.302965000 |
| H | 3.660020000 | 1.736633000 | 0.296691000 |
| C | 0.767244000 | -1.592763000 | -3.647893000 |
| C | 0.558094000 | -2.522913000 | -2.629316000 |
| H | 1.419192000 | -3.010833000 | -2.176466000 |
| C | -0.762903000 | -2.985396000 | -2.249888000 |
| C | -1.877385000 | -2.232467000 | -2.509228000 |
| H | -2.861606000 | -2.570477000 | -2.208303000 |
| H | -1.856386000 | -1.386806000 | -3.199977000 |
| Y | -0.205801000 | -0.581053000 | -1.125322000 |
| H | 1.774874000 | -1.445906000 | -4.017936000 |
| H | -0.016254000 | -1.422830000 | -4.380442000 |
| C | 0.500240000 | 2.586939000 | -0.858303000 |
| C | -0.595820000 | 1.934702000 | -1.684245000 |
| H | 1.494022000 | 2.208071000 | -1.127320000 |
| H | 0.370450000 | 2.386326000 | 0.214935000 |
| H | -1.589439000 | 2.323391000 | -1.466470000 |
| C | -0.424177000 | 1.386763000 | -2.955112000 |
| C | 0.774680000 | 0.750795000 | -3.383525000 |
| H | 0.916791000 | 0.642372000 | -4.453703000 |
| H | 1.702197000 | 0.959106000 | -2.847535000 |
| C | -1.610391000 | 1.360070000 | -3.895501000 |
| H | -1.582572000 | 2.260951000 | -4.522209000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.599153000 | 0.500907000 | -4.575185000 |
| H | -2.562674000 | 1.375558000 | -3.355353000 |
| C | -0.863534000 | -4.284938000 | -1.499707000 |
| H | -0.774839000 | -5.110680000 | -2.217858000 |
| H | -0.059866000 | -4.403590000 | -0.767407000 |
| H | -1.823757000 | -4.383409000 | -0.986852000 |

