

Insertion Modes and Origins of Product Selectivity in Rare-Earth-Catalyzed C–H Functionalization with Conjugated Dienes

Deyue Cao,^a Bowen Zheng,^b Ningjie Xu,^a Xin Wang*^a and Gen Luo*^a

^a*Institutes of Physical Science and Information Technology, Anhui University, Hefei 230601, China*

^b*School of Materials Science and Engineering, Anhui University, Hefei 230601, China*

Corresponding emails: luogen@ahu.edu.cn (G.L.); wangxin17860659070@163.com (X.W.)

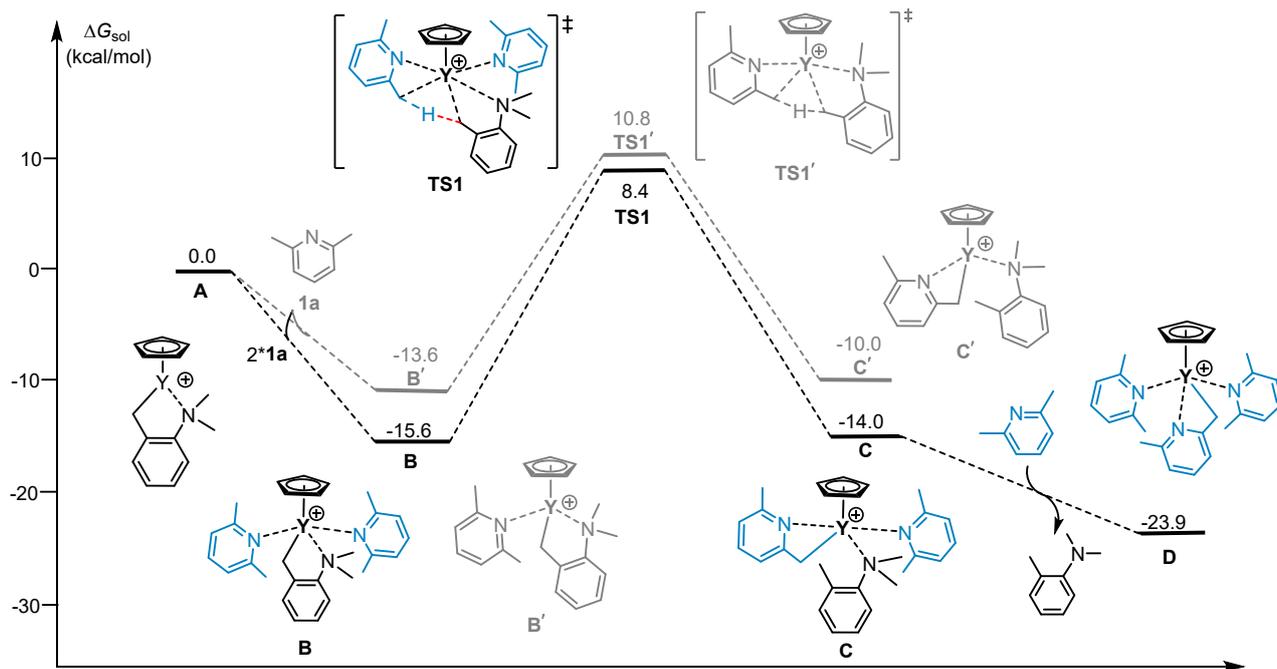


Fig. S1 Computed energy profiles for the formation of active species with or without 2,6-lutidine ligand for Y-1.

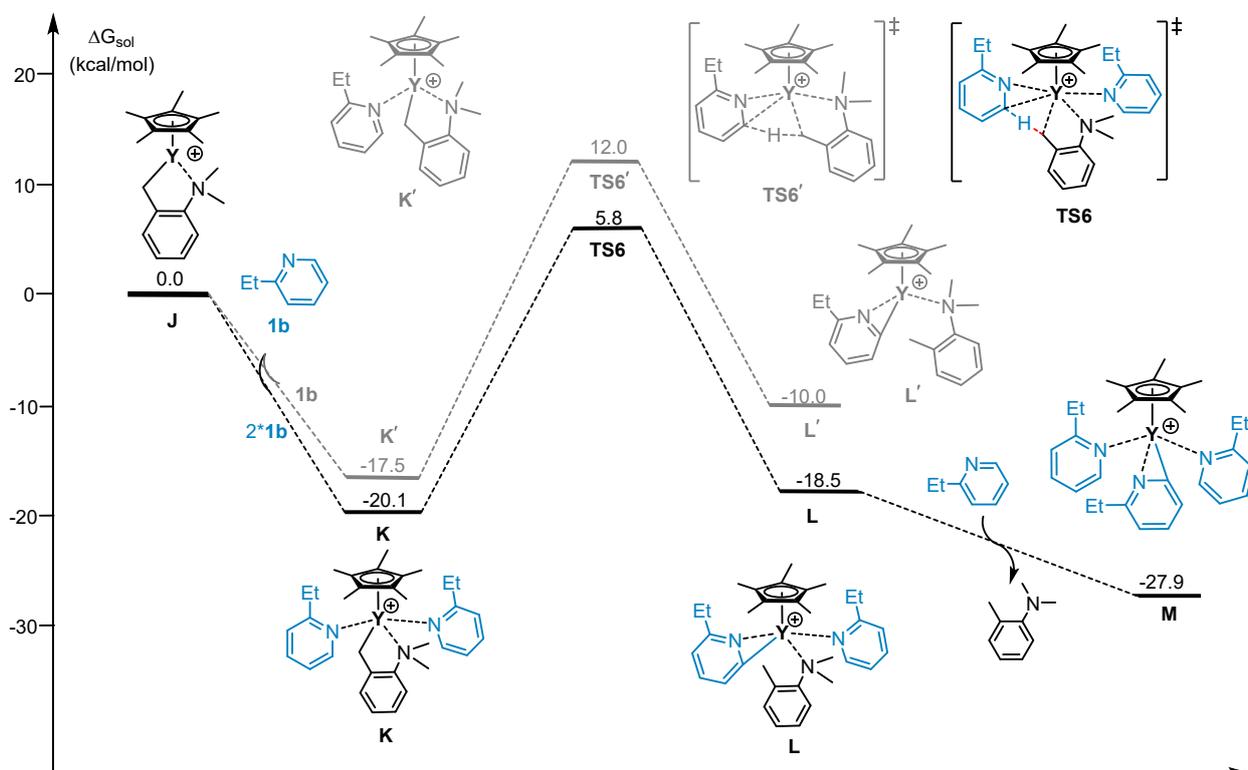


Fig. S2 Computed energy profiles for the formation of active species with or without 2-ethylpyridine ligand for Y-2.

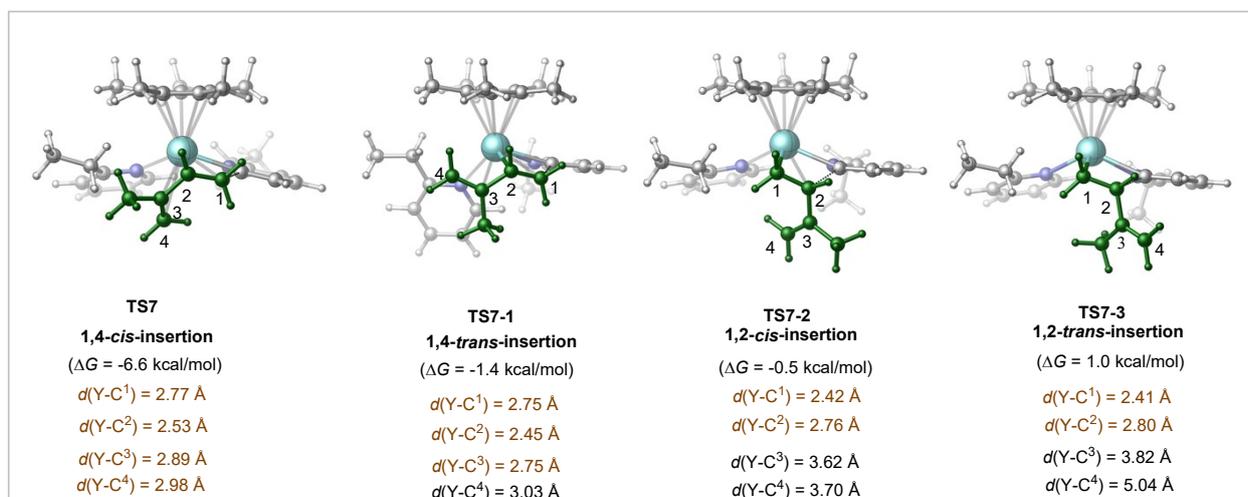
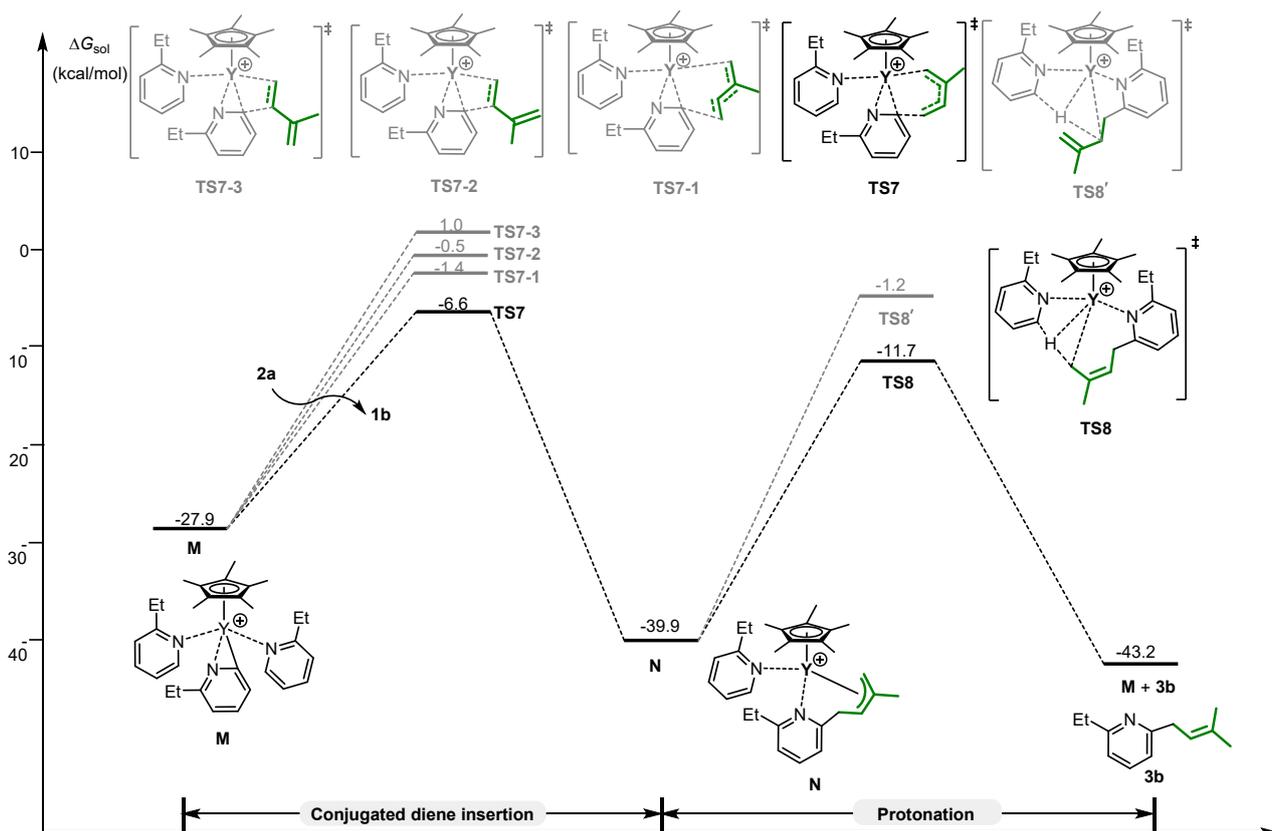


Fig. S3 Computed energy profiles for **Y-2**-catalyzed $C(sp^2)$ -H alkylation of 2-ethylpyridine (**1b**) with isoprene (**2a**) to form formal 1,4-addition product.

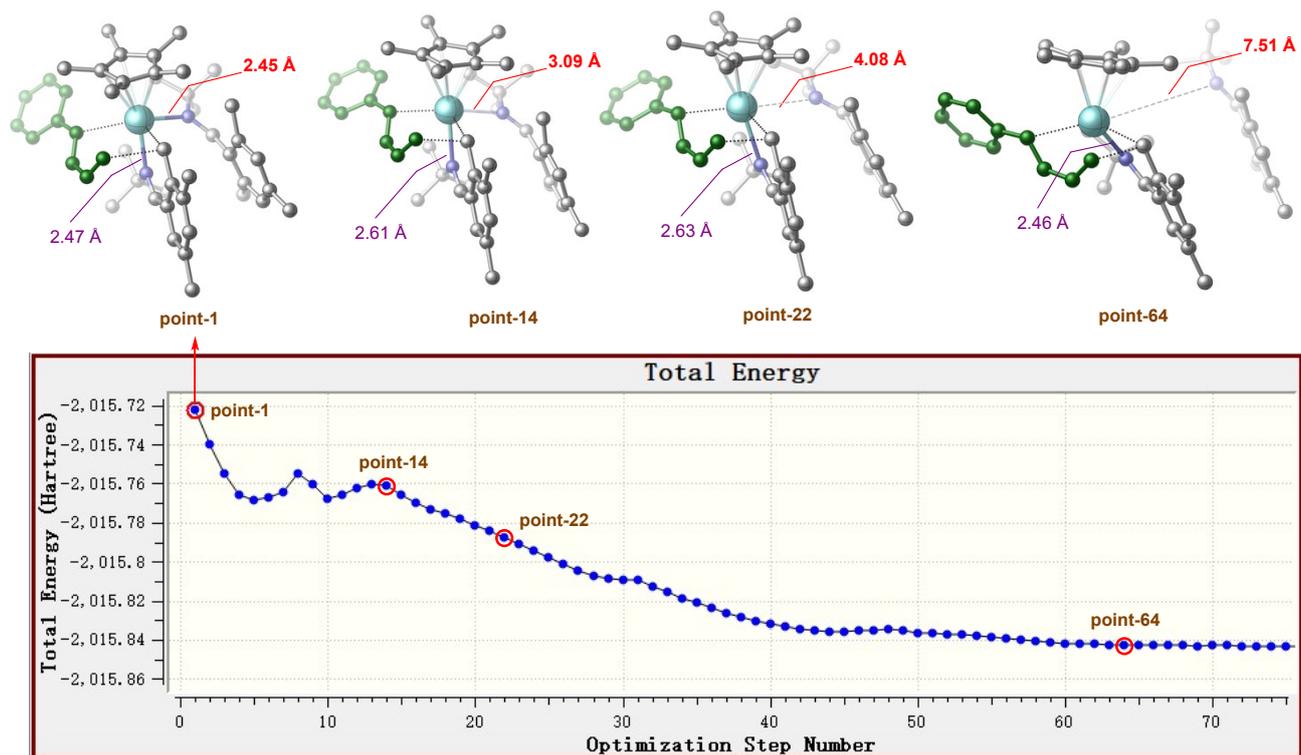


Fig. S4 Optimized energy curve and selected structures for 1,4-*cis* diene insertion with an additional **1c** ligand.

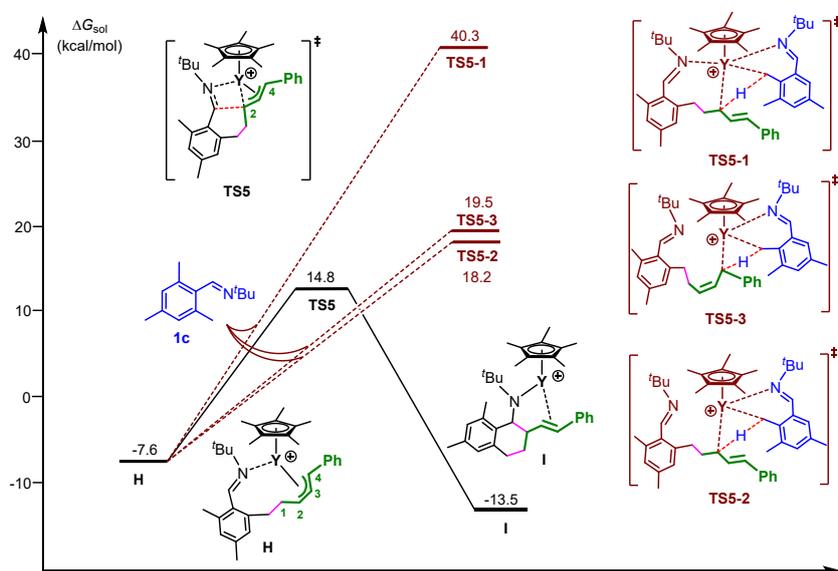


Fig. S5 Computed energy profiles for competitive cyclization (solid line) and protonation (dashed lines) processes.

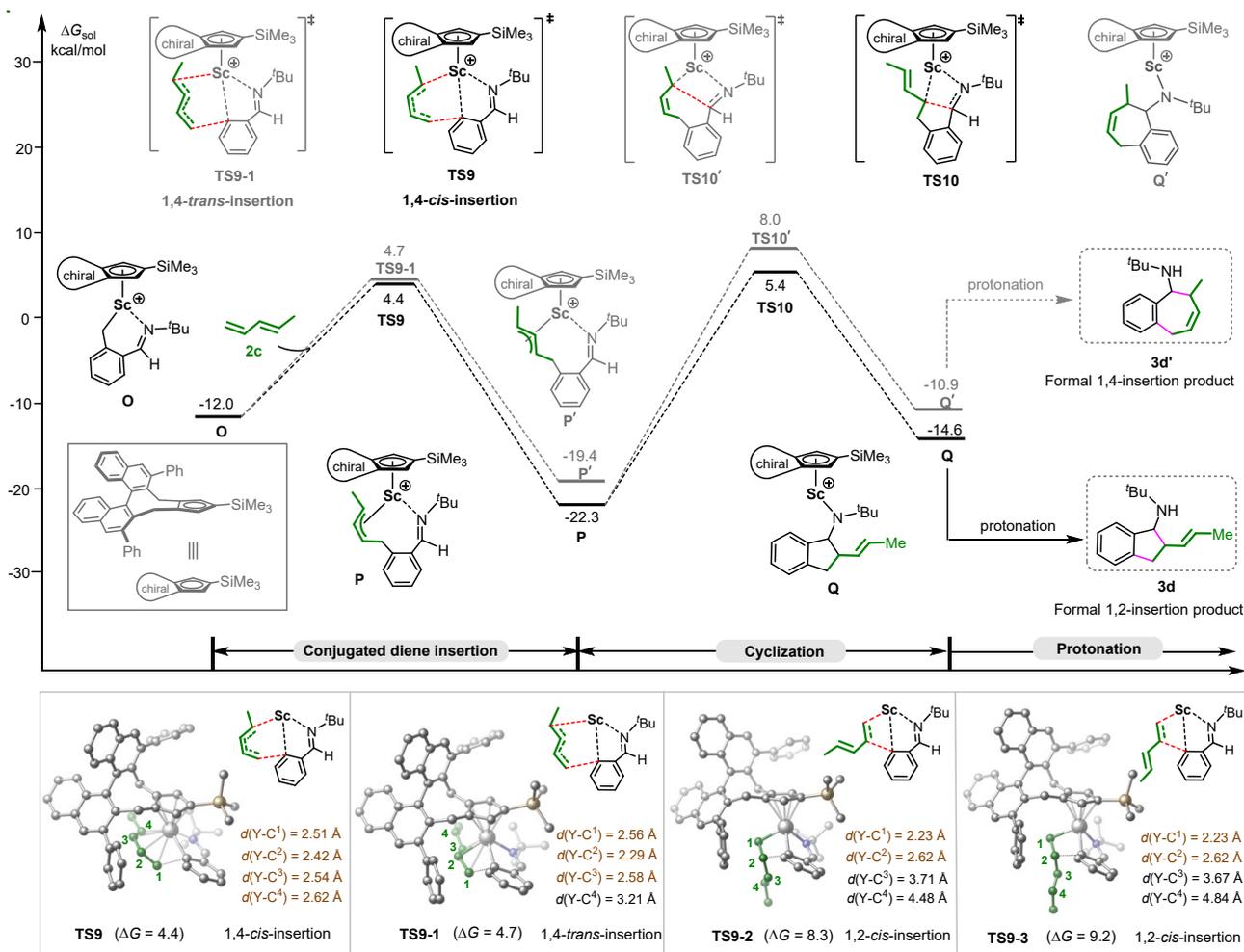


Fig. S6 Computed energy profiles for Sc-1-catalyzed annulation of *N*-*tert*-butylmesitaldimine (**1d**) with (*E*)-1,3-pentadiene (**2c**) to form formal 1,2-addition product and 3D structures of diene-insertion transition states. All hydrogen atoms in 3D structures are omitted for clarity.