110

theta3_P2_trans_1,4_isoprene E = -2046.925077 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.100074000 | -1.715696000 | 0.417128000 |
| P | -2.910676000 | 0.662458000 | 0.309895000 |
| P | 1.805553000 | -1.471650000 | 0.198487000 |
| Si | 4.633095000 | 3.816629000 | 0.368168000 |
| C | 2.801961000 | 3.813836000 | -0.178598000 |
| H | 2.720531000 | 4.373427000 | -1.121355000 |
| H | 2.227729000 | 4.392998000 | 0.559951000 |
| C | 5.674802000 | 2.875233000 | -0.893193000 |
| H | 5.393943000 | 1.816911000 | -0.955890000 |
| H | 6.736490000 | 2.912637000 | -0.620403000 |
| H | 5.581597000 | 3.309815000 | -1.896150000 |
| C | 5.190639000 | 5.614917000 | 0.463137000 |
| H | 5.104986000 | 6.114761000 | -0.509147000 |
| H | 6.239104000 | 5.684914000 | 0.777066000 |
| H | 4.593448000 | 6.186015000 | 1.184106000 |
| C | 4.782298000 | 3.002172000 | 2.066027000 |
| H | 4.153287000 | 3.506747000 | 2.809908000 |
| H | 5.816674000 | 3.053526000 | 2.426910000 |
| H | 4.500799000 | 1.942242000 | 2.046605000 |
| C | -3.094915000 | 2.281132000 | 1.186116000 |
| C | -2.096880000 | 2.639329000 | 2.106953000 |
| H | -1.292530000 | 1.943234000 | 2.338873000 |
| C | -2.150033000 | 3.866632000 | 2.762204000 |
| H | -1.380170000 | 4.126709000 | 3.484025000 |
| C | -3.194926000 | 4.755042000 | 2.501178000 |
| H | -3.236870000 | 5.712416000 | 3.013060000 |
| C | -4.189414000 | 4.403853000 | 1.591338000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -5.013192000 | 5.084565000 | 1.393990000 |
| C | -4.143580000 | 3.172168000 | 0.935224000 |
| H | -4.934341000 | 2.905519000 | 0.240218000 |
| C | -4.499901000 | 0.384689000 | -0.589426000 |
| C | -4.763271000 | 1.132471000 | -1.747258000 |
| H | -4.053717000 | 1.884215000 | -2.085046000 |
| C | -5.938670000 | 0.929887000 | -2.466781000 |
| H | -6.136237000 | 1.521911000 | -3.356455000 |
| C | -6.854762000 | -0.035786000 | -2.048512000 |
| H | -7.768657000 | -0.199089000 | -2.612936000 |
| C | -6.593077000 | -0.790525000 | -0.906589000 |
| H | -7.303494000 | -1.543705000 | -0.576544000 |
| C | -5.422968000 | -0.582670000 | -0.176454000 |
| H | -5.230999000 | -1.173488000 | 0.713854000 |
| C | -2.859947000 | -0.575643000 | 1.655283000 |
| C | -1.971050000 | -1.669606000 | 1.505026000 |
| C | -1.972977000 | -2.649999000 | 2.518725000 |
| H | -1.294792000 | -3.493500000 | 2.439243000 |
| C | -2.804255000 | -2.537678000 | 3.625229000 |
| H | -2.771571000 | -3.309207000 | 4.390568000 |
| C | -3.661419000 | -1.444617000 | 3.775835000 |
| H | -4.303135000 | -1.357274000 | 4.647250000 |
| C | -3.677979000 | -0.467317000 | 2.787562000 |
| H | -4.337404000 | 0.391513000 | 2.887356000 |
| C | -0.538025000 | -2.939810000 | 0.015103000 |
| C | -1.310740000 | -4.092030000 | -0.234434000 |
| H | -2.381117000 | -4.054760000 | -0.051336000 |
| C | -0.717294000 | -5.253519000 | -0.710274000 |
| H | -1.331321000 | -6.131747000 | -0.892754000 |
| C | 0.657664000 | -5.297862000 | -0.971030000 |
| H | 1.114634000 | -6.208054000 | -1.348601000 |
| C | 1.438814000 | -4.172952000 | -0.732868000 |
| H | 2.509139000 | -4.206157000 | -0.917790000 |
| C | 0.858725000 | -3.002069000 | -0.224153000 |
| C | 3.524462000 | -1.788111000 | -0.392187000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 4.470050000 | -2.478432000 | 0.377990000 |
| H | 4.207956000 | -2.844431000 | 1.366446000 |
| C | 5.755649000 | -2.690649000 | -0.117384000 |
| H | 6.482792000 | -3.225249000 | 0.487839000 |
| C | 6.109478000 | -2.218819000 | -1.381220000 |
| H | 7.113181000 | -2.385152000 | -1.762652000 |
| C | 5.175439000 | -1.526492000 | -2.151446000 |
| H | 5.448459000 | -1.151087000 | -3.134098000 |
| C | 3.891389000 | -1.306132000 | -1.656064000 |
| H | 3.168483000 | -0.755967000 | -2.253263000 |
| C | 1.916515000 | -1.545992000 | 2.042535000 |
| C | 1.843883000 | -2.763150000 | 2.732409000 |
| H | 1.688938000 | -3.689345000 | 2.185606000 |
| C | 1.970690000 | -2.791690000 | 4.120492000 |
| H | 1.917631000 | -3.741538000 | 4.645959000 |
| C | 2.165351000 | -1.608714000 | 4.832585000 |
| H | 2.262378000 | -1.633942000 | 5.914462000 |
| C | 2.234430000 | -0.393226000 | 4.153163000 |
| H | 2.386968000 | 0.531867000 | 4.702465000 |
| C | 2.109298000 | -0.362321000 | 2.765281000 |
| H | 2.170767000 | 0.590270000 | 2.246034000 |
| C | 0.356385000 | 1.169540000 | -4.099614000 |
| C | 0.544107000 | -0.250251000 | -3.578735000 |
| H | 1.525608000 | -0.670657000 | -3.799188000 |
| C | -0.502292000 | -1.183387000 | -3.502666000 |
| C | -1.809742000 | -0.834477000 | -3.093551000 |
| H | -2.581229000 | -1.599704000 | -3.060790000 |
| H | -2.193280000 | 0.165958000 | -3.316530000 |
| Y | -0.479262000 | -0.172157000 | -1.094624000 |
| H | 0.846233000 | 1.216920000 | -5.082878000 |
| H | -0.703221000 | 1.363864000 | -4.303587000 |
| C | 2.151370000 | 2.424947000 | -0.361682000 |
| C | 0.700528000 | 2.582182000 | -0.737487000 |
| H | 2.704811000 | 1.846817000 | -1.108644000 |
| H | 2.228690000 | 1.865057000 | 0.577280000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.051661000 | 2.914297000 | 0.079098000 |
| C | 0.165088000 | 2.613126000 | -1.986560000 |
| C | 0.941660000 | 2.313253000 | -3.248496000 |
| H | 0.943189000 | 3.230417000 | -3.856601000 |
| H | 1.988708000 | 2.091891000 | -3.021134000 |
| C | -0.167897000 | -2.651160000 | -3.638485000 |
| H | 0.890825000 | -2.855365000 | -3.455506000 |
| H | -0.768010000 | -3.284751000 | -2.978924000 |
| H | -0.388871000 | -2.950679000 | -4.671695000 |
| C | -1.233314000 | 3.144993000 | -2.195797000 |
| H | -1.857774000 | 2.489923000 | -2.815122000 |
| H | -1.750814000 | 3.339494000 | -1.252084000 |
| H | -1.169686000 | 4.097158000 | -2.741388000 |