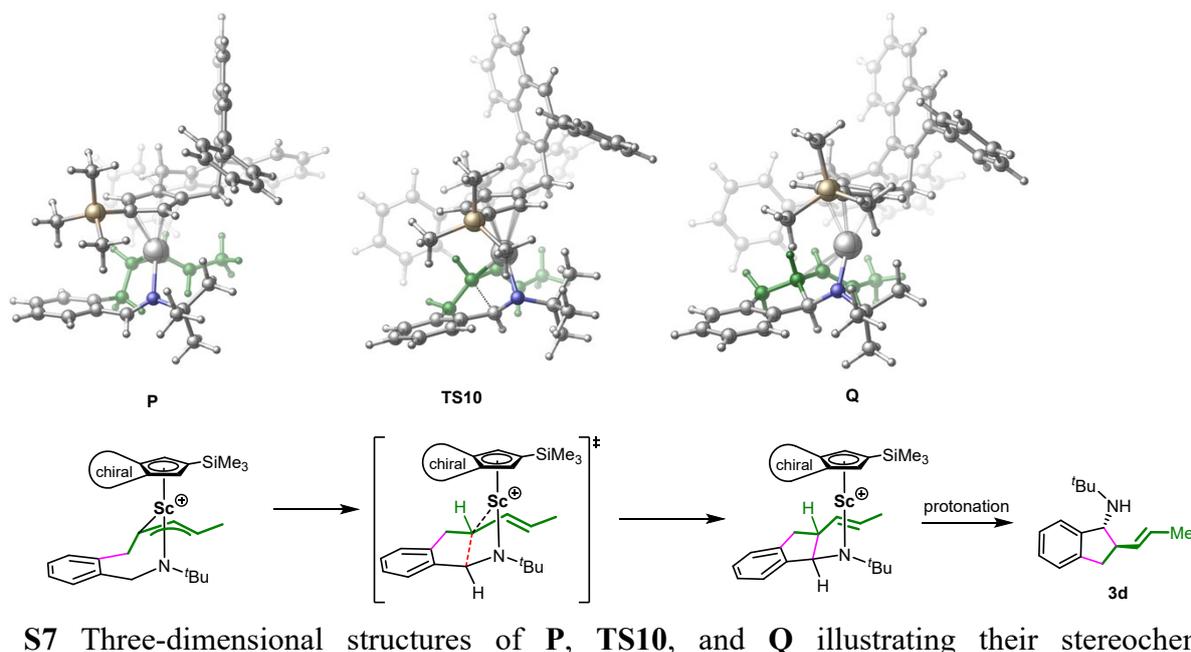


Fig. S7 Three-dimensional structures of P, TS10, and Q illustrating their stereochemical configurations.

Optimized Cartesian Coordinates of All Structures

Optimized Cartesian coordinates and their corresponding single-point energies (E(SCRF), a.u.) calculated at the M06/6-311+G(d,p)-SDD(SMD, toluene)// B3PW91/6-31G(d)-SDD level as well as the imaginary frequency (IF, cm^{-1}) of transition states.

17 (the number of atoms involved in the molecule)

1a, E(SCRF) = -327.7584403 a.u.

C	1.154544000	-0.265513000	0.000209000
C	1.198210000	1.132696000	0.000134000
C	0.000005000	1.838588000	-0.000037000
C	-1.198211000	1.132683000	-0.000137000
C	-1.154556000	-0.265507000	-0.000010000
N	0.000007000	-0.944602000	0.000159000
H	-0.000016000	2.926104000	-0.000087000
H	2.153026000	1.651274000	0.000209000
H	-2.153017000	1.651284000	-0.000245000
C	-2.411004000	-1.093995000	-0.000005000
H	-2.437522000	-1.745479000	0.880645000
H	-3.310507000	-0.471146000	-0.000722000
H	-2.436790000	-1.746475000	-0.879942000
C	2.410997000	-1.093998000	-0.000126000
H	2.434925000	-1.749738000	0.877397000
H	2.439474000	-1.742212000	-0.883166000
H	3.310468000	-0.471122000	0.004634000

13

2a, E(SCRF) = -195.1937985 a.u.

C	1.982098000	0.002458000	-0.000050000
H	2.015809000	1.088872000	-0.000231000
H	2.939649000	-0.510485000	-0.000177000
C	0.829705000	-0.680257000	0.000113000
H	0.866401000	-1.770046000	0.000221000
C	-0.515131000	-0.098572000	0.000022000
C	-1.589479000	-0.905335000	-0.000077000
H	-1.487136000	-1.988151000	-0.000068000
H	-2.602420000	-0.511333000	-0.000086000
C	-0.654000000	1.399710000	0.000042000
H	-0.172500000	1.841387000	0.881623000
H	-0.173475000	1.841297000	-0.882140000
H	-1.705481000	1.700436000	0.000557000

30

3a, E(SCRF) = -521.9906435 a.u.

C	-4.312530000	-0.283326000	0.260699000
H	-5.086618000	-0.356106000	-0.516116000
C	-0.202918000	-1.419911000	1.031976000

C	-3.102638000	0.442604000	-0.262794000
C	2.490713000	0.939834000	0.205822000
C	1.063415000	-0.864195000	0.427930000
C	1.852641000	-1.645064000	-0.427665000
C	3.000345000	-1.087073000	-0.974966000
C	3.328955000	0.227954000	-0.655558000
H	1.568312000	-2.670476000	-0.650169000
H	3.635772000	-1.668512000	-1.638953000
H	4.221327000	0.695340000	-1.062868000
H	-4.097155000	-1.296247000	0.609303000
H	-4.764130000	0.270135000	1.095691000
H	-1.083821000	0.573876000	-0.743660000
H	-2.210745000	-2.016742000	0.515890000
N	1.381346000	0.399622000	0.733830000
C	2.784823000	2.361978000	0.599836000
H	1.948313000	3.014268000	0.325446000
H	2.905141000	2.438843000	1.686360000
H	3.693679000	2.738282000	0.120825000
H	-0.018335000	-2.447302000	1.372914000
H	-0.458573000	-0.816296000	1.908374000
H	-1.101122000	-2.004263000	-0.844727000
C	-1.401157000	-1.441907000	0.053556000
C	-1.866647000	-0.073011000	-0.346117000
C	-3.375477000	1.853242000	-0.715695000
H	-2.471298000	2.344280000	-1.088737000
H	-4.129714000	1.875055000	-1.515209000
H	-3.777604000	2.461758000	0.106670000

17

1b, E(SCRF) = -326.7511984 a.u.

C	1.370135000	-1.278701000	-0.038073000
C	2.272029000	-0.242660000	0.199697000
C	1.783192000	1.060139000	0.192072000
C	0.428125000	1.265401000	-0.050883000
C	-0.400531000	0.161554000	-0.280120000
N	0.070076000	-1.095386000	-0.272224000
H	2.445352000	1.903920000	0.370997000
H	1.712123000	-2.313592000	-0.043241000
H	3.321442000	-0.455010000	0.382648000
H	0.012180000	2.269546000	-0.065423000
C	-1.880535000	0.315934000	-0.530625000
H	-2.119155000	1.372794000	-0.700763000
H	-2.131020000	-0.224882000	-1.451791000
C	-2.725515000	-0.238486000	0.620775000
H	-2.538006000	0.311262000	1.550247000

H	-3.794468000	-0.164499000	0.392004000
H	-2.480369000	-1.290922000	0.793830000

30

3b, E(SCRF) = -521.7271112 a.u.

C	-4.058154000	0.691503000	0.174605000
H	-4.972728000	0.361850000	0.686785000
C	0.202027000	0.681681000	0.539318000
C	-1.107934000	0.308118000	1.202200000
C	2.394686000	0.088786000	0.120829000
C	2.598889000	1.230968000	-0.657942000
C	1.542691000	2.120870000	-0.833513000
C	0.322021000	1.844485000	-0.229995000
N	1.216572000	-0.173609000	0.706226000
H	1.672113000	3.019484000	-1.432287000
H	3.568009000	1.417016000	-1.113103000
H	-0.526195000	2.513463000	-0.346880000
C	3.486347000	-0.929970000	0.341300000
H	4.441577000	-0.533158000	-0.023295000
H	-4.383037000	1.171854000	-0.758819000
H	-1.673235000	1.212813000	1.446362000
C	-1.908120000	-0.627647000	0.334930000
H	-1.365253000	-1.529528000	0.049168000
C	-3.162538000	-0.481858000	-0.116778000
H	3.594094000	-1.090526000	1.421419000
C	3.178103000	-2.269424000	-0.334999000
H	3.958247000	-3.007064000	-0.116237000
H	2.221317000	-2.660352000	0.024735000
H	3.111652000	-2.157473000	-1.423288000
H	-3.587324000	1.455798000	0.797689000
H	-0.864441000	-0.195681000	2.146898000
C	-3.789828000	-1.542594000	-0.983278000
H	-4.700572000	-1.946320000	-0.518914000
H	-4.093794000	-1.129958000	-1.955689000
H	-3.105581000	-2.376463000	-1.168189000

20

2b, E(SCRF) = -386.8407198 a.u.

C	-3.339113000	0.351607000	0.000172000
C	-4.431470000	-0.428414000	-0.000015000
H	-3.459919000	1.435746000	0.000444000
H	-5.432809000	-0.008259000	-0.000031000
H	-4.356175000	-1.513864000	-0.000352000
C	-1.978668000	-0.143811000	-0.000089000
H	-1.861036000	-1.227274000	-0.000228000
C	-0.894261000	0.660166000	-0.000025000

H	-1.067631000	1.737561000	0.000421000
C	0.512541000	0.265095000	-0.000059000
C	0.941513000	-1.074871000	-0.000033000
C	1.497207000	1.268046000	-0.000102000
C	2.294037000	-1.391506000	0.000068000
H	0.209801000	-1.878071000	-0.000175000
C	2.852218000	0.951855000	-0.000047000
H	1.187359000	2.311193000	-0.000198000
C	3.258036000	-0.381106000	0.000103000
H	2.600769000	-2.434619000	0.000122000
H	3.592116000	1.748394000	-0.000128000
H	4.315278000	-0.633172000	0.000292000

13

2c, E(SCRF) = -195.199502 a.u.

C	-1.357195000	0.395316000	-0.000175000
C	-2.526913000	-0.259211000	0.000077000
H	-1.358531000	1.486339000	-0.000509000
H	-3.476588000	0.267731000	0.000526000
H	-2.570953000	-1.346516000	0.000635000
C	-0.053342000	-0.245897000	-0.000198000
H	-0.045156000	-1.337533000	-0.000572000
C	1.113783000	0.418082000	0.000128000
C	2.466965000	-0.216395000	0.000028000
H	2.400871000	-1.309429000	-0.000713000
H	3.050130000	0.089771000	-0.879365000
H	3.049344000	0.088549000	0.880366000
H	1.091093000	1.509722000	0.000473000

33

A, E(SCRF) = -636.4684694 a.u.

C	-0.426374000	-1.002704000	1.660836000
C	-3.546293000	-1.613044000	-0.403386000
H	-4.241484000	-2.426774000	-0.589668000
C	-3.690717000	-0.399259000	-1.087731000
H	-4.495563000	-0.261365000	-1.803069000
C	-2.801398000	0.635737000	-0.840219000
H	-2.927504000	1.578518000	-1.362758000
C	-1.757811000	0.476526000	0.090718000
C	-0.904901000	2.214574000	1.615686000
H	-1.759108000	2.902244000	1.576325000
H	0.005854000	2.780715000	1.828625000
H	-1.077282000	1.495464000	2.415209000
C	-0.647747000	2.519493000	-0.760063000
H	-0.530684000	2.039153000	-1.740951000
H	0.227353000	3.144799000	-0.565194000

H	-1.528596000	3.172263000	-0.813062000
C	2.882368000	0.739405000	0.548158000
C	3.014258000	0.715366000	-0.866294000
H	3.085483000	1.581380000	-1.516331000
C	3.106696000	-0.640536000	-1.274015000
C	3.040643000	-1.452647000	-0.109696000
H	3.123247000	-2.534436000	-0.081966000
C	2.905006000	-0.602490000	1.017335000
H	-2.435115000	-2.719229000	1.059046000
C	-1.607677000	-0.745142000	0.832986000
C	-2.528629000	-1.779122000	0.521048000
H	-0.170469000	-0.264281000	2.423776000
H	-0.395354000	-2.007949000	2.084347000
N	-0.757653000	1.517155000	0.316634000
Y	0.698228000	-0.338863000	-0.300895000
H	3.263095000	-0.991461000	-2.289173000
H	2.839186000	1.627788000	1.168753000
H	2.865072000	-0.918190000	2.052385000

67

B, E(SCRF) = -1289.959964 a.u.

C	-1.255182000	-2.902084000	-1.836319000
H	-0.832429000	-2.112683000	-2.466060000
C	1.520858000	-1.156979000	-1.554256000
Y	0.162796000	-0.353169000	0.263309000
C	4.540846000	0.623830000	-0.054258000
H	6.538897000	-0.137687000	0.183492000
H	5.998551000	-2.332561000	-0.871472000
H	3.715304000	-2.764890000	-1.710236000
H	4.789686000	1.570583000	0.414001000
C	2.918226000	-0.858609000	-1.128770000
H	1.248939000	-0.575720000	-2.453539000
H	1.454174000	-2.208335000	-1.851955000
N	2.157828000	1.332004000	-0.338688000
C	1.993785000	2.100083000	-1.594893000
H	1.136522000	2.774475000	-1.510636000
H	2.894400000	2.696787000	-1.796602000
H	1.842728000	1.422474000	-2.436332000
C	2.396168000	2.298855000	0.745348000
H	1.503146000	2.916825000	0.866472000
H	2.608597000	1.774144000	1.679771000
H	3.232526000	2.976082000	0.523113000
C	1.089295000	-0.600315000	2.762284000
C	-0.181559000	-1.232830000	2.774955000
C	1.955517000	-1.375302000	1.950948000

C	-0.098523000	-2.391743000	1.964134000
C	1.221369000	-2.477806000	1.453281000
C	5.536231000	-0.344481000	-0.179282000
C	-2.456550000	-2.426464000	-1.078770000
C	-3.685348000	-3.053876000	-1.281336000
C	-4.798508000	-2.638369000	-0.562460000
C	-4.642506000	-1.603433000	0.346841000
C	-3.391312000	-1.003616000	0.505181000
N	-2.304868000	-1.400834000	-0.200164000
H	-5.763099000	-3.118243000	-0.701732000
H	-3.754444000	-3.868869000	-1.994455000
H	-5.479308000	-1.251434000	0.942213000
C	-3.263792000	0.128411000	1.481323000
H	-3.516108000	1.084048000	1.007755000
H	-3.948949000	-0.012760000	2.322925000
H	-2.252410000	0.203362000	1.885742000
C	5.232024000	-1.569047000	-0.769561000
C	3.944566000	-1.811304000	-1.239513000
H	-0.465651000	-3.232872000	-1.152967000
H	-1.512852000	-3.744314000	-2.483481000
C	-1.253352000	2.892390000	0.826226000
C	-1.825603000	4.135225000	0.544470000
C	-2.280694000	4.404734000	-0.738207000
C	-2.157055000	3.417170000	-1.709369000
C	-1.573543000	2.196424000	-1.375642000
N	-1.113333000	1.939539000	-0.125087000
H	-2.725725000	5.366135000	-0.978703000
H	-1.909933000	4.875165000	1.334690000
H	-2.506303000	3.584729000	-2.723248000
C	-1.472768000	1.109533000	-2.406614000
H	-0.510698000	0.586621000	-2.369430000
H	-2.266339000	0.366962000	-2.263565000
H	-1.576308000	1.515514000	-3.416483000
C	-0.821050000	2.598832000	2.235568000
H	-1.697578000	2.469816000	2.882729000
H	-0.217619000	1.690614000	2.315162000
H	-0.239124000	3.428250000	2.650957000
C	3.245606000	0.365251000	-0.505855000
H	-0.896309000	-3.105799000	1.796970000
H	1.617062000	-3.262678000	0.820422000
H	3.002332000	-1.175933000	1.760635000
H	1.375316000	0.265058000	3.350677000
H	-1.036320000	-0.931126000	3.368950000

TS1, E(SCRF) = -1289.921029 a.u., IF = *i*1225.05 cm⁻¹

C	-0.361355000	-2.734268000	-1.077352000
H	0.719565000	-1.805508000	-1.325379000
C	1.800388000	-1.050568000	-1.838594000
Y	0.222296000	-0.516358000	0.267646000
C	4.252630000	1.305006000	-0.092903000
H	6.330601000	0.943922000	0.329791000
H	6.310270000	-1.328191000	-0.703418000
H	4.232220000	-2.192455000	-1.719652000
H	4.279238000	2.289380000	0.361746000
C	3.041966000	-0.469644000	-1.246323000
H	1.338048000	-0.396728000	-2.590068000
H	2.078344000	-1.958288000	-2.388921000
N	1.812701000	1.546498000	-0.571901000
C	1.559644000	2.228275000	-1.863296000
H	0.577354000	2.709153000	-1.837802000
H	2.324230000	2.996918000	-2.043081000
H	1.594721000	1.521641000	-2.692583000
C	1.804891000	2.589614000	0.467330000
H	0.800458000	3.013840000	0.525239000
H	2.078233000	2.164146000	1.434596000
H	2.496835000	3.411335000	0.234975000
C	1.325146000	-0.275651000	2.690435000
C	0.155996000	-1.062333000	2.872889000
C	2.251328000	-1.037382000	1.936017000
C	0.361329000	-2.303659000	2.226803000
C	1.653557000	-2.285204000	1.644495000
C	5.420470000	0.542836000	-0.106491000
C	-1.786643000	-2.411680000	-0.887963000
C	-2.824707000	-2.899754000	-1.692558000
C	-4.135145000	-2.582132000	-1.362846000
C	-4.386132000	-1.794276000	-0.239820000
C	-3.315195000	-1.293282000	0.498933000
N	-2.040228000	-1.566892000	0.148537000
H	-4.960414000	-2.967831000	-1.955721000
H	-2.594158000	-3.548205000	-2.532139000
H	-5.402953000	-1.566267000	0.065293000
C	-3.560578000	-0.444869000	1.712861000
H	-4.004793000	0.520406000	1.443630000
H	-4.261392000	-0.945163000	2.390616000
H	-2.632080000	-0.264607000	2.256806000
C	5.407812000	-0.723713000	-0.684541000
C	4.234384000	-1.209923000	-1.253018000
H	-0.008933000	-3.405609000	-0.286974000

H	-0.185763000	-3.234750000	-2.035363000
C	-1.781325000	2.466849000	0.940891000
C	-2.646149000	3.533872000	0.682472000
C	-3.181692000	3.692815000	-0.586823000
C	-2.838408000	2.771577000	-1.569424000
C	-1.975093000	1.723167000	-1.255982000
N	-1.441533000	1.572257000	-0.017365000
H	-3.851415000	4.518812000	-0.809032000
H	-2.885913000	4.228721000	1.481825000
H	-3.233310000	2.856473000	-2.577023000
C	-1.648881000	0.705782000	-2.311011000
H	-0.629464000	0.314170000	-2.224827000
H	-2.341679000	-0.142014000	-2.266190000
H	-1.728263000	1.141277000	-3.311371000
C	-1.227318000	2.315012000	2.328178000
H	-2.035025000	2.127566000	3.045554000
H	-0.515967000	1.491580000	2.401165000
H	-0.722487000	3.232595000	2.650882000
C	3.068674000	0.803058000	-0.636018000
H	-0.344405000	-3.125144000	2.198891000
H	2.119249000	-3.093373000	1.092535000
H	3.251242000	-0.732392000	1.655483000
H	1.516679000	0.693073000	3.137892000
H	-0.712575000	-0.790694000	3.461506000

67

C, E(SCRF) = -1289.95609 a.u.