110

P1_thf_trans_1,4_isoprene E = -2084.07518 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -0.014479000 | -0.171821000 | 1.374792000 |
| P | 2.713262000 | -0.308393000 | 0.079813000 |
| P | -2.758718000 | -0.228744000 | 0.090978000 |
| Si | 0.240037000 | 4.529494000 | -0.382205000 |
| C | 0.010059000 | 2.692358000 | -0.919326000 |
| H | -0.716799000 | 2.287777000 | -0.191001000 |
| H | 0.994587000 | 2.220641000 | -0.734571000 |
| C | -1.454053000 | 5.358774000 | -0.409978000 |
| H | -1.892147000 | 5.393123000 | -1.414297000 |
| H | -1.369805000 | 6.395990000 | -0.062831000 |
| H | -2.162854000 | 4.849692000 | 0.254400000 |
| C | 0.945197000 | 4.562709000 | 1.359522000 |
| H | 0.301158000 | 4.020556000 | 2.061389000 |
| H | 1.031909000 | 5.595909000 | 1.717977000 |
| H | 1.943671000 | 4.113118000 | 1.401474000 |
| C | 1.407674000 | 5.375741000 | -1.595292000 |
| H | 2.394018000 | 4.897239000 | -1.597909000 |
| H | 1.553429000 | 6.425680000 | -1.313132000 |
| H | 1.021867000 | 5.365084000 | -2.621272000 |
| C | 4.039950000 | -1.377914000 | -0.630875000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 3.669531000 | -2.399281000 | -1.514812000 |
| H | 2.621562000 | -2.526206000 | -1.772986000 |
| C | 4.631407000 | -3.241394000 | -2.068656000 |
| H | 4.334076000 | -4.028140000 | -2.757431000 |
| C | 5.978002000 | -3.063906000 | -1.751357000 |
| H | 6.730728000 | -3.714285000 | -2.188311000 |
| C | 6.356712000 | -2.044028000 | -0.879477000 |
| H | 7.405213000 | -1.898864000 | -0.633649000 |
| C | 5.395058000 | -1.202655000 | -0.320996000 |
| H | 5.702585000 | -0.404846000 | 0.349132000 |
| C | 3.622921000 | 1.238382000 | 0.523744000 |
| C | 4.102817000 | 2.048091000 | -0.517444000 |
| H | 3.939699000 | 1.760670000 | -1.554388000 |
| C | 4.820768000 | 3.207298000 | -0.232038000 |
| H | 5.202822000 | 3.819556000 | -1.044640000 |
| C | 5.055142000 | 3.576208000 | 1.094129000 |
| H | 5.615983000 | 4.479972000 | 1.316025000 |
| C | 4.572070000 | 2.780591000 | 2.131582000 |
| H | 4.755997000 | 3.061630000 | 3.165140000 |
| C | 3.858348000 | 1.614311000 | 1.850304000 |
| H | 3.496985000 | 0.990168000 | 2.662637000 |
| C | 2.251742000 | -1.090803000 | 1.675747000 |
| C | 0.923318000 | -0.887497000 | 2.136473000 |
| C | 0.568536000 | -1.510962000 | 3.353812000 |
| H | -0.441659000 | -1.383246000 | 3.731038000 |
| C | 1.471232000 | -2.288237000 | 4.066745000 |
| H | 1.150679000 | -2.755528000 | 4.994800000 |
| C | 2.772540000 | -2.486964000 | 3.597896000 |
| H | 3.477210000 | -3.099028000 | 4.152810000 |
| C | 3.148658000 | -1.886635000 | 2.402109000 |
| H | 4.154758000 | -2.036368000 | 2.018922000 |
| C | -0.970154000 | 0.576354000 | 2.083080000 |
| C | -0.632069000 | 1.303020000 | 3.245918000 |
| H | 0.388079000 | 1.252066000 | 3.614805000 |
| C | -1.566459000 | 2.080987000 | 3.916331000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -1.261813000 | 2.627538000 | 4.805540000 |
| C | -2.881294000 | 2.178399000 | 3.452535000 |
| H | -3.611672000 | 2.787898000 | 3.976230000 |
| C | -3.239713000 | 1.482194000 | 2.304764000 |
| H | -4.256710000 | 1.550361000 | 1.927859000 |
| C | -2.309676000 | 0.683739000 | 1.623221000 |
| C | -4.272434000 | 0.625611000 | -0.536844000 |
| C | -5.556476000 | 0.083594000 | -0.402749000 |
| H | -5.699323000 | -0.873131000 | 0.089921000 |
| C | -6.664286000 | 0.771995000 | -0.898597000 |
| H | -7.655607000 | 0.340486000 | -0.788950000 |
| C | -6.504112000 | 2.006579000 | -1.523896000 |
| H | -7.369190000 | 2.539952000 | -1.908141000 |
| C | -5.228556000 | 2.557387000 | -1.651979000 |
| H | -5.096313000 | 3.522543000 | -2.133640000 |
| C | -4.119811000 | 1.869140000 | -1.166720000 |
| H | -3.131400000 | 2.307457000 | -1.268853000 |
| C | -3.385022000 | -1.876790000 | 0.648368000 |
| C | -3.511793000 | -2.215724000 | 1.999864000 |
| H | -3.248133000 | -1.491551000 | 2.765576000 |
| C | -3.992361000 | -3.474192000 | 2.365367000 |
| H | -4.091314000 | -3.726771000 | 3.417742000 |
| C | -4.360430000 | -4.397443000 | 1.387860000 |
| H | -4.745940000 | -5.371664000 | 1.675887000 |
| C | -4.241869000 | -4.063917000 | 0.037075000 |
| H | -4.542066000 | -4.774668000 | -0.728799000 |
| C | -3.745828000 | -2.814699000 | -0.331323000 |
| H | -3.666021000 | -2.556964000 | -1.386023000 |
| C | 1.211007000 | 0.154916000 | -3.230090000 |
| C | -0.145965000 | 0.283684000 | -3.557021000 |
| H | 1.841774000 | -0.552859000 | -3.762183000 |
| H | 1.748696000 | 1.020188000 | -2.833891000 |
| C | -0.984435000 | 1.190106000 | -2.880893000 |
| C | -0.474181000 | 2.546029000 | -2.383067000 |
| H | -1.292262000 | 3.260924000 | -2.534289000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.341106000 | 2.884686000 | -3.037929000 |
| Y | -0.022788000 | -0.188204000 | -0.956399000 |
| O | -0.026342000 | -2.558345000 | -1.079712000 |
| C | -0.080913000 | -3.382998000 | -2.282155000 |
| C | -0.010127000 | -3.427285000 | 0.109653000 |
| C | 0.267486000 | -4.788567000 | -1.820502000 |
| H | -1.097720000 | -3.325630000 | -2.685178000 |
| H | 0.620034000 | -2.961912000 | -3.005490000 |
| C | -0.324932000 | -4.819027000 | -0.411208000 |
| H | 0.989681000 | -3.360002000 | 0.546486000 |
| H | -0.744997000 | -3.037340000 | 0.814065000 |
| H | 1.354220000 | -4.924484000 | -1.785575000 |
| H | -0.151856000 | -5.550415000 | -2.483637000 |
| H | 0.116317000 | -5.594146000 | 0.221462000 |
| H | -1.407375000 | -4.978813000 | -0.447965000 |
| H | -2.035473000 | 1.170748000 | -3.164031000 |
| C | -0.783355000 | -0.700020000 | -4.512774000 |
| H | -0.160892000 | -1.581951000 | -4.689709000 |
| H | -1.778607000 | -1.021405000 | -4.183175000 |
| H | -0.917948000 | -0.201415000 | -5.480875000 |