C	-0.352312000	-2.229853000	-1.234382000
H	1.863936000	-1.351152000	-1.819158000
C	2.922762000	-1.402762000	-2.088719000
Y	-0.046441000	-0.432472000	0.377312000
C	4.314630000	1.317307000	0.239080000
H	6.297913000	1.415657000	1.052883000
H	7.032646000	-0.699884000	-0.061500000
H	5.427159000	-1.931362000	-1.481733000
H	4.038057000	2.238185000	0.736947000
C	3.803481000	-0.568894000	-1.197028000
H	3.015040000	-1.105430000	-3.142422000
H	3.218613000	-2.455307000	-2.034477000
N	2.028467000	1.132675000	-0.727577000
C	1.818774000	1.559542000	-2.133024000
H	0.822554000	1.999859000	-2.232076000
H	2.562935000	2.314568000	-2.421846000
H	1.896315000	0.713639000	-2.814068000
C	1.753567000	2.307590000	0.118780000

H	0.717062000	2.615461000	-0.039391000
H	1.902894000	2.061493000	1.173792000
H	2.391774000	3.166303000	-0.134866000
C	0.988217000	-0.248289000	2.828914000
C	-0.135924000	-1.105336000	2.943424000
C	1.969398000	-0.916368000	2.053771000
C	0.154576000	-2.303323000	2.243267000
C	1.453375000	-2.186188000	1.695150000
C	5.614401000	0.851910000	0.424413000
C	-1.812809000	-2.210061000	-1.041537000
C	-2.777328000	-2.721830000	-1.927114000
C	-4.117559000	-2.636681000	-1.587014000
C	-4.487832000	-2.039076000	-0.377727000
C	-3.504360000	-1.503889000	0.446257000
N	-2.199442000	-1.566555000	0.095542000
H	-4.878743000	-3.051158000	-2.243300000
H	-2.454787000	-3.210933000	-2.841184000
H	-5.529918000	-1.987792000	-0.078903000
C	-3.847061000	-0.841313000	1.748478000
H	-3.531973000	0.208354000	1.752861000
H	-4.923822000	-0.868163000	1.934165000
H	-3.345615000	-1.344908000	2.582513000
C	6.023736000	-0.321519000	-0.196583000
C	5.116821000	-1.009994000	-0.994141000
H	0.093785000	-3.055654000	-0.662741000
H	-0.071982000	-2.367419000	-2.282839000
C	-1.953973000	2.535552000	0.901309000
C	-2.811147000	3.602546000	0.642920000
C	-3.310614000	3.786537000	-0.642100000
C	-2.943202000	2.887434000	-1.631802000
C	-2.093543000	1.824266000	-1.316803000
N	-1.595956000	1.653533000	-0.068886000
H	-3.974814000	4.616833000	-0.864753000
H	-3.075600000	4.282717000	1.446116000
H	-3.312583000	2.991246000	-2.647378000
C	-1.757939000	0.825474000	-2.386233000
H	-0.843051000	0.255573000	-2.189505000
H	-2.568471000	0.095101000	-2.492921000
H	-1.633365000	1.320183000	-3.354691000
C	-1.383201000	2.353139000	2.277748000
H	-1.909963000	2.978114000	3.003473000
H	-1.455373000	1.315102000	2.616476000
H	-0.325124000	2.639696000	2.308735000
C	3.393736000	0.622685000	-0.558690000

H	-0.501834000	-3.160553000	2.153282000
H	1.973997000	-2.942680000	1.120035000
H	2.958491000	-0.544837000	1.817567000
H	1.105813000	0.716225000	3.310304000
H	-1.034264000	-0.909870000	3.518204000

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D, E(SCRF) = -1211.410996 a.u.

C	0.884314000	-1.927201000	-1.605815000
C	-2.287286000	-2.494700000	-1.773763000
H	-1.757487000	-2.043887000	-2.620835000
Y	0.081622000	-0.585375000	0.239636000
H	-6.413355000	-0.605723000	-0.756065000
C	-4.739315000	0.311013000	0.248791000
H	-5.334082000	1.030922000	0.802101000
C	-3.354592000	0.295835000	0.413905000
C	-0.201256000	-1.015809000	2.852055000
C	1.179828000	-1.198711000	2.575854000
H	1.997085000	-0.599063000	2.961946000
C	1.314773000	-2.363914000	1.782028000
C	0.023114000	-2.897190000	1.560133000
H	-0.201333000	-3.800777000	1.005795000
C	-0.915406000	-2.066283000	2.221530000
C	3.390562000	-2.402953000	-1.418871000
H	-4.950042000	-2.257535000	-1.934557000
C	3.596382000	0.118819000	-0.306048000
C	4.743834000	-0.641086000	-0.494924000
C	4.631865000	-1.926877000	-1.036184000
H	3.274100000	-3.382813000	-1.871435000
C	-3.144484000	-1.489049000	-1.066358000
H	5.711774000	-0.238713000	-0.213905000
H	5.520777000	-2.537351000	-1.173693000
C	-4.525235000	-1.513293000	-1.268761000
H	-1.530115000	-2.918966000	-1.108824000
H	-2.899397000	-3.311250000	-2.165761000
N	2.379066000	-0.354733000	-0.662871000
C	3.661438000	1.486043000	0.310588000
H	3.169395000	1.499566000	1.290529000
H	4.697640000	1.801860000	0.456809000
H	3.160624000	2.225629000	-0.322675000
C	2.263787000	-1.574733000	-1.263773000
H	0.748881000	-2.989243000	-1.819521000
H	0.532773000	-1.345916000	-2.470185000
C	-5.336615000	-0.598866000	-0.612158000
H	2.246476000	-2.778927000	1.417643000

H	-0.625216000	-0.259722000	3.503384000
H	-1.985923000	-2.226786000	2.270266000
C	-0.078646000	2.456088000	-1.392739000
C	-0.021800000	3.802981000	-1.744628000
C	0.252332000	4.752387000	-0.766674000
C	0.458774000	4.322519000	0.536442000
C	0.379738000	2.960446000	0.834987000
N	0.113823000	2.037003000	-0.117655000
H	0.306670000	5.807871000	-1.018107000
H	-0.185024000	4.094969000	-2.777055000
H	0.679434000	5.030170000	1.329707000
C	0.568394000	2.514173000	2.255961000
H	0.855192000	1.462473000	2.326352000
H	1.340474000	3.111038000	2.751299000
H	-0.356767000	2.646783000	2.831367000
C	-0.329552000	1.412110000	-2.440699000
H	0.586793000	0.843933000	-2.640811000
H	-1.121292000	0.713934000	-2.139084000
H	-0.646797000	1.866238000	-3.383075000
N	-2.556535000	-0.582447000	-0.242980000
C	-2.725191000	1.286418000	1.348342000
H	-3.444384000	1.611810000	2.105555000
H	-1.868744000	0.854062000	1.876215000
H	-2.384380000	2.177275000	0.810020000

57

E, E(SCRF) = -1079.821116 a.u.

C	3.099067000	-0.341540000	-1.807845000
C	2.177018000	-0.802968000	-2.679033000
C	-0.194727000	-2.274309000	-1.464016000
Y	0.698577000	-0.532985000	0.019212000
C	3.163634000	1.015239000	-1.230359000
C	2.131300000	1.882803000	-1.320669000
H	0.436584000	-0.653368000	3.316528000
C	2.330765000	-0.539434000	2.133581000
C	-2.735481000	-1.174114000	0.896163000
C	-1.551818000	-2.073493000	-0.938536000
C	-2.755800000	-2.440668000	-1.564448000
C	-3.954122000	-2.185998000	-0.917296000
C	-3.947083000	-1.562794000	0.335409000
H	-2.726069000	-2.950951000	-2.522281000
H	-4.896525000	-2.486567000	-1.368286000
H	-4.873377000	-1.380346000	0.870680000
H	3.889674000	-1.022567000	-1.501027000
C	2.911895000	-1.463426000	1.229170000

H	2.223057000	-1.822380000	-3.045420000
N	-1.571270000	-1.402135000	0.246917000
C	-2.668324000	-0.500884000	2.235657000
H	-2.144885000	0.459273000	2.169812000
H	-3.668270000	-0.314442000	2.635497000
H	-2.127752000	-1.126987000	2.955071000
C	2.043849000	-2.577478000	1.114647000
H	-0.174245000	-2.452458000	-2.541748000
H	0.289845000	-3.126337000	-0.969213000
H	2.224234000	-3.465936000	0.521294000
H	2.783710000	0.383661000	2.475964000
H	3.891590000	-1.379405000	0.777827000
H	0.088679000	-3.016154000	2.088802000
C	-0.566627000	2.663887000	0.994551000
C	-1.342288000	3.820873000	1.005142000
C	-2.239604000	4.056146000	-0.031020000
C	-2.320989000	3.129029000	-1.058684000
C	-1.525939000	1.981295000	-1.015692000
N	-0.669510000	1.740853000	0.003608000
H	-2.851404000	4.953722000	-0.042077000
H	-1.231276000	4.531231000	1.817998000
H	-2.991505000	3.281571000	-1.898879000
C	-1.632159000	0.988843000	-2.137176000
H	-2.515758000	0.352416000	-2.014730000
H	-1.728624000	1.503228000	-3.098918000
H	-0.768734000	0.317305000	-2.209689000
C	0.430307000	2.420665000	2.088335000
H	0.484224000	3.276320000	2.766110000
H	0.168325000	1.541091000	2.685427000
H	1.431706000	2.255593000	1.674802000
H	1.421790000	-0.167301000	-3.135971000
C	0.926718000	-2.344948000	1.947613000
C	1.099898000	-1.085263000	2.576132000
H	2.192255000	2.882757000	-0.901917000
H	1.247876000	1.677918000	-1.921456000
C	4.449760000	1.392492000	-0.547619000
H	5.261472000	1.417822000	-1.285978000
H	4.388492000	2.379352000	-0.081752000
H	4.740371000	0.663591000	0.216535000

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TS2, E(SCRF) = -1079.323199 a.u., IF = *i*191.88 cm⁻¹

C	2.720861000	-0.452117000	-1.809502000
C	1.746617000	-1.268088000	-2.410347000
C	0.424557000	-2.578329000	-1.174932000

Y	0.891220000	-0.253299000	0.059408000
C	2.665397000	0.980866000	-1.660006000
C	1.498416000	1.693807000	-1.762254000
H	0.578892000	0.348129000	3.298602000
C	2.447339000	0.481723000	2.066762000
C	-2.276373000	-1.563234000	1.057254000
C	-0.936971000	-2.477739000	-0.645601000
C	-2.031785000	-3.182016000	-1.174134000
C	-3.255616000	-3.090044000	-0.530465000
C	-3.377396000	-2.289645000	0.609210000
H	-1.896474000	-3.817750000	-2.043649000
H	-4.111725000	-3.650384000	-0.896897000
H	-4.318760000	-2.226065000	1.145291000
H	3.656283000	-0.933369000	-1.536737000
C	3.186065000	-0.526184000	1.403738000
H	2.090745000	-2.228134000	-2.774016000
N	-1.089942000	-1.640935000	0.414822000
C	-2.358617000	-0.692291000	2.275839000
H	-1.979893000	0.313565000	2.068957000
H	-3.388549000	-0.606407000	2.631063000
H	-1.755615000	-1.113306000	3.089038000
C	2.506952000	-1.757527000	1.575226000
H	0.466377000	-3.237335000	-2.037901000
H	1.134078000	-2.937678000	-0.420896000
H	2.846009000	-2.723711000	1.218874000
H	2.744758000	1.518366000	2.169640000
H	4.135165000	-0.393401000	0.901911000
H	0.642947000	-2.262757000	2.687169000
C	-1.032709000	2.777001000	0.642083000
C	-2.030395000	3.747679000	0.562598000
C	-3.075495000	3.588835000	-0.338591000
C	-3.071658000	2.468963000	-1.155951000
C	-2.051051000	1.523870000	-1.029527000
N	-1.053190000	1.655804000	-0.123805000
H	-3.861722000	4.334257000	-0.417154000
H	-1.971666000	4.624692000	1.199188000
H	-3.847292000	2.317415000	-1.900489000
C	-2.074601000	0.331622000	-1.942401000
H	-2.741149000	-0.448832000	-1.560027000
H	-2.440257000	0.617615000	-2.933694000
H	-1.088847000	-0.122104000	-2.080042000
C	0.117053000	2.979870000	1.581730000
H	0.138927000	4.007565000	1.953547000
H	0.051962000	2.317206000	2.450466000

H	1. 069223000	2. 782798000	1. 077693000
H	0. 960773000	-0. 830106000	-3. 024362000
C	1. 356587000	-1. 515617000	2. 363110000
C	1. 310495000	-0. 133355000	2. 661145000
H	1. 484534000	2. 772201000	-1. 641257000
H	0. 612722000	1. 274701000	-2. 239127000
C	3. 951266000	1. 692305000	-1. 324123000
H	4. 516777000	1. 846599000	-2. 251898000
H	3. 770847000	2. 675031000	-0. 879547000
H	4. 591641000	1. 113642000	-0. 652933000

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F, E(SCRF) = -1079.860439 a.u.

C	1. 336312000	1. 673545000	-1. 735707000
C	1. 278018000	0. 353940000	-2. 475593000
C	2. 528536000	-0. 490249000	-2. 269648000
Y	0. 005583000	0. 706644000	0. 144217000
C	0. 244229000	2. 567103000	-1. 732640000
C	-1. 079766000	2. 108772000	-1. 769379000
H	-0. 938415000	0. 554606000	3. 317281000
C	-0. 418629000	2. 397020000	2. 152400000
C	1. 764153000	-2. 089142000	0. 996418000
C	2. 709259000	-1. 147620000	-0. 920868000
C	3. 942805000	-1. 735463000	-0. 627937000
C	4. 080044000	-2. 506832000	0. 516762000
C	2. 964587000	-2. 712867000	1. 323135000
H	4. 774854000	-1. 598470000	-1. 312114000
H	5. 032847000	-2. 966861000	0. 763364000
H	3. 016599000	-3. 356870000	2. 195600000
H	2. 332098000	2. 107884000	-1. 659088000
C	0. 805110000	2. 817745000	1. 583838000
H	1. 145654000	0. 527012000	-3. 555280000
N	1. 655829000	-1. 265872000	-0. 078705000
C	0. 524644000	-2. 398779000	1. 790031000
H	-0. 254472000	-1. 635618000	1. 697833000
H	0. 089580000	-3. 343079000	1. 437487000
H	0. 747148000	-2. 520896000	2. 854064000
C	1. 772254000	1. 810446000	1. 816466000
H	2. 538188000	-1. 304323000	-3. 009301000
H	3. 415269000	0. 115632000	-2. 494341000
H	2. 814484000	1. 847385000	1. 521697000
H	-1. 332566000	2. 978053000	2. 178953000
H	0. 979754000	3. 764703000	1. 091963000
H	1. 638018000	-0. 118378000	2. 917816000
C	-3. 372341000	-0. 208731000	0. 314212000

C	-4.592815000	-0.882186000	0.277856000
C	-4.667629000	-2.134362000	-0.315779000
C	-3.517540000	-2.660833000	-0.886727000
C	-2.324699000	-1.938370000	-0.836852000
N	-2.237868000	-0.734953000	-0.214338000
H	-5.605633000	-2.681375000	-0.346815000
H	-5.470380000	-0.417083000	0.715461000
H	-3.534608000	-3.623435000	-1.387970000
C	-1.124651000	-2.483095000	-1.554265000
H	-0.186496000	-2.240929000	-1.050774000
H	-1.189971000	-3.570391000	-1.653437000
H	-1.076980000	-2.071592000	-2.571659000
C	-3.298992000	1.143325000	0.955255000
H	-4.284818000	1.616738000	0.976120000
H	-2.947544000	1.076310000	1.990507000
H	-2.629543000	1.810588000	0.397342000
H	0.390722000	-0.258773000	-2.216396000
C	1.146458000	0.768563000	2.538946000
C	-0.215636000	1.119227000	2.738121000
H	-1.890557000	2.830412000	-1.704001000
H	-1.338646000	1.200621000	-2.315934000
C	0.503127000	4.037521000	-1.521038000
H	0.488702000	4.525702000	-2.504139000
H	-0.271448000	4.515696000	-0.912712000
H	1.483677000	4.231323000	-1.076757000

57

TS3', E(SCRf) = -1079.800584 a.u., IF = *i*1221.23 cm⁻¹

C	-0.250320000	-2.250168000	0.518266000
H	-0.540123000	-1.541653000	-0.650893000
C	-1.132418000	-0.932878000	-1.877870000
Y	-0.030347000	0.421283000	0.045973000
C	0.483730000	3.012240000	0.415574000
C	-0.871110000	2.944659000	0.011262000
H	-1.725995000	3.223167000	0.614585000
C	-0.908426000	2.518946000	-1.340182000
C	3.521077000	0.516732000	0.587956000
C	2.914327000	-1.323155000	-0.704575000
C	4.209461000	-1.436586000	-1.207478000
C	5.176288000	-0.516027000	-0.819817000
C	4.833757000	0.448456000	0.117608000
H	4.454738000	-2.254186000	-1.878077000
H	6.189460000	-0.579124000	-1.206801000
H	5.576013000	1.139149000	0.506478000
H	-1.033289000	-2.974049000	0.265158000