123

theta3_thf_C2_trans_1,4_isoprene E = -2279.226566 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | -1.099355000 | 1.297764000 | 1.133856000 |
| P | -2.979656000 | -0.756480000 | -0.030934000 |
| P | 1.822352000 | 1.864581000 | 0.419069000 |
| Si | 5.137200000 | -3.874316000 | -1.176980000 |
| C | 3.853311000 | -2.759797000 | -2.039666000 |
| H | 3.351176000 | -3.378482000 | -2.798318000 |
| H | 4.388588000 | -1.979273000 | -2.600589000 |
| C | 4.310688000 | -5.499669000 | -0.680602000 |
| H | 3.443574000 | -5.338505000 | -0.028745000 |
| H | 5.009591000 | -6.152626000 | -0.143908000 |
| H | 3.960659000 | -6.048918000 | -1.563117000 |
| C | 6.533337000 | -4.221355000 | -2.397393000 |
| H | 6.157510000 | -4.696347000 | -3.311659000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 7.281366000 | -4.894553000 | -1.961334000 |
| H | 7.050519000 | -3.299801000 | -2.690464000 |
| C | 5.835383000 | -3.022571000 | 0.360175000 |
| H | 6.262439000 | -2.043118000 | 0.114340000 |
| H | 6.631165000 | -3.627624000 | 0.811385000 |
| H | 5.066047000 | -2.869591000 | 1.127355000 |
| C | -4.130943000 | -1.163516000 | -1.417947000 |
| C | -3.784250000 | -0.757326000 | -2.714051000 |
| H | -2.848036000 | -0.230161000 | -2.882142000 |
| C | -4.627708000 | -1.022966000 | -3.790548000 |
| H | -4.347464000 | -0.703232000 | -4.790978000 |
| C | -5.825603000 | -1.707815000 | -3.585724000 |
| H | -6.481145000 | -1.922111000 | -4.425241000 |
| C | -6.176308000 | -2.119463000 | -2.301217000 |
| H | -7.108272000 | -2.653157000 | -2.135303000 |
| C | -5.336206000 | -1.849060000 | -1.220859000 |
| H | -5.621532000 | -2.176585000 | -0.225482000 |
| C | -3.530546000 | -1.895582000 | 1.318380000 |
| C | -3.290836000 | -3.271457000 | 1.182590000 |
| H | -2.782197000 | -3.652043000 | 0.300675000 |
| C | -3.722663000 | -4.160765000 | 2.164893000 |
| H | -3.548129000 | -5.226683000 | 2.041880000 |
| C | -4.384604000 | -3.685436000 | 3.298830000 |
| H | -4.721527000 | -4.379793000 | 4.063716000 |
| C | -4.618283000 | -2.318687000 | 3.442233000 |
| H | -5.138549000 | -1.943363000 | 4.319477000 |
| C | -4.195857000 | -1.425355000 | 2.456225000 |
| H | -4.393344000 | -0.363192000 | 2.567742000 |
| C | -3.459203000 | 0.922884000 | 0.515165000 |
| C | -2.430298000 | 1.738538000 | 1.057368000 |
| C | -2.806353000 | 3.050865000 | 1.433162000 |
| H | -2.051410000 | 3.715620000 | 1.841556000 |
| C | -4.106764000 | 3.513509000 | 1.289640000 |
| H | -4.340065000 | 4.533175000 | 1.587160000 |
| C | -5.107130000 | 2.695215000 | 0.757480000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -6.123815000 | 3.058492000 | 0.642062000 |
| C | -4.767912000 | 1.404986000 | 0.370926000 |
| H | -5.526123000 | 0.753887000 | -0.057092000 |
| C | -0.346309000 | 1.819662000 | 2.198162000 |
| C | -0.905836000 | 1.969989000 | 3.488799000 |
| H | -1.946367000 | 1.696299000 | 3.637553000 |
| C | -0.166641000 | 2.455580000 | 4.557879000 |
| H | -0.639995000 | 2.549395000 | 5.532299000 |
| C | 1.175015000 | 2.809176000 | 4.393958000 |
| H | 1.756612000 | 3.191581000 | 5.227359000 |
| C | 1.758389000 | 2.652143000 | 3.143348000 |
| H | 2.805011000 | 2.907947000 | 3.005575000 |
| C | 1.023119000 | 2.165141000 | 2.051385000 |
| C | 3.629560000 | 1.820479000 | 0.829833000 |
| C | 4.471176000 | 2.926937000 | 0.654102000 |
| H | 4.083491000 | 3.850962000 | 0.237531000 |
| C | 5.815041000 | 2.857376000 | 1.021720000 |
| H | 6.454169000 | 3.724487000 | 0.877988000 |
| C | 6.332755000 | 1.690562000 | 1.579464000 |
| H | 7.378730000 | 1.640498000 | 1.869244000 |
| C | 5.499951000 | 0.588138000 | 1.769063000 |
| H | 5.892665000 | -0.324594000 | 2.207871000 |
| C | 4.160865000 | 0.650347000 | 1.390519000 |
| H | 3.525687000 | -0.215203000 | 1.553001000 |
| C | 1.653036000 | 3.453162000 | -0.517464000 |
| C | 0.879679000 | 4.515769000 | -0.039022000 |
| H | 0.375569000 | 4.427223000 | 0.918931000 |
| C | 0.775960000 | 5.698499000 | -0.773599000 |
| H | 0.177822000 | 6.519661000 | -0.387310000 |
| C | 1.453284000 | 5.836658000 | -1.984400000 |
| H | 1.384284000 | 6.764424000 | -2.545891000 |
| C | 2.233048000 | 4.782862000 | -2.465626000 |
| H | 2.777361000 | 4.888760000 | -3.400556000 |
| C | 2.325228000 | 3.595162000 | -1.741990000 |
| H | 2.955134000 | 2.789066000 | -2.114038000 |