C	0.424185000	2.319469000	-1.772309000
H	1.009057000	-3.950173000	0.215719000
N	2.553824000	-0.310466000	0.122411000
C	3.203544000	1.468750000	1.706943000
H	3.555319000	2.483047000	1.491704000
H	2.136935000	1.513675000	1.930131000
H	3.717989000	1.137156000	2.617984000
C	1.285253000	2.621688000	-0.688810000
H	2.440258000	-3.251477000	-1.416224000
H	1.194221000	-2.086944000	-1.763354000
H	2.366702000	2.613900000	-0.728355000
H	-1.800915000	2.390406000	-1.941003000
H	0.737205000	2.029337000	-2.769798000
H	0.838882000	3.371559000	1.374289000
C	-2.491827000	-0.676328000	-1.337111000
C	-3.683601000	-1.182069000	-1.857815000
C	-4.877591000	-0.870095000	-1.217648000
C	-4.853030000	-0.075519000	-0.073810000
C	-3.632423000	0.384548000	0.420287000
N	-2.477731000	0.069434000	-0.202348000
H	-5.822790000	-1.239467000	-1.606083000
H	-3.664849000	-1.792799000	-2.754998000
H	-5.772237000	0.182691000	0.443141000
C	-3.575858000	1.238448000	1.654771000
H	-3.840794000	2.277164000	1.420484000
H	-4.289815000	0.888228000	2.406781000
H	-2.577367000	1.237361000	2.100473000
C	1.900922000	-2.402706000	-0.984177000
H	-0.788617000	-0.114399000	-2.526565000
C	1.142593000	-2.864916000	0.285655000
H	-1.075529000	-1.848959000	-2.472498000
H	1.780329000	-2.698242000	1.160909000
C	-0.583752000	-1.612199000	1.795425000
C	0.236560000	-0.712757000	2.442265000
H	-0.064848000	-0.282240000	3.393736000
H	1.300318000	-0.670307000	2.211190000
C	-1.939377000	-1.925264000	2.377614000
H	-2.716898000	-2.007305000	1.612816000
H	-1.873714000	-2.902907000	2.873905000
H	-2.250547000	-1.195040000	3.129646000

57

TS3, E(SCRF) = -1079.814985 a.u., IF = *i*1150.47 cm⁻¹

C	1.901682000	1.780013000	1.505331000
H	2.131393000	1.471379000	0.189140000

C	2.623236000	0.782907000	-1.100642000
Y	0.158409000	0.766626000	-0.281760000
C	0.593138000	2.254509000	1.942895000
C	-0.456481000	1.391872000	2.174621000
H	-0.504569000	0.979253000	-3.515522000
C	0.237914000	2.624122000	-2.208663000
C	-2.246477000	-1.576528000	-1.031420000
C	-2.350180000	-1.106909000	1.247761000
C	-3.664468000	-1.573005000	1.312194000
C	-4.280894000	-2.044012000	0.160809000
C	-3.546881000	-2.079034000	-1.018566000
H	-4.180658000	-1.588408000	2.267564000
H	-5.303405000	-2.409807000	0.189173000
H	-3.969207000	-2.494782000	-1.928514000
H	-1.418688000	1.825785000	2.442656000
C	-0.346857000	3.268340000	-1.094994000
H	0.207329000	-0.191661000	3.446867000
N	-1.675717000	-1.042613000	0.076468000
C	-1.437395000	-1.665428000	-2.296231000
H	-1.487792000	-2.684365000	-2.697348000
H	-1.823106000	-0.999529000	-3.074889000
H	-0.379598000	-1.439448000	-2.128921000
C	-1.612151000	2.672879000	-0.853372000
H	-1.478519000	-1.783360000	3.039958000
H	-2.315906000	-0.262760000	3.214956000
H	-2.327307000	2.972232000	-0.096425000
H	1.186145000	2.882897000	-2.663740000
H	0.069605000	4.117600000	-0.570697000
H	-2.693125000	1.047754000	-1.917654000
C	2.897802000	-0.579655000	-0.626334000
C	4.178443000	-1.101008000	-0.404584000
C	4.300395000	-2.403656000	0.050335000
C	3.146142000	-3.153432000	0.278881000
C	1.894998000	-2.575191000	0.080957000
N	1.773376000	-1.291066000	-0.340261000
H	5.280737000	-2.843490000	0.212761000
H	5.050094000	-0.490802000	-0.619301000
H	3.212274000	-4.183414000	0.614199000
C	0.650515000	-3.375495000	0.331009000
H	0.008030000	-2.899258000	1.077520000
H	0.059206000	-3.479267000	-0.584676000
H	0.901004000	-4.378060000	0.686435000
C	-1.637863000	-0.811985000	2.549976000
H	3.506074000	1.423883000	-1.159394000

H	2.156745000	0.777429000	-2.092829000
C	-0.302783000	-0.080458000	2.477902000
H	0.374781000	-0.621962000	1.786128000
C	-1.801506000	1.653831000	-1.813163000
C	-0.648681000	1.611654000	-2.646880000
H	2.682148000	2.542569000	1.558914000
H	2.244713000	0.856924000	1.985679000
C	0.390822000	3.738632000	2.095227000
H	0.690676000	4.016468000	3.114934000
H	1.018243000	4.318214000	1.412438000
H	-0.653686000	4.037532000	1.967464000

61

G, E(SCRf) = -1028.11966 a.u.

Y	-0.661202000	0.084712000	-0.167944000
C	0.664930000	-0.165963000	-2.114590000
N	0.320497000	2.262441000	-0.270972000
C	1.571947000	1.981715000	-0.092162000
H	2.269621000	2.777505000	0.179660000
C	-0.205937000	3.648443000	-0.251572000
C	0.801997000	4.693874000	0.229538000
H	0.317406000	5.674702000	0.249463000
H	1.159015000	4.484717000	1.244849000
H	1.665534000	4.777606000	-0.439788000
C	-0.649569000	3.968946000	-1.688059000
H	-1.385866000	3.241690000	-2.050913000
H	-1.111665000	4.960821000	-1.727720000
H	0.204992000	3.961149000	-2.372736000
C	-1.425592000	3.633093000	0.680807000
H	-2.179761000	2.907508000	0.342582000
H	-1.137458000	3.388828000	1.710185000
H	-1.914171000	4.612501000	0.692907000
C	-2.122330000	-1.167886000	1.538318000
C	-1.529873000	-2.385122000	-0.339570000
C	-2.989822000	-0.782950000	0.469716000
H	0.607957000	-0.917173000	-2.899779000
H	0.507571000	0.850796000	-2.498486000
C	1.773820000	-0.330959000	-1.196236000
C	2.477760000	-1.566160000	-1.189762000
C	2.135452000	0.629476000	-0.173968000
C	3.501390000	-1.850944000	-0.306541000
H	2.216766000	-2.292345000	-1.955712000
C	3.220907000	0.342893000	0.723511000
C	3.858156000	-0.878001000	0.654749000
H	4.666134000	-1.093979000	1.349839000

C	-2.223590000	-0.709379000	2.967449000
H	-2.894392000	-1.366333000	3.536891000
H	-1.256456000	-0.727459000	3.482508000
H	-2.629202000	0.304859000	3.054648000
C	-0.208997000	-2.922052000	1.847607000
H	0.153115000	-2.352973000	2.710775000
H	-0.657881000	-3.843507000	2.241484000
H	0.663645000	-3.216674000	1.255782000
C	-0.924736000	-3.444230000	-1.213318000
H	0.119257000	-3.645092000	-0.953406000
H	-1.471676000	-4.390249000	-1.103643000
H	-0.959184000	-3.172205000	-2.272732000
C	-3.330304000	-1.520654000	-2.015762000
H	-2.653626000	-1.731167000	-2.850359000
H	-4.117134000	-2.286344000	-2.037681000
H	-3.819931000	-0.561558000	-2.217953000
C	-4.172737000	0.140834000	0.579793000
H	-5.078661000	-0.424127000	0.836887000
H	-4.042790000	0.897189000	1.361721000
H	-4.388361000	0.662961000	-0.359561000
C	-2.617533000	-1.533131000	-0.692455000
C	3.672546000	1.351549000	1.750601000
H	4.130339000	2.233212000	1.281905000
H	2.851030000	1.707834000	2.383855000
H	4.427789000	0.914060000	2.408475000
C	4.252454000	-3.150615000	-0.369166000
H	5.309046000	-2.974885000	-0.605520000
H	4.224681000	-3.669051000	0.596701000
H	3.844263000	-3.820987000	-1.130408000
C	-1.213099000	-2.151553000	1.034720000

81

TS4, E(SCRF) = -1414960584 a.u., IF = $i328.81 \text{ cm}^{-1}$

C	-0.539995000	-0.991550000	-2.031359000
C	-0.953544000	0.356162000	-2.152460000
C	0.767494000	-1.491611000	-1.801185000
C	1.970384000	-0.803364000	-1.695105000
C	-2.078320000	1.155342000	-0.469445000
Y	0.348596000	0.427116000	0.039585000
C	-4.349836000	0.599569000	-1.361250000
C	-3.316433000	-0.928903000	0.224315000
C	-4.466204000	-1.744131000	0.148973000
C	-5.538804000	-1.440708000	-0.676449000
C	-5.450454000	-0.255960000	-1.418495000
H	-4.507549000	-2.647974000	0.754164000

H	-6.286532000	0.021812000	-2.057941000
C	-2.308206000	-1.442904000	1.139400000
H	-2.692072000	-2.285030000	1.722660000
C	-0.325725000	-1.916591000	2.363408000
C	-0.471619000	-3.426491000	2.119864000
H	0.211206000	-3.968938000	2.781929000
H	-1.478477000	-3.799080000	2.331619000
H	-0.219453000	-3.685761000	1.085309000
C	1.149581000	-1.543916000	2.201924000
H	1.315287000	-0.471345000	2.376912000
H	1.775174000	-2.062950000	2.934850000
H	1.540939000	-1.831638000	1.213935000
C	-0.810815000	-1.545292000	3.769810000
H	-0.699807000	-0.472121000	3.955618000
H	-1.866388000	-1.805339000	3.904938000
H	-0.233205000	-2.085348000	4.527644000
N	-1.076185000	-1.100855000	1.346576000
H	-1.334278000	-1.733185000	-2.047700000
H	-1.863663000	0.558388000	-2.704233000
H	-0.204261000	1.142803000	-2.333154000
C	0.274900000	2.831952000	1.220543000
H	0.808605000	-2.567492000	-1.631087000
H	2.024166000	0.214860000	-2.096505000
C	3.275318000	-1.450807000	-1.497058000
C	3.418689000	-2.693718000	-0.852991000
C	4.438267000	-0.832158000	-1.990215000
C	4.668153000	-3.288477000	-0.711116000
H	2.545675000	-3.208989000	-0.458493000
C	5.688984000	-1.425796000	-1.844616000
H	4.354260000	0.110323000	-2.525804000
C	5.811728000	-2.656432000	-1.201400000
H	4.750316000	-4.250964000	-0.212957000
H	6.568618000	-0.929169000	-2.245146000
H	6.786513000	-3.121575000	-1.086971000
C	-3.246287000	0.270612000	-0.535922000
C	0.693398000	3.056189000	-0.127303000
H	-1.797559000	1.323958000	0.582569000
H	-2.229680000	2.129335000	-0.926619000
C	2.369756000	1.886364000	0.953260000
C	1.307101000	2.112060000	1.887943000
C	-6.752008000	-2.325212000	-0.767262000
H	-7.664956000	-1.772931000	-0.515859000
H	-6.881067000	-2.716971000	-1.783308000
H	-6.678962000	-3.178911000	-0.087215000

C	-4.395930000	1.887597000	-2.146844000
H	-4.366897000	2.762463000	-1.484830000
H	-3.564123000	1.991182000	-2.853973000
H	-5.319433000	1.950762000	-2.728479000
C	-0.925963000	3.438459000	1.889110000
H	-1.335277000	2.798424000	2.679158000
H	-0.656898000	4.392762000	2.361851000
H	-1.734817000	3.651879000	1.183405000
C	0.024907000	3.961054000	-1.124098000
H	-1.052829000	4.045987000	-0.955259000
H	0.435699000	4.977123000	-1.050426000
H	0.177139000	3.637274000	-2.160287000
C	2.886889000	2.699381000	-1.472433000
H	2.362276000	2.605242000	-2.431430000
H	3.309725000	3.712961000	-1.448469000
H	3.729644000	2.003721000	-1.477479000
C	3.718622000	1.308319000	1.278993000
H	4.165589000	0.783138000	0.429158000
H	4.416884000	2.102082000	1.577258000
H	3.673523000	0.597739000	2.111137000
C	1.379593000	1.907079000	3.376150000
H	2.094308000	1.129088000	3.662320000
H	1.713883000	2.832455000	3.864541000
H	0.409247000	1.652421000	3.816140000
C	1.992643000	2.486545000	-0.283909000

81

TS4-1, E(SCRF) = -1414.9623479 a.u., IF = *i*347.71 cm⁻¹

C	0.176163000	0.352220000	-2.136053000
C	1.030516000	-0.787635000	-2.109404000
C	-1.250580000	0.323679000	-2.081186000
C	-2.009743000	1.344391000	-1.539731000
C	2.115505000	-1.186940000	-0.425110000
Y	-0.274889000	-0.321914000	0.220155000
C	4.397616000	-0.840021000	-1.377859000
C	3.445821000	0.937842000	-0.016034000
C	4.625617000	1.688890000	-0.223207000
C	5.671186000	1.230884000	-1.007857000
C	5.527321000	-0.045122000	-1.569006000
H	4.709937000	2.667629000	0.245394000
H	6.342004000	-0.444059000	-2.170755000
C	2.486893000	1.617980000	0.834635000
H	2.917266000	2.521554000	1.276509000
C	0.587718000	2.321179000	2.078260000
C	0.641903000	3.757447000	1.538024000

H	0.053389000	4.417019000	2.184248000
H	1.659364000	4.159632000	1.511477000
H	0.226494000	3.814841000	0.525388000
C	-0.876778000	1.889511000	2.178631000
H	-0.970005000	0.863412000	2.562596000
H	-1.429982000	2.520431000	2.881266000
H	-1.403672000	1.983017000	1.215399000
C	1.239555000	2.229049000	3.463948000
H	1.196904000	1.205448000	3.851822000
H	2.289921000	2.537675000	3.436648000
H	0.720507000	2.884502000	4.171211000
N	1.252166000	1.353355000	1.135943000
H	0.655971000	1.332531000	-2.086391000
H	1.984029000	-0.692453000	-2.620021000
H	0.559854000	-1.757472000	-2.288230000
C	-0.274955000	-2.652266000	1.480000000
H	-1.758510000	-0.585951000	-2.409820000
H	-1.470873000	2.239110000	-1.210733000
C	-3.465438000	1.482922000	-1.577561000
C	-4.281582000	0.714044000	-2.428430000
C	-4.088272000	2.444041000	-0.759437000
C	-5.663841000	0.872945000	-2.426244000
H	-3.828559000	0.012879000	-3.124290000
C	-5.469939000	2.604506000	-0.760229000
H	-3.475975000	3.076613000	-0.118862000
C	-6.266080000	1.812621000	-1.588303000
H	-6.273185000	0.274552000	-3.098256000
H	-5.926397000	3.354695000	-0.120074000
H	-7.344657000	1.941111000	-1.596536000
C	3.317945000	-0.354685000	-0.597756000
C	-0.866457000	-2.924643000	0.204532000
H	1.825364000	-1.187559000	0.641933000
H	2.286867000	-2.231163000	-0.675917000
C	-2.302716000	-1.547497000	1.378864000
C	-1.171295000	-1.818763000	2.210808000
C	6.912685000	2.046694000	-1.242535000
H	7.810879000	1.499726000	-0.933249000
H	7.031369000	2.288260000	-2.305553000
H	6.885765000	2.988765000	-0.687276000
C	4.384645000	-2.226115000	-1.976243000
H	4.342496000	-2.999070000	-1.197859000
H	3.535526000	-2.395292000	-2.648372000
H	5.293932000	-2.401798000	-2.557103000
C	0.936492000	-3.330073000	2.055916000

H	1.481862000	-2.691667000	2.760730000
H	0.641319000	-4.232025000	2.609128000
H	1.642454000	-3.650185000	1.283445000
C	-0.364957000	-3.931862000	-0.790969000
H	0.728707000	-3.965883000	-0.842801000
H	-0.697444000	-4.941494000	-0.514720000
H	-0.742364000	-3.743206000	-1.801736000
C	-3.171567000	-2.430014000	-0.907023000
H	-2.746648000	-2.700252000	-1.879929000
H	-3.854509000	-3.243542000	-0.626150000
H	-3.782329000	-1.532623000	-1.042808000
C	-3.561089000	-0.831607000	1.785420000
H	-4.003539000	-0.265854000	0.958892000
H	-4.319105000	-1.548557000	2.128723000
H	-3.392033000	-0.131607000	2.610410000
C	-1.032636000	-1.492420000	3.672711000
H	-1.710778000	-0.694057000	3.989804000
H	-1.282279000	-2.373364000	4.279359000
H	-0.013055000	-1.200241000	3.951557000
C	-2.119789000	-2.253327000	0.149069000

81

TS4-2, E(SCRF) = -1414.945573 a.u., IF = *i*324.86 cm⁻¹

C	0.878272000	0.001852000	-1.183145000
C	0.062136000	-1.052790000	-1.775961000
C	2.321304000	-0.179230000	-0.910403000
C	3.025595000	-1.308457000	-1.114877000
C	0.396679000	0.635600000	0.706461000
Y	-1.631110000	-0.600526000	-0.222352000
C	1.947948000	2.489825000	1.411764000
C	-0.012200000	3.047973000	0.078113000
C	0.398866000	4.398956000	0.080650000
C	1.560837000	4.817074000	0.710601000
C	2.307848000	3.838673000	1.379166000
H	-0.220993000	5.136105000	-0.426256000
H	3.205575000	4.144804000	1.913273000
C	-1.272887000	2.828961000	-0.608745000
H	-1.671576000	3.758002000	-1.028030000
C	-3.247794000	1.907808000	-1.567376000
C	-2.987274000	2.524531000	-2.948762000
H	-3.912429000	2.530514000	-3.534473000
H	-2.641848000	3.560703000	-2.883008000
H	-2.236603000	1.948981000	-3.502191000
C	-3.813086000	0.494603000	-1.767708000
H	-4.066489000	0.003929000	-0.811313000

H	-4.755167000	0.522221000	-2.323519000
H	-3.140602000	-0.139214000	-2.372063000
C	-4.254561000	2.743141000	-0.766285000
H	-4.436928000	2.302084000	0.220259000
H	-3.896894000	3.767203000	-0.617704000
H	-5.210339000	2.800418000	-1.297811000
N	-1.973133000	1.751390000	-0.785437000
H	0.680719000	0.989265000	-1.605644000
H	-0.348580000	-0.770440000	-2.753361000
H	0.487050000	-2.054829000	-1.790664000
C	-2.165383000	-1.767529000	2.048864000
H	2.833616000	0.713529000	-0.558330000
H	2.501636000	-2.185676000	-1.491890000
C	4.458843000	-1.509149000	-0.894938000
C	5.347137000	-0.468852000	-0.566891000
C	4.978287000	-2.808605000	-1.021181000
C	6.696792000	-0.725953000	-0.360675000
H	4.986334000	0.553506000	-0.492082000
C	6.329451000	-3.067397000	-0.811128000
H	4.309159000	-3.624785000	-1.286242000
C	7.193774000	-2.026223000	-0.478043000
H	7.369153000	0.091574000	-0.114408000
H	6.707889000	-4.080879000	-0.911916000
H	8.250265000	-2.222579000	-0.317805000
C	0.783644000	2.064190000	0.729479000
C	-1.113457000	-2.545786000	1.470150000
H	-0.578110000	0.595246000	1.259880000
H	1.070129000	0.006539000	1.286496000
C	-2.995552000	-2.809832000	0.160802000
C	-3.331099000	-1.934752000	1.241998000
C	2.001951000	6.254954000	0.698446000
H	2.144618000	6.634370000	1.716783000
H	2.958135000	6.369182000	0.173907000
H	1.269445000	6.896567000	0.200280000
C	2.783685000	1.541826000	2.237610000
H	2.197754000	1.109283000	3.058330000
H	3.190489000	0.707423000	1.656323000
H	3.629482000	2.069325000	2.686793000
C	-2.117640000	-1.036953000	3.362895000
H	-2.766184000	-0.153105000	3.373770000
H	-2.457198000	-1.687859000	4.179835000
H	-1.105851000	-0.706851000	3.620304000
C	0.250572000	-2.772213000	2.059055000
H	0.510543000	-2.006404000	2.796758000

H	0.292673000	-3.738753000	2.578358000
H	1.040970000	-2.782531000	1.299586000
C	-0.916999000	-4.234834000	-0.504713000
H	0.170076000	-4.116958000	-0.456149000
H	-1.146788000	-5.241651000	-0.130350000
H	-1.206236000	-4.211267000	-1.560909000
C	-3.948024000	-3.364354000	-0.862632000
H	-3.455170000	-3.569072000	-1.819752000
H	-4.376355000	-4.315222000	-0.518309000
H	-4.791363000	-2.692992000	-1.058957000
C	-4.704891000	-1.424984000	1.583808000
H	-5.370601000	-1.403848000	0.714120000
H	-5.183328000	-2.076596000	2.327366000
H	-4.687764000	-0.417504000	2.016980000
C	-1.628960000	-3.193902000	0.309187000

81

TS4-3, E(SCRF) = -1414.247380 a.u., IF = $i326.11 \text{ cm}^{-1}$

C	0.767420000	-0.422672000	-1.125257000
C	-0.305525000	-1.111616000	-1.843588000
C	1.989344000	-1.194083000	-0.843662000
C	3.227283000	-0.706662000	-1.055158000
C	0.394863000	0.222661000	0.784017000
Y	-1.846600000	-0.334259000	-0.261890000
C	2.399944000	1.503771000	1.607700000
C	0.718773000	2.679560000	0.295963000
C	1.499439000	3.852672000	0.384744000
C	2.715479000	3.881098000	1.050238000
C	3.132655000	2.692024000	1.661335000
H	1.130671000	4.764553000	-0.081230000
H	4.067885000	2.693931000	2.218247000
C	-0.530043000	2.869444000	-0.419515000
H	-0.637316000	3.896396000	-0.782776000
C	-2.654374000	2.604753000	-1.460182000
C	-2.189634000	3.180829000	-2.804885000
H	-3.056642000	3.487595000	-3.399254000
H	-1.555398000	4.063853000	-2.680473000
H	-1.628019000	2.435685000	-3.379699000
C	-3.600935000	1.428711000	-1.736614000
H	-4.001187000	0.986439000	-0.807330000
H	-4.484295000	1.754917000	-2.293780000
H	-3.130238000	0.656735000	-2.370551000
C	-3.395381000	3.660084000	-0.629220000
H	-3.723844000	3.247053000	0.331254000
H	-2.760785000	4.528388000	-0.424472000

H	-4.279073000	4.016947000	-1.168702000
N	-1.499707000	2.046813000	-0.675601000
H	0.976476000	0.586553000	-1.481441000
H	-0.577476000	-0.615881000	-2.783440000
H	-0.167565000	-2.184869000	-1.975009000
C	-2.666131000	-1.551440000	1.899387000
H	1.841071000	-2.227339000	-0.532118000
H	3.311256000	0.328366000	-1.389665000
C	4.503735000	-1.408061000	-0.909355000
C	4.609094000	-2.741904000	-0.475467000
C	5.687264000	-0.714328000	-1.212691000
C	5.850987000	-3.351864000	-0.349653000
H	3.714650000	-3.312005000	-0.238377000
C	6.931511000	-1.325182000	-1.088052000
H	5.625242000	0.316920000	-1.554345000
C	7.017779000	-2.646964000	-0.654935000
H	5.912120000	-4.383889000	-0.014807000
H	7.833340000	-0.769962000	-1.331196000
H	7.986805000	-3.128512000	-0.557473000
C	1.179494000	1.473588000	0.894360000
C	-1.957073000	-2.552462000	1.163887000
H	-0.566831000	0.439141000	1.322719000
H	0.843794000	-0.597480000	1.342887000
C	-3.854346000	-2.004437000	-0.029328000
C	-3.843391000	-1.216278000	1.164341000
C	3.549157000	5.130256000	1.135377000
H	3.057999000	5.976341000	0.646101000
H	3.738973000	5.408922000	2.178389000
H	4.525240000	4.986962000	0.656853000
C	2.909754000	0.308880000	2.374870000
H	2.198662000	0.002567000	3.152593000
H	3.091445000	-0.553915000	1.727417000
H	3.852746000	0.547926000	2.873700000
C	-2.335929000	-1.065656000	3.283974000
H	-2.654991000	-0.030428000	3.451871000
H	-2.843651000	-1.679565000	4.040107000
H	-1.263685000	-1.120391000	3.499345000
C	-0.742945000	-3.298597000	1.639170000
H	-0.125925000	-2.700791000	2.318476000
H	-1.035224000	-4.201988000	2.191147000
H	-0.107014000	-3.625433000	0.809512000
C	-2.398238000	-3.930247000	-1.007896000
H	-1.332363000	-4.175874000	-1.044042000
H	-2.930552000	-4.850631000	-0.732101000

H	-2.710312000	-3.672125000	-2.025566000
C	-4.970671000	-2.082608000	-1.034500000
H	-4.605739000	-2.283495000	-2.048286000
H	-5.661488000	-2.898048000	-0.781663000
H	-5.568007000	-1.165096000	-1.070634000
C	-4.949973000	-0.322781000	1.655264000
H	-5.584178000	0.043706000	0.840619000
H	-5.609918000	-0.868409000	2.343135000
H	-4.576683000	0.549025000	2.205940000
C	-2.691823000	-2.834550000	-0.024495000

81

H, E(SCRF) = 1415.011535 a.u.

C	-0.609972000	-1.133924000	-1.658689000
C	-0.992897000	0.263617000	-2.093788000
C	0.681205000	-1.637135000	-1.662763000
C	1.882911000	-0.883455000	-1.748493000
C	-1.998504000	0.978617000	-1.150874000
Y	0.587506000	0.262239000	0.128649000
C	-4.358656000	0.467131000	-1.826012000
C	-3.507977000	-0.602177000	0.185714000
C	-4.772124000	-1.205245000	0.358275000
C	-5.822145000	-1.014408000	-0.531290000
C	-5.585370000	-0.171412000	-1.619007000
H	-4.930815000	-1.852970000	1.218087000
H	-6.389494000	0.008774000	-2.329869000
C	-2.558231000	-1.009699000	1.226981000
H	-3.065322000	-1.618534000	1.980302000
C	-0.686074000	-1.603089000	2.540112000
C	-1.079835000	-3.088756000	2.519481000
H	-0.508662000	-3.628595000	3.281928000
H	-2.138108000	-3.252103000	2.742861000
H	-0.860579000	-3.540131000	1.545388000
C	0.835507000	-1.526919000	2.371689000
H	1.211774000	-0.491869000	2.437157000
H	1.351581000	-2.054325000	3.179591000
H	1.167258000	-2.019707000	1.443087000
C	-1.102537000	-0.945791000	3.860322000
H	-0.834064000	0.115117000	3.875733000
H	-2.183863000	-1.022586000	4.015850000
H	-0.608649000	-1.437622000	4.705170000
N	-1.285898000	-0.846659000	1.379410000
H	-1.435960000	-1.823923000	-1.515307000
H	-1.410431000	0.250308000	-3.110648000
H	-0.104661000	0.918110000	-2.215295000

C	0.534813000	2.638539000	1.300550000
H	0.773253000	-2.686854000	-1.375767000
H	1.884193000	-0.025290000	-2.425377000
C	3.211602000	-1.499133000	-1.564215000
C	3.434381000	-2.583227000	-0.694425000
C	4.322792000	-1.000563000	-2.268769000
C	4.701121000	-3.140550000	-0.539050000
H	2.604461000	-3.012491000	-0.134848000
C	5.592090000	-1.549406000	-2.105662000
H	4.179667000	-0.187998000	-2.977897000
C	5.791187000	-2.622814000	-1.237865000
H	4.837082000	-3.983610000	0.133896000
H	6.426997000	-1.145140000	-2.672291000
H	6.779767000	-3.055249000	-1.113884000
C	-3.297854000	0.250278000	-0.925468000
C	0.869804000	2.854771000	-0.075254000
H	-1.575945000	1.211106000	-0.155158000
H	-2.200383000	1.966909000	-1.574394000
C	2.636744000	1.746105000	0.915168000
C	1.630693000	1.966487000	1.913610000
C	-7.157970000	-1.678278000	-0.337134000
H	-7.966386000	-0.938907000	-0.307590000
H	-7.378865000	-2.366584000	-1.161506000
H	-7.191924000	-2.250660000	0.594301000
C	-4.226525000	1.402824000	-3.003011000
H	-4.085210000	2.442680000	-2.680621000
H	-3.385039000	1.146198000	-3.655817000
H	-5.130145000	1.378080000	-3.617593000
C	-0.662443000	3.201963000	2.013975000
H	-0.949362000	2.600176000	2.882481000
H	-0.453580000	4.215818000	2.381511000
H	-1.540653000	3.277141000	1.363289000
C	0.124844000	3.747112000	-1.030227000
H	-0.933869000	3.841753000	-0.770259000
H	0.546959000	4.760738000	-1.005329000
H	0.188822000	3.408373000	-2.070801000
C	2.988058000	2.507672000	-1.550501000
H	2.376259000	2.495484000	-2.459908000
H	3.496734000	3.481203000	-1.525952000
H	3.760959000	1.741642000	-1.653577000
C	4.007177000	1.178599000	1.158069000
H	4.399649000	0.654879000	0.281133000
H	4.717491000	1.978073000	1.408989000
H	4.019420000	0.470545000	1.993764000

C	1. 826276000	1. 784989000	3. 393504000
H	2. 491672000	0. 949098000	3. 634897000
H	2. 289811000	2. 684856000	3. 819718000
H	0. 884555000	1. 632689000	3. 930276000
C	2. 174935000	2. 318057000	-0. 303771000

81

TS5, E(SCRF) = -1414.260611 a.u., IF = $i222.14 \text{ cm}^{-1}$

C	0. 667663000	-1. 471913000	1. 195329000
C	0. 910644000	-0. 286267000	2. 135634000
C	-0. 687374000	-1. 982642000	1. 023067000
C	-1. 868880000	-1. 420298000	1. 438220000
C	2. 007756000	0. 680232000	1. 631322000
Y	-0. 408919000	0. 430523000	-0. 159470000
N	1. 257136000	-0. 321580000	-1. 488898000
C	1. 734589000	-1. 221529000	-0. 573041000
C	4. 146560000	-1. 718967000	-0. 353423000
C	5. 422582000	-1. 532972000	0. 180403000
C	5. 574442000	-0. 585594000	1. 197391000
H	4. 000444000	-2. 454857000	-1. 142158000
H	6. 561009000	-0. 432766000	1. 630517000
C	3. 059807000	-0. 964063000	0. 095183000
H	1. 646693000	-2. 275397000	-0. 850849000
C	0. 689008000	-0. 834217000	-2. 776119000
C	1. 228902000	-2. 205219000	-3. 203465000
H	0. 904184000	-2. 414536000	-4. 228309000
H	2. 323884000	-2. 215081000	-3. 193183000
H	0. 865099000	-3. 031122000	-2. 581019000
C	-0. 849368000	-0. 925682000	-2. 689345000
H	-1. 319864000	0. 057477000	-2. 503132000
H	-1. 294808000	-1. 259095000	-3. 633600000
H	-1. 173718000	-1. 653691000	-1. 928031000
C	1. 087669000	0. 197781000	-3. 837056000
H	0. 767026000	1. 200697000	-3. 541220000
H	2. 176254000	0. 217358000	-3. 946252000
H	0. 641406000	-0. 038914000	-4. 810002000
C	4. 504253000	0. 164639000	1. 689435000
H	1. 377930000	-2. 275777000	1. 370870000
H	1. 181448000	-0. 656575000	3. 132047000
H	-0. 008749000	0. 300874000	2. 339142000
C	-0. 442051000	3. 014008000	-0. 678395000
H	-0. 750661000	-2. 896513000	0. 429597000
H	-1. 843026000	-0. 625720000	2. 187183000
C	-3. 213780000	-1. 932476000	1. 145761000
C	-3. 490384000	-2. 797056000	0. 071478000

C	-4.275897000	-1.563697000	1.990334000
C	-4.777068000	-3.278721000	-0.141923000
H	-2.696700000	-3.098299000	-0.608141000
C	-5.563752000	-2.046276000	1.776229000
H	-4.081194000	-0.913958000	2.840802000
C	-5.819880000	-2.904679000	0.707925000
H	-4.969245000	-3.947361000	-0.976558000
H	-6.366374000	-1.756357000	2.448530000
H	-6.824268000	-3.281379000	0.537513000
C	3.228934000	-0.034987000	1.129198000
C	-0.744247000	2.873014000	0.717837000
H	1.628214000	1.334130000	0.812395000
H	2.242911000	1.390806000	2.426825000
C	-2.511950000	1.996789000	-0.481270000
C	-1.538909000	2.488589000	-1.415843000
C	6.604191000	-2.311304000	-0.333090000
H	7.195725000	-1.707764000	-1.033312000
H	7.272332000	-2.608313000	0.482126000
H	6.291543000	-3.216677000	-0.862479000
C	4.741314000	1.153692000	2.803918000
H	4.478369000	2.177223000	2.508613000
H	4.160983000	0.911705000	3.703394000
H	5.795348000	1.162351000	3.094299000
C	0.739346000	3.749115000	-1.245599000
H	0.976411000	3.425659000	-2.263075000
H	0.539674000	4.828472000	-1.284308000
H	1.644701000	3.612451000	-0.644448000
C	0.016399000	3.513348000	1.846471000
H	1.072166000	3.664470000	1.602362000
H	-0.402971000	4.504002000	2.067381000
H	-0.035043000	2.936123000	2.776808000
C	-2.807593000	2.105202000	2.108108000
H	-2.170402000	1.860290000	2.966548000
H	-3.320596000	3.043355000	2.359960000
H	-3.579124000	1.334218000	2.025513000
C	-3.881128000	1.484979000	-0.833990000
H	-4.265176000	0.775128000	-0.094548000
H	-4.599208000	2.314074000	-0.892404000
H	-3.897419000	0.984217000	-1.808011000
C	-1.771613000	2.664320000	-2.890338000
H	-2.389151000	1.870275000	-3.323448000
H	-2.304905000	3.607678000	-3.069317000
H	-0.840389000	2.713628000	-3.461228000
C	-2.030665000	2.265212000	0.832689000

TS5', E(SCRIF) = -1414.947499 a.u., IF = *i*218.48 cm⁻¹

Y	-1.171848000	-0.147404000	0.135237000
N	0.506103000	0.712303000	1.276790000
C	1.289823000	1.030992000	0.201316000
C	0.287476000	0.905246000	-1.734125000
C	1.913349000	-1.705344000	-1.270318000
C	2.213473000	0.122958000	-3.084810000
C	2.024878000	-1.340026000	-2.775674000
C	1.455414000	1.119615000	-2.604159000
C	3.656680000	1.071785000	0.661921000
C	4.942555000	0.564887000	0.828983000
C	5.188325000	-0.732805000	0.375044000
H	3.445178000	2.077631000	1.019952000
H	6.181835000	-1.159212000	0.500149000
C	2.626284000	0.323237000	0.071326000
H	1.418186000	2.099265000	0.010019000
C	0.008452000	1.735258000	2.247333000
C	0.558815000	3.147157000	2.040454000
H	0.185168000	3.798254000	2.838000000
H	1.652044000	3.161106000	2.092858000
H	0.244919000	3.586358000	1.087613000
C	-1.531658000	1.794664000	2.174223000
H	-1.995822000	0.805836000	2.351695000
H	-1.950876000	2.429552000	2.962207000
H	-1.890730000	2.230976000	1.224332000
C	0.425311000	1.227730000	3.635705000
H	0.025909000	0.225268000	3.818703000
H	1.516003000	1.168897000	3.698705000
H	0.064067000	1.897001000	4.425706000
C	4.205436000	-1.493347000	-0.256164000
H	3.042996000	0.383806000	-3.737567000
H	2.874430000	-1.891326000	-3.191552000
H	1.139535000	-1.733005000	-3.301496000
C	-1.445721000	-2.662093000	0.747593000
H	1.692468000	2.147607000	-2.872538000
H	-0.140110000	-0.081948000	-2.020691000
C	-0.793682000	1.918844000	-1.720004000
C	-0.551331000	3.290892000	-1.501684000
C	-2.146419000	1.511979000	-1.836155000
C	-1.601585000	4.195451000	-1.394913000
H	0.471989000	3.651208000	-1.438573000
C	-3.202811000	2.424724000	-1.700334000
H	-2.378487000	0.503327000	-2.192788000

C	-2.933104000	3.768582000	-1.470510000
H	-1.382718000	5.249852000	-1.248379000
H	-4.226952000	2.082730000	-1.821834000
H	-3.743781000	4.485375000	-1.382116000
C	2.908874000	-0.958496000	-0.426272000
C	-2.004939000	-2.540333000	-0.567587000
H	0.890726000	-1.525150000	-0.904309000
H	2.050848000	-2.786773000	-1.173353000
C	-3.366864000	-1.385196000	0.901146000
C	-2.289017000	-1.954584000	1.653138000
C	6.027816000	1.375697000	1.485593000
H	6.307821000	0.948556000	2.456539000
H	6.934771000	1.398577000	0.870768000
H	5.711954000	2.409514000	1.656366000
C	4.559820000	-2.877407000	-0.744545000
H	3.942137000	-3.650207000	-0.269403000
H	4.437305000	-2.984939000	-1.828992000
H	5.602854000	-3.110947000	-0.513906000
C	-0.284161000	-3.525871000	1.152753000
H	0.379379000	-3.030562000	1.870346000
H	-0.645061000	-4.447342000	1.628702000
H	0.321857000	-3.826152000	0.294085000
C	-1.551972000	-3.278169000	-1.797692000
H	-0.482166000	-3.506304000	-1.775712000
H	-2.080471000	-4.236719000	-1.885571000
H	-1.753394000	-2.721264000	-2.719841000
C	-4.197472000	-1.538521000	-1.564672000
H	-3.733491000	-1.510989000	-2.556990000
H	-4.931088000	-2.355651000	-1.586103000
H	-4.765252000	-0.611419000	-1.430888000
C	-4.565547000	-0.677138000	1.470098000
H	-4.962755000	0.086343000	0.791750000
H	-5.379882000	-1.389322000	1.658509000
H	-4.346307000	-0.189307000	2.425565000
C	-2.159603000	-1.981359000	3.150247000
H	-2.644049000	-1.125598000	3.632237000
H	-2.637759000	-2.883050000	3.556441000
H	-1.114008000	-2.001254000	3.474243000
C	-3.198536000	-1.763334000	-0.464697000

81

I, E(SCRF) = -1415.011129 a.u.