| | | | |
|---|--------------|--------------|--------------|
| C | 1.063480000 | -1.447291000 | 2.017078000 |
| C | 0.262024000 | -2.318212000 | 2.677176000 |
| C | 0.267180000 | -3.762487000 | 2.390902000 |
| C | 1.365988000 | -4.482377000 | 2.132770000 |
| H | 1.311596000 | -5.554131000 | 1.963820000 |
| H | 2.356430000 | -4.033926000 | 2.122893000 |
| Y | -0.150116000 | -0.256582000 | -0.417617000 |
| H | -0.695080000 | -4.266891000 | 2.474708000 |
| O | -0.707292000 | 1.268834000 | -2.185479000 |
| C | 0.015782000 | 1.420645000 | -3.444005000 |
| C | -1.636785000 | 2.402414000 | -2.036014000 |
| C | -0.878518000 | 2.295159000 | -4.300805000 |
| H | 0.971353000 | 1.908655000 | -3.231431000 |
| H | 0.191298000 | 0.425605000 | -3.844676000 |
| C | -1.435052000 | 3.275359000 | -3.267844000 |
| H | -2.643402000 | 1.982143000 | -1.979162000 |
| H | -1.401043000 | 2.905410000 | -1.099351000 |
| H | -1.680077000 | 1.700375000 | -4.754092000 |
| H | -0.321323000 | 2.786472000 | -5.103608000 |
| H | -2.371060000 | 3.745245000 | -3.582746000 |
| H | -0.706785000 | 4.065953000 | -3.062314000 |
| H | 1.154144000 | -0.420705000 | 2.368200000 |
| H | 1.787995000 | -1.810866000 | 1.288598000 |
| C | 2.781618000 | -2.090601000 | -1.152134000 |
| C | 1.693704000 | -1.465702000 | -2.023785000 |
| H | 2.334316000 | -2.845164000 | -0.491086000 |
| H | 3.282070000 | -1.355379000 | -0.508823000 |
| H | 2.115482000 | -0.937088000 | -2.882281000 |
| C | 0.463514000 | -2.106219000 | -2.267847000 |
| C | -0.331351000 | -2.653641000 | -1.241531000 |
| H | -1.230528000 | -3.200899000 | -1.513259000 |
| H | 0.145015000 | -3.008215000 | -0.320598000 |
| C | -0.146346000 | -2.077109000 | -3.654229000 |
| H | -0.144507000 | -3.105306000 | -4.038455000 |
| H | -1.189896000 | -1.743110000 | -3.663921000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.439066000 | -1.481032000 | -4.359916000 |
| C | -0.645928000 | -1.876005000 | 3.787290000 |
| H | -0.642923000 | -0.790478000 | 3.910497000 |
| H | -1.673383000 | -2.213092000 | 3.611123000 |
| H | -0.320149000 | -2.336038000 | 4.729654000 |

123

theta3_thf_TS2_trans_1,4_isoprene E = -2279.197198 a.u. Imaginary frequency=202i

| | | | |
|----|--------------|--------------|--------------|
| N | -1.366688000 | 1.302556000 | 0.914308000 |
| P | -2.893156000 | -1.176032000 | 0.041348000 |
| P | 1.434710000 | 2.283892000 | 0.168141000 |
| Si | 5.628731000 | -4.267379000 | -0.063379000 |
| C | 4.427197000 | -3.603445000 | -1.386517000 |
| H | 3.846298000 | -4.451342000 | -1.777690000 |
| H | 5.019993000 | -3.233220000 | -2.235905000 |
| C | 4.643174000 | -5.028187000 | 1.358701000 |
| H | 4.035995000 | -4.281933000 | 1.886592000 |
| H | 5.314726000 | -5.477518000 | 2.100267000 |
| H | 3.972026000 | -5.820402000 | 1.004583000 |
| C | 6.717461000 | -5.579173000 | -0.868202000 |
| H | 6.120848000 | -6.406290000 | -1.271350000 |
| H | 7.421869000 | -6.004874000 | -0.143477000 |
| H | 7.307157000 | -5.162586000 | -1.693633000 |
| C | 6.698892000 | -2.855785000 | 0.596594000 |
| H | 7.247105000 | -2.355250000 | -0.211079000 |
| H | 7.441558000 | -3.234285000 | 1.309345000 |
| H | 6.103424000 | -2.099003000 | 1.122475000 |
| C | -3.875320000 | -2.025898000 | -1.277697000 |
| C | -3.343627000 | -2.127916000 | -2.569061000 |
| H | -2.352030000 | -1.738304000 | -2.776598000 |
| C | -4.066764000 | -2.737126000 | -3.593559000 |
| H | -3.637202000 | -2.810617000 | -4.589216000 |
| C | -5.331838000 | -3.261536000 | -3.335724000 |
| H | -5.895744000 | -3.741938000 | -4.130546000 |
| C | -5.867778000 | -3.175843000 | -2.050820000 |
| H | -6.851649000 | -3.587430000 | -1.842158000 |