C	-1.057711000	-1.571857000	-1.114553000
C	-1.068241000	-0.319768000	-2.023895000
C	0.307578000	-2.094884000	-0.744825000

C	1.509009000	-1.791576000	-1.301105000
C	-2.212672000	0.682330000	-1.741784000
Y	0.879509000	0.415092000	0.366245000
N	-1.024844000	-0.418445000	1.007647000
C	-1.837519000	-1.336443000	0.201787000
C	-4.356831000	-1.566526000	0.415620000
C	-5.659795000	-1.226108000	0.050184000
C	-5.826468000	-0.230290000	-0.918540000
H	-4.198716000	-2.351722000	1.153758000
H	-6.835455000	0.050523000	-1.215655000
C	-3.255031000	-0.926530000	-0.156137000
H	-1.893777000	-2.313421000	0.709146000
C	-1.358945000	-0.230463000	2.432447000
C	-1.633096000	-1.552171000	3.166830000
H	-1.725191000	-1.377871000	4.244667000
H	-2.568083000	-2.012544000	2.835302000
H	-0.819771000	-2.271692000	3.007593000
C	-0.108032000	0.407595000	3.065055000
H	0.133820000	1.388264000	2.612933000
H	-0.249735000	0.627666000	4.128049000
H	0.768386000	-0.266516000	3.018132000
C	-2.540673000	0.734416000	2.635390000
H	-2.336939000	1.698918000	2.155923000
H	-3.456320000	0.329478000	2.198342000
H	-2.721910000	0.910950000	3.702809000
C	-4.746288000	0.407880000	-1.532164000
H	-1.582697000	-2.377687000	-1.647675000
H	-1.106129000	-0.646557000	-3.069137000
H	-0.109688000	0.239424000	-1.977864000
C	1.344993000	2.632959000	-0.948321000
H	0.288651000	-2.830684000	0.060938000
H	1.539921000	-1.174208000	-2.202106000
C	2.810608000	-2.320766000	-0.853044000
C	3.017531000	-2.799951000	0.453708000
C	3.889471000	-2.344755000	-1.752378000
C	4.259573000	-3.295069000	0.841364000
H	2.199054000	-2.805401000	1.172670000
C	5.128482000	-2.848614000	-1.365587000
H	3.744535000	-1.991592000	-2.770809000
C	5.318573000	-3.322191000	-0.067156000
H	4.400374000	-3.665310000	1.853144000
H	5.945937000	-2.875382000	-2.080584000
H	6.285898000	-3.712738000	0.235216000
C	-3.441771000	0.044689000	-1.147769000

C	2.519187000	1.837848000	-1.165128000
H	-1.850459000	1.448125000	-1.039498000
H	-2.450614000	1.213489000	-2.667314000
C	2.432218000	2.386546000	1.076980000
C	1.292955000	2.977246000	0.435489000
C	-6.853120000	-1.910555000	0.662581000
H	-7.528072000	-1.186958000	1.134969000
H	-7.436542000	-2.445716000	-0.096363000
H	-6.553726000	-2.636164000	1.425064000
C	-5.001600000	1.459203000	-2.582968000
H	-4.568318000	2.429147000	-2.308463000
H	-4.578466000	1.178255000	-3.556071000
H	-6.074874000	1.610472000	-2.728449000
C	0.473222000	3.210933000	-2.028092000
H	-0.524206000	3.472905000	-1.662752000
H	0.922575000	4.133410000	-2.419960000
H	0.350231000	2.533179000	-2.879497000
C	3.058589000	1.427620000	-2.506141000
H	2.264455000	1.208749000	-3.229085000
H	3.663379000	2.235649000	-2.939349000
H	3.706110000	0.548034000	-2.436396000
C	4.531153000	1.049062000	0.297645000
H	4.688949000	0.185353000	-0.356173000
H	5.339865000	1.763122000	0.091011000
H	4.665900000	0.711100000	1.330561000
C	2.867104000	2.622565000	2.498287000
H	3.372350000	1.754030000	2.935980000
H	3.578405000	3.457622000	2.545602000
H	2.029612000	2.883449000	3.152822000
C	0.326743000	3.945917000	1.060486000
H	0.210343000	3.786522000	2.137486000
H	0.682215000	4.977003000	0.930617000
H	-0.669862000	3.892145000	0.609829000
C	3.192748000	1.697657000	0.082991000

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I', E(SCRF) = -1414.99028 a.u.

Y	-1.594620000	0.023095000	0.433143000
N	0.466381000	0.219907000	1.062546000
C	1.488841000	0.916454000	0.275826000
C	0.760958000	1.348727000	-1.039321000
C	2.037702000	-1.336635000	-1.746660000
C	2.224803000	0.939730000	-3.037082000
C	2.087107000	-0.563737000	-3.092686000
C	1.671959000	1.783765000	-2.159730000

C	3.911711000	0.750769000	0.827757000
C	5.187701000	0.190889000	0.812686000
C	5.385256000	-0.933959000	0.009936000
H	3.743624000	1.634882000	1.440809000
H	6.366692000	-1.404460000	-0.012564000
C	2.846649000	0.228211000	0.081107000
H	1.739262000	1.856994000	0.789692000
C	0.694294000	-0.057928000	2.495282000
C	1.259084000	1.147794000	3.262842000
H	1.247172000	0.951677000	4.341057000
H	2.295577000	1.351395000	2.985192000
H	0.664011000	2.050602000	3.075140000
C	-0.700254000	-0.355941000	3.083638000
H	-1.181426000	-1.229079000	2.605056000
H	-0.649091000	-0.625203000	4.143356000
H	-1.364756000	0.530784000	3.045965000
C	1.579067000	-1.294440000	2.727935000
H	1.159692000	-2.168177000	2.216172000
H	2.587541000	-1.131770000	2.341912000
H	1.656166000	-1.523308000	3.798183000
C	4.369237000	-1.458987000	-0.789544000
H	2.864871000	1.374803000	-3.803445000
H	2.940647000	-0.943956000	-3.665676000
H	1.202440000	-0.831921000	-3.691941000
C	-2.246134000	-2.399279000	-0.164720000
H	1.884007000	2.849154000	-2.233593000
H	0.239052000	0.450734000	-1.423179000
C	-0.324991000	2.375294000	-0.741537000
C	-0.094074000	3.524440000	0.032486000
C	-1.623794000	2.189055000	-1.259892000
C	-1.122841000	4.421505000	0.306269000
H	0.900913000	3.725281000	0.419009000
C	-2.664027000	3.091045000	-0.978985000
H	-1.796673000	1.394348000	-1.991929000
C	-2.416032000	4.202962000	-0.181275000
H	-0.915179000	5.305033000	0.903978000
H	-3.646278000	2.932745000	-1.414587000
H	-3.209986000	4.911605000	0.035351000
C	3.088140000	-0.865613000	-0.771794000
C	-2.546403000	-1.634041000	-1.336415000
H	1.047598000	-1.272322000	-1.285566000
H	2.178729000	-2.398012000	-1.978323000
C	-4.046676000	-1.019194000	0.309787000
C	-3.174888000	-2.014971000	0.853945000

C	6.314495000	0.772060000	1.624899000
H	6.729247000	0.031189000	2.318923000
H	7.137735000	1.104270000	0.981010000
H	5.984449000	1.633564000	2.213833000
C	4.676052000	-2.655912000	-1.657585000
H	4.052501000	-3.521213000	-1.398739000
H	4.518884000	-2.451375000	-2.723453000
H	5.719382000	-2.961347000	-1.538176000
C	-1.266463000	-3.537202000	-0.081207000
H	-0.871698000	-3.674201000	0.930588000
H	-1.750106000	-4.480587000	-0.368561000
H	-0.410474000	-3.396796000	-0.748084000
C	-1.942373000	-1.837327000	-2.698663000
H	-0.915124000	-2.210289000	-2.645010000
H	-2.521727000	-2.578520000	-3.265631000
H	-1.934626000	-0.920079000	-3.298541000
C	-4.441679000	0.012889000	-2.048349000
H	-3.806216000	0.439444000	-2.832566000
H	-5.179602000	-0.621130000	-2.557952000
H	-4.999935000	0.831051000	-1.582052000
C	-5.238985000	-0.425418000	1.007621000
H	-5.470851000	0.585188000	0.653324000
H	-6.135499000	-1.035196000	0.832732000
H	-5.102105000	-0.374037000	2.093500000
C	-3.363043000	-2.700025000	2.180185000
H	-3.672527000	-2.012411000	2.975411000
H	-4.147780000	-3.463804000	2.099779000
H	-2.456621000	-3.213510000	2.515868000
C	-3.669798000	-0.795329000	-1.044532000

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B', E(SCRF) = -963.1718463 a.u.

C	2.371844000	1.266199000	-2.191874000
H	1.309040000	1.004633000	-2.275129000
C	-1.026861000	0.123952000	-2.060251000
Y	-0.029970000	0.278541000	0.098120000
C	-3.608429000	-1.169026000	0.453301000
H	-5.596397000	-0.426889000	0.764377000
H	-5.414762000	1.269747000	-1.061776000
H	-3.342216000	1.440954000	-2.379258000
H	-3.707081000	-1.910103000	1.238861000
C	-2.290823000	-0.125190000	-1.349671000
H	-0.551063000	-0.754114000	-2.514066000
H	-1.121154000	0.909807000	-2.811479000
N	-1.261385000	-1.920145000	0.021234000

C	-1.054982000	-2.981767000	-0.991467000
H	-0.079281000	-3.453052000	-0.835588000
H	-1.839676000	-3.745046000	-0.903819000
H	-1.094394000	-2.564444000	-1.996883000
C	-1.315879000	-2.552790000	1.351618000
H	-2.118183000	-3.299239000	1.421920000
H	-0.371309000	-3.071724000	1.533397000
H	-1.471473000	-1.803235000	2.134829000
C	-0.594198000	1.534947000	2.336814000
C	0.674427000	2.058531000	1.963221000
C	-1.544167000	1.960138000	1.372713000
C	0.506542000	2.797065000	0.768567000
C	-0.861399000	2.731432000	0.394906000
C	-4.681457000	-0.333262000	0.187281000
C	3.110362000	0.379467000	-1.233247000
C	4.476546000	0.144958000	-1.398146000
C	5.158595000	-0.618993000	-0.461289000
C	4.458065000	-1.136190000	0.624959000
C	3.094414000	-0.886319000	0.733470000
N	2.429919000	-0.144649000	-0.186406000
H	6.222903000	-0.806724000	-0.570759000
H	4.991598000	0.571936000	-2.252788000
H	4.959307000	-1.731549000	1.381271000
C	2.292949000	-1.449489000	1.872134000
H	2.940891000	-1.811398000	2.674783000
H	1.631017000	-0.693137000	2.317557000
H	1.687968000	-2.303199000	1.542264000
C	-4.576878000	0.615550000	-0.837089000
C	-3.411920000	0.712103000	-1.575651000
H	2.437942000	2.313505000	-1.870696000
H	2.804243000	1.207472000	-3.194973000
C	-2.415832000	-1.071408000	-0.285315000
H	1.282655000	3.348668000	0.250096000
H	-1.317049000	3.222517000	-0.456659000
H	-2.607221000	1.747439000	1.383931000
H	-0.811990000	0.974445000	3.240494000
H	1.599267000	1.953752000	2.519733000

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TS1', E(SCRF) = -963.1305255 a.u., IF = *i*1337.44 cm⁻¹

C	1.482791000	0.551618000	-2.170642000
H	0.140340000	-0.072764000	-2.124658000
C	-1.082052000	-0.806679000	-2.114257000
Y	-0.086276000	0.550946000	-0.148746000
C	-2.929629000	-1.508907000	1.187668000

H	-5.002117000	-1.151631000	1.604350000
H	-5.466907000	-0.231167000	-0.669998000
H	-3.661138000	-0.118413000	-2.341287000
H	-2.741925000	-1.913760000	2.176328000
C	-2.136722000	-0.945290000	-1.070997000
H	-0.593652000	-1.751354000	-2.374327000
H	-1.511421000	-0.389839000	-3.029586000
N	-0.525952000	-1.815120000	0.589185000
C	-0.079729000	-3.091831000	-0.010060000
H	1.006138000	-3.176639000	0.088389000
H	-0.556228000	-3.937934000	0.502991000
H	-0.344999000	-3.139711000	-1.064460000
C	-0.238278000	-1.849738000	2.033167000
H	-0.740972000	-2.684464000	2.540514000
H	0.839202000	-1.976886000	2.166632000
H	-0.554414000	-0.918193000	2.518273000
C	-0.757520000	2.373060000	1.606977000
C	0.262901000	2.988937000	0.831833000
C	-1.891454000	2.190296000	0.773723000
C	-0.240427000	3.183999000	-0.476092000
C	-1.567356000	2.681715000	-0.517986000
C	-4.208284000	-1.079812000	0.866867000
C	2.515343000	-0.001669000	-1.269938000
C	3.621449000	-0.757068000	-1.680071000
C	4.542552000	-1.167025000	-0.726459000
C	4.353750000	-0.822732000	0.614223000
C	3.215819000	-0.110473000	0.980934000
N	2.300737000	0.249384000	0.053314000
H	5.420751000	-1.734270000	-1.023029000
H	3.763711000	-0.976329000	-2.733591000
H	5.082216000	-1.103461000	1.368266000
C	2.981782000	0.327497000	2.398127000
H	3.474498000	-0.337565000	3.112778000
H	3.389055000	1.335193000	2.550497000
H	1.915298000	0.374385000	2.640489000
C	-4.467340000	-0.566085000	-0.408334000
C	-3.450293000	-0.499144000	-1.345158000
H	1.493848000	1.648933000	-2.159657000
H	1.611267000	0.230454000	-3.207517000
C	-1.887165000	-1.439810000	0.245966000
H	0.282422000	3.668562000	-1.292797000
H	-2.236816000	2.717350000	-1.370103000
H	-2.844717000	1.769306000	1.072914000
H	-0.703810000	2.147380000	2.667437000

H 1. 240812000 3. 290923000 1. 187812000
50

C', E(SCRF) = -963.1648883 a.u.

C	1. 573267000	0. 585756000	-2. 099996000
H	-0. 750747000	-0. 629045000	-2. 268717000
C	-1. 841232000	-0. 808077000	-2. 250874000
Y	0. 011759000	0. 641082000	-0. 252282000
C	-2. 592385000	-1. 602371000	1. 456697000
H	-4. 466546000	-1. 320186000	2. 459717000
H	-5. 587133000	-0. 355829000	0. 446524000
H	-4. 320839000	-0. 132993000	-1. 659670000
H	-2. 130564000	-2. 028568000	2. 339733000
C	-2. 489502000	-0. 939850000	-0. 889350000
H	-1. 979345000	-1. 721649000	-2. 844039000
H	-2. 307153000	0. 005620000	-2. 814423000
N	-0. 448334000	-1. 816084000	0. 214481000
C	-0. 120629000	-2. 958044000	-0. 670218000
H	0. 964425000	-3. 010544000	-0. 791196000
H	-0. 483198000	-3. 896204000	-0. 229575000
H	-0. 574182000	-2. 837276000	-1. 651526000
C	0. 177880000	-2. 054589000	1. 526656000
H	-0. 198302000	-2. 967863000	2. 007607000
H	1. 254500000	-2. 164079000	1. 378201000
H	-0. 002059000	-1. 213977000	2. 207738000
C	-0. 489906000	2. 589235000	1. 432892000
C	0. 361762000	3. 163919000	0. 451852000
C	-1. 728625000	2. 282057000	0. 814335000
C	-0. 347452000	3. 210672000	-0. 771592000
C	-1. 636174000	2. 656942000	-0. 552084000
C	-3. 922221000	-1. 204387000	1. 527083000
C	2. 522501000	-0. 042133000	-1. 186032000
C	3. 502014000	-1. 001752000	-1. 511987000
C	4. 347872000	-1. 461315000	-0. 517963000
C	4. 217736000	-0. 982788000	0. 793976000
C	3. 195931000	-0. 091281000	1. 090656000
N	2. 342252000	0. 323712000	0. 123524000
H	5. 135627000	-2. 171149000	-0. 757321000
H	3. 617774000	-1. 317150000	-2. 544332000
H	4. 904593000	-1. 300209000	1. 571863000
C	3. 003058000	0. 473548000	2. 468727000
H	3. 602086000	-0. 063223000	3. 208688000
H	3. 304121000	1. 528049000	2. 490069000
H	1. 953691000	0. 434876000	2. 783076000
C	-4. 548555000	-0. 669486000	0. 403022000

C	-3.831828000	-0.542961000	-0.779335000
H	1.746650000	1.666653000	-2.169753000
H	1.546873000	0.151302000	-3.100586000
C	-1.860829000	-1.482119000	0.263132000
H	0.017012000	3.623023000	-1.705023000
H	-2.433554000	2.591117000	-1.284253000
H	-2.601519000	1.861391000	1.301333000
H	-0.254450000	2.461943000	2.484615000
H	1.370129000	3.524552000	0.616639000

48

J, E(SCRF) = -832.8411063 a.u.

N	1.998120000	-1.704911000	-0.222470000
C	0.987405000	0.293308000	-2.050866000
H	1.237207000	-0.566710000	-2.681788000
H	0.690802000	1.140547000	-2.668141000
C	1.952269000	0.641932000	-1.003386000
C	2.405784000	-0.314153000	-0.031978000
C	3.203710000	0.081599000	1.056873000
H	3.570389000	-0.657677000	1.761828000
C	3.549256000	1.412852000	1.233274000
H	4.170746000	1.703803000	2.074540000
C	3.101978000	2.369251000	0.313177000
H	3.376773000	3.412831000	0.438856000
C	2.321483000	1.991038000	-0.765566000
H	1.994597000	2.737609000	-1.484551000
C	2.059421000	-2.540007000	0.990525000
H	3.090031000	-2.740406000	1.312132000
H	1.585248000	-3.503779000	0.779459000
H	1.539299000	-2.058985000	1.829519000
C	2.733018000	-2.383035000	-1.315117000
H	2.760788000	-1.751102000	-2.202313000
H	2.236482000	-3.327103000	-1.559883000
H	3.765201000	-2.590750000	-1.004947000
C	-2.742627000	-0.655309000	0.277404000
C	-2.114989000	-0.051762000	1.410682000
C	-1.575913000	1.208129000	0.997850000
C	-1.887996000	1.388762000	-0.387636000
C	-2.599959000	0.236428000	-0.834102000
C	-2.119503000	-0.591933000	2.814716000
H	-1.244685000	-0.269981000	3.390900000
H	-2.157309000	-1.686886000	2.844567000
H	-3.002246000	-0.234097000	3.361004000
C	-0.950010000	2.238874000	1.896725000
H	-1.712561000	2.934078000	2.271909000

H	-0.195237000	2.838170000	1.377630000
H	-0.470816000	1.790561000	2.773502000
C	-1.650399000	2.639968000	-1.180340000
H	-1.590446000	2.440550000	-2.254129000
H	-0.728656000	3.149420000	-0.881868000
H	-2.474153000	3.349792000	-1.027281000
C	-3.197564000	0.046096000	-2.199991000
H	-4.200750000	0.489888000	-2.247014000
H	-3.309431000	-1.011360000	-2.463879000
H	-2.597766000	0.522366000	-2.982114000
C	-3.515212000	-1.946782000	0.278922000
H	-4.570822000	-1.764305000	0.519781000
H	-3.501074000	-2.445990000	-0.696727000
H	-3.144028000	-2.658546000	1.025393000
Y	-0.227316000	-0.607669000	-0.232207000

82

K, E(SCRF) = -1486.424037 a.u.

Y	-0.230067000	-0.230287000	0.079714000
C	-1.435899000	-0.396271000	-1.998557000
H	0.502171000	-1.644222000	-2.606623000
C	1.518573000	-1.830122000	-2.280252000
C	-5.414963000	1.041312000	-1.101150000
H	-6.102276000	-0.598337000	-2.320458000
H	-3.825350000	-1.385978000	-2.862657000
H	-4.444335000	2.564001000	0.046619000
H	-6.410642000	1.407905000	-0.868992000
C	-2.805637000	0.111528000	-1.709320000
H	-0.890424000	0.298061000	-2.666632000
H	-1.514891000	-1.344585000	-2.544785000
C	-5.239801000	-0.079134000	-1.910908000
C	-1.505795000	-2.419390000	0.845288000
C	-2.115884000	-1.375398000	1.601103000
C	-1.151003000	-0.883671000	2.532202000
C	-0.171450000	-2.590637000	1.325983000
C	0.047701000	-1.642862000	2.369599000
C	0.738514000	-3.723693000	0.945097000
H	0.471872000	-4.632299000	1.501873000
H	0.670989000	-3.972189000	-0.119365000
H	1.788572000	-3.509726000	1.166330000
C	1.196311000	-1.628567000	3.340428000
H	1.587406000	-0.623684000	3.546497000
H	0.878689000	-2.041756000	4.307474000
H	2.032741000	-2.241399000	2.995067000
C	-3.582141000	-1.053990000	1.602099000

H	-4.114661000	-1.756505000	2.258682000
H	-3.793968000	-0.048186000	1.976812000
H	-4.029159000	-1.132339000	0.607738000
C	-2.209297000	-3.317023000	-0.131470000
H	-2.995610000	-2.787245000	-0.677459000
H	-1.521389000	-3.743442000	-0.869400000
H	-2.684365000	-4.160451000	0.388746000
N	-1.818978000	1.881065000	-0.322761000
C	-1.331097000	2.873712000	-1.305855000
H	-2.085826000	3.657305000	-1.463349000
H	-0.412941000	3.341894000	-0.938412000
H	-1.138182000	2.391852000	-2.266193000
C	-2.063919000	2.587393000	0.945939000
H	-2.550265000	1.918309000	1.657534000
H	-1.107646000	2.921689000	1.359095000
H	-2.693241000	3.478797000	0.814520000
C	3.105111000	-1.540402000	-0.618909000
C	4.036102000	-2.258075000	-1.378508000
C	3.685190000	-2.768570000	-2.620451000
C	2.391434000	-2.546638000	-3.085019000
C	-3.955984000	-0.525429000	-2.210132000
N	1.846728000	-1.328652000	-1.069477000
H	4.403066000	-3.331351000	-3.210584000
H	5.032755000	-2.420158000	-0.979266000
H	2.056428000	-2.921762000	-4.046569000
C	-3.012285000	1.226403000	-0.867252000
C	3.508657000	-1.011523000	0.732981000
H	3.771629000	-1.865024000	1.371598000
H	2.647074000	-0.530891000	1.203482000
C	4.694963000	-0.041278000	0.701121000
H	4.937759000	0.289032000	1.716182000
H	5.592839000	-0.510265000	0.286005000
H	4.474112000	0.846590000	0.100227000
C	2.098376000	2.468587000	-0.332044000
C	2.828679000	3.583220000	0.091055000
C	2.847382000	3.937641000	1.436040000
C	2.131045000	3.165118000	2.346086000
C	1.421788000	2.077714000	1.855588000
N	1.390210000	1.729500000	0.555299000
H	3.414247000	4.803279000	1.767251000
H	3.380687000	4.170551000	-0.634092000
H	2.114043000	3.396735000	3.406009000
H	0.843425000	1.451412000	2.530906000
C	2.095254000	2.019110000	-1.773986000

H	1. 127124000	1. 552530000	-1. 992269000
H	2. 834937000	1. 213388000	-1. 877935000
C	2. 380276000	3. 100691000	-2. 815186000
H	2. 261056000	2. 685582000	-3. 820516000
H	1. 694229000	3. 949285000	-2. 719504000
H	3. 404798000	3. 480439000	-2. 746070000
C	-1. 435090000	0. 019275000	3. 700955000
H	-2. 250004000	0. 722751000	3. 505759000
H	-1. 738110000	-0. 575037000	4. 574410000
H	-0. 560513000	0. 601368000	4. 015926000
C	-4. 297105000	1. 694615000	-0. 586543000

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K', E(SCRF) = -1159.642595 a.u.

N	1. 026918000	-2. 270847000	0. 497044000
C	1. 155459000	-0. 838714000	-2. 046437000
H	0. 547127000	-1. 723298000	-2. 272674000
H	1. 382646000	-0. 305956000	-2. 971112000
C	2. 355493000	-1. 093246000	-1. 234490000
C	2. 311124000	-1. 733470000	0. 044855000
C	3. 468369000	-1. 851343000	0. 833507000
H	3. 428514000	-2. 365848000	1. 787923000
C	4. 679962000	-1. 332995000	0. 403184000
H	5. 565639000	-1. 438981000	1. 022214000
C	4. 748484000	-0. 690803000	-0. 838568000
H	5. 695230000	-0. 293731000	-1. 194726000
C	3. 615609000	-0. 574031000	-1. 624802000
H	3. 682379000	-0. 092830000	-2. 596981000
C	0. 933227000	-2. 478424000	1. 951812000
H	1. 576666000	-3. 297298000	2. 301276000
H	-0. 098015000	-2. 740615000	2. 205349000
H	1. 217162000	-1. 569664000	2. 495266000
C	0. 667631000	-3. 530520000	-0. 190145000
H	0. 792110000	-3. 422970000	-1. 267488000
H	-0. 375433000	-3. 782115000	0. 026485000
H	1. 313915000	-4. 349707000	0. 153229000
C	-0. 921467000	2. 330465000	0. 660058000
C	0. 145970000	2. 052052000	1. 571485000
C	1. 373101000	2. 107811000	0. 842914000
C	1. 062941000	2. 416989000	-0. 520333000
C	-0. 351657000	2. 551500000	-0. 628760000
C	0. 015978000	1. 895732000	3. 062616000
H	0. 819687000	1. 285845000	3. 490652000
H	-0. 937245000	1. 442124000	3. 358117000
H	0. 065826000	2. 872693000	3. 561801000

C	2.756816000	2.027837000	1.425758000
H	3.149127000	3.034532000	1.623667000
H	3.464569000	1.531304000	0.754078000
H	2.774048000	1.488464000	2.378610000
C	2.062173000	2.739252000	-1.592814000
H	1.681582000	2.511245000	-2.593523000
H	2.998099000	2.188933000	-1.458919000
H	2.309612000	3.809406000	-1.576504000
C	-1.101783000	2.990522000	-1.853691000
H	-1.163793000	4.086289000	-1.899442000
H	-2.130775000	2.614618000	-1.865634000
H	-0.612638000	2.662023000	-2.777224000
C	-2.361355000	2.563367000	1.022672000
H	-2.566168000	3.639250000	1.103514000
H	-3.055778000	2.164448000	0.274451000
H	-2.621791000	2.122474000	1.990429000
C	-3.197933000	-0.958986000	0.141066000
C	-4.477112000	-1.207512000	-0.355680000
C	-4.719300000	-1.112225000	-1.723605000
C	-3.672453000	-0.770027000	-2.574789000
C	-2.425516000	-0.533711000	-2.013187000
N	-2.185890000	-0.619000000	-0.690421000
H	-5.713379000	-1.304173000	-2.117444000
H	-5.278890000	-1.472515000	0.324177000
H	-3.812374000	-0.684697000	-3.647204000
H	-1.576178000	-0.264252000	-2.636887000
C	-2.848503000	-1.082514000	1.605084000
H	-2.279936000	-2.015175000	1.737931000
H	-2.163276000	-0.259390000	1.859932000
C	-4.019075000	-1.072751000	2.585668000
H	-4.664895000	-1.947323000	2.457309000
H	-3.645713000	-1.096039000	3.613812000
H	-4.630683000	-0.171771000	2.471083000
Y	0.139455000	0.012515000	-0.063645000

82

TS6, E(SCRF) = -1486.379445 a.u., IF = *i*1315.52 cm⁻¹

Y	-0.192395000	-0.205940000	0.088777000
C	-1.462716000	-0.284811000	-2.247311000
H	-0.440369000	-1.146498000	-1.745396000
C	0.811989000	-1.819743000	-1.496720000
C	-5.353006000	1.109028000	-0.976557000
H	-6.120120000	-0.535222000	-2.141495000
H	-3.885482000	-1.304427000	-2.853547000
H	-4.308159000	2.634951000	0.098517000

H	-6.330311000	1.474338000	-0.674980000
C	-2.795361000	0.195167000	-1.770049000
H	-0.883978000	0.519012000	-2.727942000
H	-1.626437000	-1.023049000	-3.043034000
C	-5.233666000	-0.011359000	-1.794692000
C	-1.632663000	-2.195461000	1.092313000
C	-2.055526000	-1.048379000	1.825919000
C	-0.959799000	-0.610740000	2.632601000
C	-0.284940000	-2.483397000	1.461688000
C	0.138196000	-1.496062000	2.398113000
C	0.475529000	-3.725506000	1.102272000
H	0.330503000	-4.494516000	1.873198000
H	0.139959000	-4.152753000	0.153255000
H	1.553222000	-3.549877000	1.023025000
C	1.431833000	-1.526954000	3.162441000
H	1.784534000	-0.529463000	3.447446000
H	1.320492000	-2.101324000	4.092447000
H	2.231509000	-2.003748000	2.587599000
C	-3.480780000	-0.597108000	1.961940000
H	-4.010284000	-1.254256000	2.666454000
H	-3.565227000	0.418926000	2.360013000
H	-4.027849000	-0.629193000	1.015869000
C	-2.516311000	-3.057656000	0.236788000
H	-3.292081000	-2.473328000	-0.267711000
H	-1.948521000	-3.591803000	-0.532441000
H	-3.025364000	-3.817167000	0.846109000
N	-1.716689000	1.964229000	-0.443942000
C	-1.269018000	2.951493000	-1.452531000
H	-2.016280000	3.750280000	-1.561262000
H	-0.322596000	3.398644000	-1.133879000
H	-1.137979000	2.479173000	-2.427241000
C	-1.889509000	2.689111000	0.826400000
H	-2.345614000	2.035299000	1.570732000
H	-0.908651000	3.016329000	1.181792000
H	-2.515269000	3.585964000	0.714995000
C	3.049929000	-1.743995000	-0.763045000
C	3.384641000	-2.761012000	-1.660990000
C	2.406516000	-3.304817000	-2.491138000
C	1.098079000	-2.830926000	-2.412571000
C	-3.972078000	-0.448616000	-2.187797000
N	1.778129000	-1.296267000	-0.715926000
H	2.666988000	-4.097587000	-3.188233000
H	4.405091000	-3.130201000	-1.700312000
H	0.317005000	-3.240014000	-3.047912000

C	-2.937040000	1.306180000	-0.909933000
C	4.062577000	-1.139353000	0.176519000
H	4.376806000	-1.909736000	0.894595000
H	3.563601000	-0.358034000	0.758463000
C	5.307749000	-0.572577000	-0.514709000
H	5.991652000	-0.148878000	0.227708000
H	5.857264000	-1.344176000	-1.063488000
H	5.048306000	0.219559000	-1.225626000
C	2.240326000	2.323027000	-0.371565000
C	3.139132000	3.326945000	-0.000934000
C	3.250966000	3.708453000	1.331979000
C	2.451280000	3.077367000	2.279960000
C	1.573838000	2.095583000	1.840583000
N	1.457619000	1.717168000	0.553933000
H	3.949884000	4.487572000	1.623255000
H	3.748830000	3.808025000	-0.757361000
H	2.496227000	3.337979000	3.332327000
H	0.924241000	1.586801000	2.545958000
C	2.125113000	1.850830000	-1.801471000
H	1.086509000	1.549302000	-1.985629000
H	2.716136000	0.931593000	-1.904540000
C	2.550198000	2.849838000	-2.876882000
H	2.337095000	2.438439000	-3.868190000
H	2.014472000	3.801009000	-2.785243000
H	3.624252000	3.059303000	-2.842794000
C	-1.058178000	0.371764000	3.768810000
H	-1.521949000	1.326268000	3.494606000
H	-1.669007000	-0.049573000	4.578545000
H	-0.078793000	0.589975000	4.207888000
C	-4.203016000	1.765658000	-0.542314000

65

TS6', E(SCRF) = -1159.592335 a.u., IF = *i*1347.87 cm⁻¹

N	0.790515000	-2.304049000	0.562821000
C	1.067820000	-1.090183000	-2.097263000
H	0.682154000	-2.040585000	-2.485139000
H	1.380235000	-0.490732000	-2.957820000
C	2.225946000	-1.289053000	-1.169441000
C	2.110423000	-1.893495000	0.118608000
C	3.241171000	-2.043962000	0.938827000
H	3.149648000	-2.528145000	1.905507000
C	4.487090000	-1.598710000	0.521613000
H	5.351869000	-1.734684000	1.164176000
C	4.619471000	-0.986951000	-0.727922000
H	5.591889000	-0.641475000	-1.067238000

C	3.509639000	-0.835335000	-1.544757000
H	3.622506000	-0.379983000	-2.525014000
C	0.630534000	-2.422656000	2.020502000
H	1.163459000	-3.289094000	2.435939000
H	-0.433232000	-2.546072000	2.243833000
H	1.001639000	-1.524487000	2.529664000
C	0.294043000	-3.537371000	-0.080553000
H	0.432995000	-3.490460000	-1.159378000
H	-0.772558000	-3.650003000	0.132688000
H	0.834852000	-4.413572000	0.302236000
C	-0.754700000	2.433536000	0.675944000
C	0.276105000	2.103860000	1.610257000
C	1.519647000	2.077310000	0.906519000
C	1.253438000	2.384883000	-0.465056000
C	-0.150209000	2.608766000	-0.603729000
C	0.096035000	1.945156000	3.095696000
H	0.886559000	1.336823000	3.549362000
H	-0.866662000	1.489624000	3.356350000
H	0.126184000	2.921553000	3.597582000
C	2.884066000	1.922684000	1.518746000
H	3.323529000	2.906310000	1.732804000
H	3.580855000	1.395975000	0.858486000
H	2.853886000	1.377012000	2.467810000
C	2.290055000	2.637038000	-1.522959000
H	1.922044000	2.407048000	-2.528648000
H	3.198433000	2.050073000	-1.356462000
H	2.585824000	3.694840000	-1.526184000
C	-0.842284000	3.111417000	-1.838385000
H	-0.842178000	4.209573000	-1.859574000
H	-1.886722000	2.787680000	-1.886430000
H	-0.348057000	2.774366000	-2.755519000
C	-2.192964000	2.712212000	1.007502000
H	-2.351643000	3.787498000	1.164971000
H	-2.871727000	2.402233000	0.205876000
H	-2.510050000	2.208260000	1.926501000
C	-3.391448000	-0.877004000	0.032027000
C	-4.327687000	-0.900963000	-1.001497000
C	-3.922151000	-0.643455000	-2.312675000
C	-2.583815000	-0.370789000	-2.584219000
C	-1.685291000	-0.363703000	-1.517768000
N	-2.099822000	-0.613335000	-0.259593000
H	-4.655179000	-0.657359000	-3.115493000
H	-5.368818000	-1.112783000	-0.784736000
H	-2.246033000	-0.169954000	-3.596894000

H	-0.297211000	-0.611120000	-1.868485000
C	-3.724733000	-1.133293000	1.480854000
H	-3.178649000	-2.034396000	1.796400000
H	-3.300199000	-0.309144000	2.069938000
C	-5.204932000	-1.295104000	1.811881000
H	-5.644841000	-2.159725000	1.303196000
H	-5.332045000	-1.450389000	2.887349000
H	-5.780516000	-0.404569000	1.536718000
Y	0.149008000	0.061091000	0.014013000

82

L, E(SCRF) = -1486.41847 a.u.

Y	-0.006430000	-0.091619000	0.242209000
C	-2.781157000	-1.299446000	-2.266960000
H	-1.764156000	-1.281250000	-1.861606000
C	0.620619000	-1.677323000	-1.353752000
C	-5.646017000	1.350059000	-0.412694000
H	-7.076819000	-0.181600000	-0.924684000
H	-5.371241000	-1.645421000	-1.953041000
H	-4.041425000	2.684569000	-0.023906000
H	-6.374568000	2.017138000	0.039130000
C	-3.718360000	-0.338398000	-1.584384000
H	-2.713346000	-1.093606000	-3.344234000
H	-3.155509000	-2.323078000	-2.167928000
C	-6.036746000	0.129986000	-0.950275000
C	-1.313876000	-1.887390000	1.672471000
C	-1.763005000	-0.631146000	2.180681000
C	-0.661076000	-0.001837000	2.835060000
C	0.060416000	-2.037312000	2.017397000
C	0.470099000	-0.869013000	2.729167000
C	0.871551000	-3.282782000	1.811229000
H	0.657733000	-4.014915000	2.601739000
H	0.650359000	-3.764858000	0.853429000
H	1.946924000	-3.084202000	1.839129000
C	1.791232000	-0.685833000	3.422947000
H	2.084087000	0.366407000	3.507495000
H	1.752509000	-1.088689000	4.444202000
H	2.602270000	-1.207291000	2.905628000
C	-3.193077000	-0.184798000	2.282890000
H	-3.642316000	-0.578344000	3.205799000
H	-3.292092000	0.905100000	2.325412000
H	-3.806232000	-0.537201000	1.449331000
C	-2.178893000	-2.946381000	1.050946000
H	-3.053529000	-2.518692000	0.551091000
H	-1.631296000	-3.544316000	0.315313000

H	-2.553346000	-3.638314000	1.817976000
N	-1.926279000	1.322919000	-1.047240000
C	-1.507879000	1.608000000	-2.440801000
H	-2.136131000	2.395602000	-2.880031000
H	-0.468747000	1.949746000	-2.446662000
H	-1.579985000	0.713267000	-3.056606000
C	-1.680008000	2.541015000	-0.253687000
H	-1.989182000	2.388671000	0.784809000
H	-0.610568000	2.772434000	-0.282090000
H	-2.207714000	3.419691000	-0.651092000
C	2.959127000	-1.859598000	-0.924437000
C	3.082805000	-2.818516000	-1.925591000
C	1.951486000	-3.213947000	-2.647470000
C	0.714014000	-2.649480000	-2.359874000
C	-5.072986000	-0.690690000	-1.525831000
N	1.742696000	-1.320252000	-0.685121000
H	2.049964000	-3.965001000	-3.428358000
H	4.049731000	-3.259731000	-2.142409000
H	-0.170789000	-2.957455000	-2.911504000
C	-3.329056000	0.897187000	-1.020697000
C	4.107651000	-1.383905000	-0.068392000
H	3.918583000	-1.716481000	0.961966000
H	4.067971000	-0.287354000	-0.027277000
C	5.499372000	-1.839417000	-0.497108000
H	6.256482000	-1.409409000	0.165972000
H	5.604964000	-2.928476000	-0.447106000
H	5.733861000	-1.522578000	-1.519791000
C	2.572714000	2.215818000	-0.752793000
C	3.619058000	3.103896000	-0.476310000
C	3.727895000	3.691917000	0.776574000
C	2.771395000	3.387379000	1.743256000
C	1.769413000	2.491287000	1.406584000
N	1.663183000	1.899444000	0.197922000
H	4.539874000	4.380067000	0.994244000
H	4.343515000	3.328781000	-1.252972000
H	2.799749000	3.827634000	2.734549000
H	1.007920000	2.227475000	2.134388000
C	2.441851000	1.618758000	-2.131122000
H	1.593891000	0.927317000	-2.154145000
H	3.326923000	1.002697000	-2.336843000
C	2.294024000	2.669348000	-3.239527000
H	2.165146000	2.176616000	-4.208387000
H	1.428571000	3.319533000	-3.069618000
H	3.177620000	3.311205000	-3.312835000

C	-0.770636000	1.214694000	3.714248000
H	-1.276512000	2.061918000	3.232634000
H	-1.353095000	0.981154000	4.615633000
H	0.207870000	1.561076000	4.063210000
C	-4.306008000	1.725957000	-0.452585000

65

L', E(SCRF) = -1159.629466 a.u.