| | | | |
|---|--------------|--------------|--------------|
| C | -5.146415000 | -2.564934000 | -1.026778000 |
| H | -5.571704000 | -2.515963000 | -0.028502000 |
| C | -3.510623000 | -2.014257000 | 1.574732000 |
| C | -3.414918000 | -3.410736000 | 1.677875000 |
| H | -3.050670000 | -3.997396000 | 0.837063000 |
| C | -3.815963000 | -4.060395000 | 2.842877000 |
| H | -3.747983000 | -5.143199000 | 2.906727000 |
| C | -4.309522000 | -3.324243000 | 3.921257000 |
| H | -4.622807000 | -3.831916000 | 4.829328000 |
| C | -4.408644000 | -1.937542000 | 3.824445000 |
| H | -4.805133000 | -1.360069000 | 4.655490000 |
| C | -4.012432000 | -1.283093000 | 2.656927000 |
| H | -4.108383000 | -0.203800000 | 2.581206000 |
| C | -3.577595000 | 0.523156000 | 0.146601000 |
| C | -2.719319000 | 1.546361000 | 0.632338000 |
| C | -3.289600000 | 2.837580000 | 0.748358000 |
| H | -2.684267000 | 3.648503000 | 1.139718000 |
| C | -4.601554000 | 3.100554000 | 0.380911000 |
| H | -4.984622000 | 4.113290000 | 0.481456000 |
| C | -5.421738000 | 2.088430000 | -0.121475000 |
| H | -6.446484000 | 2.292919000 | -0.416309000 |
| C | -4.897385000 | 0.806976000 | -0.228652000 |
| H | -5.522124000 | 0.005594000 | -0.613116000 |
| C | -0.774004000 | 2.122653000 | 1.897979000 |
| C | -1.456805000 | 2.428348000 | 3.096439000 |
| H | -2.464785000 | 2.045972000 | 3.229205000 |
| C | -0.876276000 | 3.190305000 | 4.099085000 |
| H | -1.439372000 | 3.400585000 | 5.004992000 |
| C | 0.431345000 | 3.660149000 | 3.959342000 |
| H | 0.899961000 | 4.244058000 | 4.746131000 |
| C | 1.128399000 | 3.371642000 | 2.791937000 |
| H | 2.147153000 | 3.729680000 | 2.684560000 |
| C | 0.541907000 | 2.635607000 | 1.752488000 |
| C | 3.230052000 | 2.602114000 | 0.483541000 |
| C | 3.722390000 | 3.887723000 | 0.762926000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 3.042710000 | 4.734646000 | 0.800250000 |
| C | 5.084534000 | 4.092668000 | 0.968504000 |
| H | 5.450902000 | 5.091885000 | 1.188094000 |
| C | 5.976705000 | 3.022882000 | 0.883640000 |
| H | 7.039248000 | 3.186528000 | 1.041267000 |
| C | 5.503475000 | 1.748351000 | 0.579733000 |
| H | 6.195013000 | 0.914710000 | 0.492653000 |
| C | 4.138712000 | 1.542365000 | 0.376798000 |
| H | 3.779728000 | 0.550080000 | 0.119963000 |
| C | 1.005489000 | 3.741492000 | -0.906465000 |
| C | -0.203392000 | 4.426649000 | -0.750677000 |
| H | -0.881002000 | 4.148945000 | 0.048481000 |
| C | -0.536249000 | 5.481152000 | -1.601593000 |
| H | -1.474931000 | 6.010140000 | -1.458719000 |
| C | 0.335489000 | 5.864408000 | -2.619679000 |
| H | 0.080336000 | 6.691954000 | -3.276004000 |
| C | 1.545302000 | 5.188064000 | -2.781901000 |
| H | 2.238576000 | 5.488750000 | -3.563158000 |
| C | 1.878195000 | 4.132738000 | -1.934581000 |
| H | 2.834103000 | 3.629875000 | -2.061739000 |
| C | 1.902795000 | -0.572451000 | 1.944444000 |
| C | 0.774430000 | -0.887957000 | 2.659411000 |
| C | -0.173963000 | -1.850205000 | 2.161484000 |
| C | 0.196996000 | -2.895510000 | 1.315207000 |
| H | -0.530920000 | -3.674865000 | 1.120940000 |
| H | 1.233735000 | -3.215616000 | 1.306270000 |
| Y | -0.001005000 | -0.377429000 | 0.012090000 |
| H | -1.183221000 | -1.832086000 | 2.561437000 |
| O | -0.428299000 | 0.632878000 | -2.201191000 |
| C | 0.623707000 | 0.993714000 | -3.140387000 |
| C | -1.653183000 | 1.341850000 | -2.583364000 |
| C | -0.108975000 | 1.346685000 | -4.419191000 |
| H | 1.158092000 | 1.860886000 | -2.744408000 |
| H | 1.305898000 | 0.148021000 | -3.211162000 |
| C | -1.326292000 | 2.094636000 | -3.872088000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -2.430017000 | 0.585705000 | -2.721885000 |
| H | -1.936891000 | 2.000633000 | -1.762837000 |
| H | -0.407260000 | 0.441333000 | -4.959984000 |
| H | 0.503509000 | 1.959942000 | -5.086356000 |
| H | -2.174312000 | 2.100918000 | -4.562691000 |
| H | -1.060916000 | 3.132672000 | -3.647662000 |
| H | 2.619416000 | 0.152144000 | 2.315261000 |
| H | 2.264994000 | -1.223089000 | 1.143144000 |
| C | 3.455974000 | -2.496605000 | -0.922201000 |
| C | 2.526236000 | -2.102565000 | -2.034008000 |
| H | 2.885653000 | -2.853052000 | -0.056618000 |
| H | 4.047225000 | -1.633881000 | -0.582997000 |
| H | 3.030741000 | -1.764443000 | -2.941675000 |
| C | 1.187182000 | -2.322577000 | -2.111964000 |
| C | 0.352335000 | -2.873144000 | -1.008818000 |
| H | -0.676486000 | -3.059567000 | -1.333334000 |
| H | 0.768268000 | -3.817803000 | -0.661346000 |
| C | 0.498902000 | -2.198839000 | -3.454237000 |
| H | 0.154601000 | -3.192869000 | -3.768092000 |
| H | -0.383556000 | -1.552445000 | -3.418074000 |
| H | 1.171309000 | -1.824293000 | -4.233448000 |
| C | 0.459249000 | -0.198225000 | 3.954898000 |
| H | 0.963481000 | 0.766018000 | 4.049403000 |
| H | -0.615232000 | -0.051058000 | 4.086585000 |
| H | 0.802772000 | -0.846150000 | 4.772694000 |

123

theta3_thf_P2_trans_1,4_isoprene E = -2279.257585 a.u.

| | | | |
|----|--------------|--------------|--------------|
| N | 1.499483000 | 1.463299000 | -0.727914000 |
| P | 2.983045000 | -1.081003000 | 0.030626000 |
| P | -1.406079000 | 2.244839000 | -0.202649000 |
| Si | -6.241361000 | -3.631828000 | 0.266498000 |
| C | -4.584857000 | -3.241131000 | 1.131572000 |
| H | -4.255075000 | -4.154408000 | 1.648463000 |
| H | -4.770397000 | -2.499509000 | 1.923044000 |
| C | -5.997679000 | -5.066622000 | -0.936206000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -5.289147000 | -4.819299000 | -1.736154000 |
| H | -6.946354000 | -5.335120000 | -1.416451000 |
| H | -5.625395000 | -5.962621000 | -0.424853000 |
| C | -7.493390000 | -4.100518000 | 1.596241000 |
| H | -7.162586000 | -4.975452000 | 2.168568000 |
| H | -8.465521000 | -4.347220000 | 1.152657000 |
| H | -7.654311000 | -3.280157000 | 2.305983000 |
| C | -6.838720000 | -2.108610000 | -0.680438000 |
| H | -6.931920000 | -1.234796000 | -0.023858000 |
| H | -7.823816000 | -2.291322000 | -1.126485000 |
| H | -6.155703000 | -1.848813000 | -1.498808000 |
| C | 3.831898000 | -2.014817000 | 1.389744000 |
| C | 3.243701000 | -2.044565000 | 2.662280000 |
| H | 2.284877000 | -1.560477000 | 2.827143000 |
| C | 3.871584000 | -2.698331000 | 3.720586000 |
| H | 3.403196000 | -2.713290000 | 4.701349000 |
| C | 5.092825000 | -3.340505000 | 3.519065000 |
| H | 5.580480000 | -3.855963000 | 4.341873000 |
| C | 5.683020000 | -3.321647000 | 2.256550000 |
| H | 6.634939000 | -3.819432000 | 2.092178000 |
| C | 5.059801000 | -2.662703000 | 1.197147000 |
| H | 5.532649000 | -2.655340000 | 0.219837000 |
| C | 3.820365000 | -1.715956000 | -1.493229000 |
| C | 3.688118000 | -3.073263000 | -1.824918000 |
| H | 3.126628000 | -3.741880000 | -1.175921000 |
| C | 4.290331000 | -3.580817000 | -2.973361000 |
| H | 4.190570000 | -4.636084000 | -3.213252000 |
| C | 5.018891000 | -2.736339000 | -3.812892000 |
| H | 5.485870000 | -3.131800000 | -4.710709000 |
| C | 5.150650000 | -1.387139000 | -3.491697000 |
| H | 5.724141000 | -0.726572000 | -4.136596000 |
| C | 4.558435000 | -0.877127000 | -2.334916000 |
| H | 4.681794000 | 0.171699000 | -2.082214000 |
| C | 3.617384000 | 0.635112000 | 0.215880000 |
| C | 2.791821000 | 1.699531000 | -0.230411000 |

| | | | |
|---|--------------|-------------|--------------|
| C | 3.311154000 | 3.006276000 | -0.090685000 |
| H | 2.715296000 | 3.848440000 | -0.426469000 |
| C | 4.562748000 | 3.242602000 | 0.462249000 |
| H | 4.915366000 | 4.267106000 | 0.553789000 |
| C | 5.359813000 | 2.186095000 | 0.906175000 |
| H | 6.338524000 | 2.368530000 | 1.339607000 |
| C | 4.875006000 | 0.890026000 | 0.777896000 |
| H | 5.482084000 | 0.054487000 | 1.115587000 |
| C | 0.994643000 | 2.402900000 | -1.654216000 |
| C | 1.791757000 | 2.867276000 | -2.721737000 |
| H | 2.817868000 | 2.518635000 | -2.792573000 |
| C | 1.289774000 | 3.734193000 | -3.681941000 |
| H | 1.933762000 | 4.064190000 | -4.493166000 |
| C | -0.038459000 | 4.161324000 | -3.621537000 |
| H | -0.440487000 | 4.830801000 | -4.376326000 |
| C | -0.844884000 | 3.716763000 | -2.580696000 |
| H | -1.880001000 | 4.040583000 | -2.534792000 |
| C | -0.344986000 | 2.862548000 | -1.587994000 |
| C | -3.149953000 | 2.595244000 | -0.712715000 |
| C | -3.661062000 | 3.903236000 | -0.714300000 |
| H | -3.032965000 | 4.733952000 | -0.404340000 |
| C | -4.977275000 | 4.145373000 | -1.100056000 |
| H | -5.358987000 | 5.162855000 | -1.100050000 |
| C | -5.803063000 | 3.087084000 | -1.480423000 |
| H | -6.830304000 | 3.278143000 | -1.778719000 |
| C | -5.309762000 | 1.784146000 | -1.468133000 |
| H | -5.950949000 | 0.954388000 | -1.752169000 |
| C | -3.991619000 | 1.540042000 | -1.083260000 |
| H | -3.616631000 | 0.521857000 | -1.073249000 |
| C | -1.180130000 | 3.503882000 | 1.145851000 |
| C | -0.113671000 | 4.408274000 | 1.149132000 |
| H | 0.587563000 | 4.417305000 | 0.321018000 |
| C | 0.038781000 | 5.319317000 | 2.195718000 |
| H | 0.868359000 | 6.021348000 | 2.179992000 |
| C | -0.878603000 | 5.344759000 | 3.244589000 |

| | | | |
|---|--------------|--------------|--------------|
| H | -0.766570000 | 6.063648000 | 4.051649000 |
| C | -1.952929000 | 4.452760000 | 3.244479000 |
| H | -2.684158000 | 4.478790000 | 4.048355000 |
| C | -2.099523000 | 3.534762000 | 2.206341000 |
| H | -2.957943000 | 2.866009000 | 2.202702000 |
| C | -1.348649000 | -0.353878000 | -2.329720000 |
| C | -0.193119000 | -1.057826000 | -2.732918000 |
| C | 0.198370000 | -2.257507000 | -2.117174000 |
| C | -0.819830000 | -3.348579000 | -1.818639000 |
| H | -0.715779000 | -4.100539000 | -2.616888000 |
| H | -1.829247000 | -2.945917000 | -1.934975000 |
| Y | 0.108686000 | -0.292137000 | -0.243022000 |
| H | 1.176304000 | -2.634269000 | -2.414366000 |
| O | 0.211578000 | 0.217153000 | 2.203951000 |
| C | -0.861388000 | 0.146622000 | 3.175012000 |
| C | 1.218269000 | 1.171022000 | 2.691112000 |
| C | -0.211660000 | 0.501277000 | 4.498915000 |
| H | -1.637639000 | 0.868944000 | 2.896945000 |
| H | -1.273743000 | -0.861916000 | 3.142534000 |
| C | 0.758819000 | 1.607724000 | 4.080851000 |
| H | 2.173818000 | 0.643155000 | 2.705023000 |
| H | 1.275898000 | 1.997231000 | 1.982687000 |
| H | 0.324791000 | -0.364924000 | 4.903427000 |
| H | -0.942733000 | 0.829371000 | 5.243214000 |
| H | 1.602470000 | 1.716622000 | 4.768041000 |
| H | 0.238241000 | 2.568202000 | 4.024812000 |
| H | -1.652754000 | 0.530276000 | -2.883345000 |
| H | -2.178361000 | -0.922334000 | -1.899936000 |
| C | -3.454504000 | -2.742847000 | 0.208982000 |
| C | -2.163764000 | -2.617291000 | 0.976849000 |
| H | -3.333314000 | -3.434225000 | -0.630341000 |
| H | -3.752914000 | -1.776272000 | -0.221785000 |
| H | -2.275955000 | -2.101589000 | 1.932729000 |
| C | -0.990634000 | -3.253783000 | 0.749183000 |
| C | -0.719949000 | -4.093921000 | -0.483174000 |

| | | | |
|---|--------------|--------------|--------------|
| H | 0.278606000 | -4.540034000 | -0.395419000 |
| H | -1.423225000 | -4.939947000 | -0.499702000 |
| C | 0.750998000 | -0.402826000 | -3.713068000 |
| H | 0.647092000 | 0.684169000 | -3.745432000 |
| H | 1.797083000 | -0.657688000 | -3.516363000 |
| H | 0.506958000 | -0.787311000 | -4.712949000 |
| C | 0.073595000 | -3.332329000 | 1.812518000 |
| H | -0.138253000 | -2.704346000 | 2.683041000 |
| H | 0.143982000 | -4.370328000 | 2.168506000 |
| H | 1.069803000 | -3.084230000 | 1.428132000 |