N	0.908209000	-2.253164000	0.255639000
C	1.836371000	-1.039246000	-2.319932000
H	2.005198000	-1.872066000	-3.015668000
H	2.101517000	-0.123968000	-2.858534000
C	2.697085000	-1.192178000	-1.082747000
C	2.286830000	-1.825035000	0.118528000
C	3.202248000	-1.970419000	1.172791000
H	2.902471000	-2.463848000	2.090519000
C	4.509282000	-1.512584000	1.055181000
H	5.201242000	-1.649192000	1.881013000
C	4.924349000	-0.890354000	-0.120621000
H	5.943798000	-0.531099000	-0.224274000
C	4.021903000	-0.734921000	-1.165080000
H	4.346628000	-0.258003000	-2.086743000
C	0.472651000	-2.524276000	1.635322000
H	0.946184000	-3.420386000	2.059644000
H	-0.608441000	-2.684153000	1.627025000
H	0.702499000	-1.677513000	2.294299000
C	0.552162000	-3.412478000	-0.592686000
H	0.874135000	-3.255103000	-1.620777000
H	-0.533397000	-3.539726000	-0.583634000
H	1.029591000	-4.325675000	-0.212448000
C	-0.975545000	2.440186000	0.550510000
C	-0.037347000	2.094802000	1.571780000
C	1.272820000	2.126679000	0.998843000
C	1.137116000	2.472023000	-0.380545000
C	-0.253207000	2.666922000	-0.656144000
C	-0.355168000	1.885490000	3.027356000
H	0.376111000	1.239272000	3.526837000
H	-1.346862000	1.444954000	3.178299000
H	-0.348406000	2.841138000	3.568496000
C	2.569348000	1.974481000	1.744469000
H	2.938032000	2.952823000	2.081723000
H	3.357645000	1.531410000	1.126582000
H	2.463615000	1.352556000	2.640127000
C	2.267292000	2.764133000	-1.328067000
H	1.993082000	2.576096000	-2.372262000

H	3.161658000	2.174303000	-1.100994000
H	2.558376000	3.821403000	-1.266177000
C	-0.833367000	3.184997000	-1.940905000
H	-0.855861000	4.283194000	-1.940761000
H	-1.859140000	2.836970000	-2.094419000
H	-0.248353000	2.876615000	-2.813769000
C	-2.447944000	2.664265000	0.736348000
H	-2.659152000	3.731522000	0.885871000
H	-3.027803000	2.338469000	-0.133394000
H	-2.837774000	2.135769000	1.611860000
C	-3.376081000	-1.034271000	0.104862000
C	-4.317967000	-1.169153000	-0.910438000
C	-3.960448000	-0.874113000	-2.230694000
C	-2.670896000	-0.443167000	-2.522842000
C	-1.742977000	-0.317897000	-1.481537000
N	-2.127856000	-0.624756000	-0.217310000
H	-4.700273000	-0.978528000	-3.021221000
H	-5.325652000	-1.496170000	-0.678280000
H	-2.388179000	-0.200254000	-3.543702000
H	0.741554000	-1.035432000	-2.173381000
C	-3.653443000	-1.325384000	1.559865000
H	-3.053915000	-2.199678000	1.855154000
H	-3.258838000	-0.485917000	2.148029000
C	-5.113286000	-1.572207000	1.928443000
H	-5.514851000	-2.462322000	1.432237000
H	-5.206052000	-1.730826000	3.007112000
H	-5.745297000	-0.717768000	1.662895000
Y	0.060045000	0.115354000	-0.103537000

76

M, E(SCRF) = -1407861238 a.u.

Y	-0.036207000	-0.387158000	0.226542000
C	0.997532000	-1.137145000	-1.734910000
C	-0.370260000	-2.885424000	0.996015000
C	-1.369311000	-2.144485000	1.697425000
C	-0.710763000	-1.295819000	2.639796000
C	0.903366000	-2.494543000	1.501279000
C	0.697198000	-1.512208000	2.515141000
C	2.219084000	-3.121395000	1.141747000
H	2.376727000	-4.046025000	1.713819000
H	2.275210000	-3.383803000	0.080288000
H	3.061959000	-2.458938000	1.363259000
C	1.768292000	-0.977365000	3.426616000
H	1.407820000	-0.152487000	4.050114000
H	2.111091000	-1.759943000	4.116534000

H	2.654661000	-0.623891000	2.886064000
C	-2.852225000	-2.369813000	1.607337000
H	-3.168665000	-3.153084000	2.309603000
H	-3.428869000	-1.471016000	1.851067000
H	-3.160464000	-2.695902000	0.608615000
C	-0.616505000	-3.998594000	0.017748000
H	-1.547948000	-3.861058000	-0.541306000
H	0.194251000	-4.087048000	-0.711850000
H	-0.695971000	-4.962912000	0.538265000
C	3.226698000	-0.356239000	-1.384502000
C	3.634867000	-0.932259000	-2.583050000
C	2.704868000	-1.626054000	-3.365873000
C	1.384653000	-1.733273000	-2.944362000
N	1.933084000	-0.474515000	-1.010730000
H	3.025848000	-2.079842000	-4.301156000
H	4.666668000	-0.847825000	-2.906893000
H	0.659858000	-2.275552000	-3.546869000
C	4.139759000	0.403388000	-0.453267000
H	4.122201000	-0.106261000	0.520470000
H	3.690234000	1.389824000	-0.272842000
C	5.583585000	0.570591000	-0.915641000
H	6.152865000	1.139873000	-0.174279000
H	6.083746000	-0.395980000	-1.041146000
H	5.645432000	1.111995000	-1.866373000
C	0.682911000	3.011895000	-0.181298000
C	1.166503000	4.275875000	0.174598000
C	1.457953000	4.563474000	1.501417000
C	1.258901000	3.572715000	2.461751000
C	0.784601000	2.341249000	2.038205000
N	0.500273000	2.051790000	0.752028000
H	1.836395000	5.542120000	1.783063000
H	1.314766000	5.024695000	-0.597862000
H	1.470922000	3.744494000	3.511906000
H	0.627405000	1.537961000	2.751618000
C	0.345124000	2.715100000	-1.620104000
H	0.152772000	1.644200000	-1.752289000
H	1.224398000	2.934455000	-2.239512000
C	-0.852734000	3.522706000	-2.135935000
H	-1.048590000	3.277669000	-3.184667000
H	-1.757280000	3.306833000	-1.558115000
H	-0.665988000	4.600009000	-2.076700000
C	-1.396605000	-0.511678000	3.725102000
H	-2.389108000	-0.160772000	3.421410000
H	-1.546203000	-1.135846000	4.616669000

H	-0.823004000	0.363123000	4.052916000
C	-2.869076000	1.203735000	0.545471000
C	-4.110317000	1.813283000	0.469111000
C	-4.861358000	1.622086000	-0.691120000
C	-4.335269000	0.833014000	-1.703760000
C	-3.074284000	0.240476000	-1.556784000
N	-2.348392000	0.435104000	-0.433737000
H	-5.839008000	2.082810000	-0.801848000
H	-2.253627000	1.334918000	1.433041000
H	-4.474434000	2.419214000	1.292256000
H	-4.893036000	0.667425000	-2.620624000
C	-2.514756000	-0.628614000	-2.651195000
H	-2.516358000	-0.053628000	-3.587175000
H	-1.468096000	-0.864297000	-2.426369000
C	-3.310802000	-1.924192000	-2.858914000
H	-4.353626000	-1.723181000	-3.126479000
H	-2.867390000	-2.512037000	-3.668717000
H	-3.310033000	-2.540717000	-1.954224000

72

TS7, E(SCRF) = -1276.276578 a.u., IF = *i*167.98 cm⁻¹

Y	-0.011275000	-0.477313000	-0.228827000
C	2.265845000	-0.681829000	-1.219646000
C	-1.346445000	-1.714891000	-2.479411000
C	-1.032039000	-0.508754000	-3.026707000
C	-0.362055000	-2.488976000	-1.733711000
C	1.004629000	-2.367616000	-1.979012000
H	3.074053000	-0.036784000	2.172840000
H	3.239302000	-1.639649000	1.454391000
H	2.985698000	-1.472801000	3.192481000
C	0.577191000	1.208367000	3.017408000
H	0.387642000	1.168036000	4.098986000
H	-0.044093000	2.020378000	2.620254000
H	1.626037000	1.493455000	2.892461000
C	-2.288735000	0.000299000	2.735790000
H	-2.391496000	1.041595000	2.409180000
H	-2.278787000	0.013443000	3.834241000
H	-3.192546000	-0.538847000	2.437256000
C	-2.029909000	-2.995841000	1.626862000
H	-2.217940000	-3.488305000	2.590632000
H	-1.798758000	-3.790602000	0.909730000
H	-2.976089000	-2.537206000	1.317782000
C	1.075824000	-3.641394000	1.359849000
H	0.470871000	-4.241038000	0.670828000
H	2.086284000	-3.570381000	0.943738000

H	1. 156631000	-4. 219705000	2. 290286000
C	3. 126266000	1. 409032000	-0. 549495000
C	4. 384660000	1. 053311000	-1. 021459000
C	4. 580034000	-0. 199281000	-1. 606072000
C	3. 510866000	-1. 077614000	-1. 713437000
C	1. 211758000	-1. 131382000	2. 030859000
N	2. 097314000	0. 526423000	-0. 667625000
H	5. 565691000	-0. 480733000	-1. 968765000
H	5. 212829000	1. 746910000	-0. 930123000
H	3. 646652000	-2. 054349000	-2. 170505000
C	2. 844788000	2. 750473000	0. 080207000
H	2. 349819000	3. 385132000	-0. 670662000
H	2. 115604000	2. 598212000	0. 884429000
C	4. 060057000	3. 497712000	0. 628072000
H	4. 750527000	3. 799976000	-0. 165923000
H	3. 736228000	4. 410373000	1. 137592000
H	4. 614296000	2. 889464000	1. 351062000
C	0. 480191000	-2. 289291000	1. 630046000
C	2. 699928000	-1. 064137000	2. 213914000
H	1. 678015000	-3. 075568000	-1. 507240000
C	-0. 913995000	-1. 996647000	1. 751743000
C	0. 274410000	-0. 116833000	2. 378092000
C	-1. 039470000	-0. 655771000	2. 220454000
H	-1. 763429000	0. 076649000	-3. 575447000
C	-0. 767447000	2. 769170000	-0. 393506000
C	-1. 346149000	4. 029411000	-0. 431417000
C	-2. 735301000	4. 109174000	-0. 440535000
C	-3. 472418000	2. 930491000	-0. 424945000
C	-2. 821090000	1. 694731000	-0. 398953000
N	-1. 469096000	1. 621084000	-0. 369826000
H	-3. 238270000	5. 071848000	-0. 462212000
H	0. 310756000	2. 662233000	-0. 378521000
H	-0. 722114000	4. 916910000	-0. 447063000
H	-4. 555897000	2. 965239000	-0. 435669000
C	-3. 580945000	0. 395536000	-0. 456769000
H	-3. 567765000	0. 055190000	-1. 500122000
H	-3. 016432000	-0. 356898000	0. 110501000
C	-5. 024153000	0. 432555000	0. 042860000
H	-5. 664736000	1. 046012000	-0. 599034000
H	-5. 445552000	-0. 577433000	0. 039813000
H	-5. 089610000	0. 821544000	1. 064392000
H	-0. 712209000	-3. 293585000	-1. 092648000
H	1. 334710000	-1. 982206000	-2. 939811000
H	-0. 006576000	-0. 135585000	-3. 064177000

C	-2.730504000	-2.298695000	-2.585704000
H	-2.684578000	-3.224016000	-3.173230000
H	-3.137461000	-2.570828000	-1.604358000
H	-3.429847000	-1.621302000	-3.083224000

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TS7-1, E(SCRF) = -1276.272268 a.u., IF = $i230.16 \text{ cm}^{-1}$

Y	-0.260422000	-0.469946000	0.304482000
C	-1.855745000	1.343065000	1.028148000
C	-1.509635000	0.115865000	2.686352000
C	-0.722868000	-1.054919000	2.641609000
C	-1.512780000	-2.763516000	-0.256685000
C	-2.822179000	0.122881000	-2.272116000
H	-2.185313000	0.790221000	-2.861397000
H	-3.388175000	0.737972000	-1.564539000
H	-3.549964000	-0.318969000	-2.966430000
C	-0.104820000	-1.094900000	-3.328628000
H	-0.664736000	-1.446498000	-4.205609000
H	0.899677000	-1.521594000	-3.407426000
H	-0.010697000	-0.007144000	-3.429820000
C	0.575134000	-3.666822000	-1.500906000
H	1.364164000	-3.299671000	-2.162959000
H	0.128980000	-4.540975000	-1.994307000
H	1.053548000	-4.033788000	-0.585351000
C	-1.686864000	-3.942754000	0.657356000
H	-2.165899000	-4.772894000	0.120218000
H	-2.327429000	-3.717134000	1.516615000
H	-0.736147000	-4.328127000	1.042470000
C	-3.788614000	-1.588280000	0.225338000
H	-3.747146000	-1.931406000	1.265230000
H	-4.144157000	-0.552902000	0.229362000
H	-4.558323000	-2.191029000	-0.275540000
C	-1.278434000	2.859975000	-0.689455000
C	-2.380723000	3.653350000	-0.376723000
C	-3.236951000	3.266311000	0.653237000
C	-2.976397000	2.100468000	1.368926000
C	-2.029341000	-0.953139000	-1.588996000
N	-1.048564000	1.735902000	0.028584000
H	-4.107560000	3.872425000	0.891751000
H	-2.576007000	4.556718000	-0.946524000
H	-3.633397000	1.796539000	2.179464000
C	-0.335475000	3.198424000	-1.814149000
H	0.409976000	2.399792000	-1.892309000
H	-0.900253000	3.196909000	-2.756377000
C	0.360859000	4.555298000	-1.654049000

H	0.960351000	4.591550000	-0.738305000
H	1.028078000	4.739061000	-2.502019000
H	-0.359206000	5.379117000	-1.615771000
C	-2.467115000	-1.727782000	-0.474429000
C	-0.800304000	-1.505630000	-2.059581000
C	-0.479722000	-2.628977000	-1.234714000
H	-1.226490000	-2.003979000	2.471786000
C	2.130856000	1.894667000	0.593387000
C	3.304642000	2.618548000	0.753101000
C	4.492323000	2.042021000	0.315400000
C	4.449075000	0.775203000	-0.257556000
C	3.231593000	0.102416000	-0.379161000
N	2.075474000	0.663656000	0.051325000
H	5.437371000	2.568803000	0.414140000
H	1.181212000	2.320097000	0.904309000
H	3.280110000	3.604889000	1.204833000
H	5.359296000	0.304909000	-0.611418000
C	3.123305000	-1.266100000	-0.996498000
H	2.577007000	-1.905613000	-0.288230000
H	2.476574000	-1.177848000	-1.879352000
C	4.431144000	-1.945189000	-1.390475000
H	5.095628000	-2.079261000	-0.529816000
H	4.224596000	-2.937457000	-1.802633000
H	4.970754000	-1.379857000	-2.157976000
H	-2.580108000	-0.020747000	2.803836000
C	1.444887000	-2.095532000	2.213545000
H	2.523256000	-2.155278000	2.328904000
H	0.952800000	-2.958897000	1.768216000
H	-1.126231000	0.985627000	3.216846000
C	0.723909000	-1.091593000	2.791594000
C	1.424710000	0.018037000	3.536427000
H	1.148654000	-0.028233000	4.597116000
H	2.511042000	-0.071436000	3.457929000
H	1.145412000	1.018708000	3.185145000

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TS7-2, E(SCRF) = -1276.262829 a.u., IF = $i273.64 \text{ cm}^{-1}$

Y	-0.059990000	0.392727000	0.211609000
C	2.343145000	-0.059285000	0.670194000
C	1.388735000	0.034439000	2.533085000
C	0.084714000	0.613791000	2.619100000
C	-1.007313000	2.852973000	0.068006000
C	1.981362000	2.310527000	-2.152976000
H	2.053954000	1.501548000	-2.886845000
H	2.829225000	2.211927000	-1.466760000

H	2.119561000	3.252361000	-2.700901000
C	-0.788149000	1.175441000	-3.292906000
H	-1.059572000	1.935117000	-4.038722000
H	-1.601728000	0.440699000	-3.283377000
H	0.111275000	0.674833000	-3.667650000
C	-3.077181000	1.976811000	-1.268209000
H	-3.321828000	1.010452000	-1.723876000
H	-3.440362000	2.752858000	-1.955539000
H	-3.664861000	2.071636000	-0.349660000
C	-1.741880000	3.544278000	1.181389000
H	-2.034835000	4.558933000	0.879314000
H	-1.128147000	3.645692000	2.082161000
H	-2.661166000	3.021669000	1.467941000
C	1.387955000	3.721854000	0.630915000
H	1.138735000	3.722836000	1.697617000
H	2.403613000	3.325791000	0.527256000
H	1.419139000	4.772228000	0.310896000
C	2.791701000	-1.203931000	-1.340850000
C	4.158735000	-0.986804000	-1.177042000
C	4.613574000	-0.257197000	-0.079441000
C	3.699932000	0.205687000	0.863480000
C	0.662033000	2.306373000	-1.435284000
N	1.926068000	-0.727445000	-0.418153000
H	5.675224000	-0.052608000	0.035640000
H	4.856178000	-1.369958000	-1.915938000
H	4.040552000	0.768035000	1.728934000
C	2.244485000	-1.985208000	-2.502809000
H	1.279081000	-1.555197000	-2.797765000
H	2.913534000	-1.869208000	-3.362989000
C	2.083706000	-3.477702000	-2.179506000
H	1.418228000	-3.631103000	-1.322710000
H	1.670466000	-4.014000000	-3.040144000
H	3.049457000	-3.931614000	-1.934068000
C	0.394296000	2.945110000	-0.185671000
C	0.656748000	-2.341148000	2.595499000
H	-0.283974000	-2.108278000	2.099221000
H	0.802272000	-3.383345000	2.865101000
C	1.580792000	-1.411584000	2.880332000
C	-0.570895000	1.804443000	-1.945160000
C	-1.604386000	2.143852000	-1.018496000
H	-0.690680000	-0.001898000	3.073104000
H	0.034611000	1.666727000	2.891443000
C	-1.614541000	-2.140490000	-1.213109000
C	-2.510705000	-3.089655000	-1.680806000

C	-3.757119000	-3.166507000	-1.064848000
C	-4.045688000	-2.301176000	-0.014856000
C	-3.094080000	-1.370282000	0.407527000
N	-1.886590000	-1.294021000	-0.201733000
H	-4.495579000	-3.891145000	-1.396163000
H	-0.630083000	-2.046638000	-1.664716000
H	-2.237259000	-3.743241000	-2.502355000
H	-5.009847000	-2.344892000	0.478680000
C	-3.336543000	-0.439057000	1.569550000
H	-2.831112000	-0.859621000	2.451041000
H	-2.827984000	0.512131000	1.360416000
C	-4.798394000	-0.165241000	1.918042000
H	-5.307467000	-1.061540000	2.287058000
H	-4.854538000	0.583932000	2.713407000
H	-5.355013000	0.216593000	1.055530000
C	2.856558000	-1.757169000	3.597370000
H	2.901730000	-2.821763000	3.842222000
H	3.735642000	-1.510388000	2.989411000
H	2.941253000	-1.188710000	4.532516000
H	2.215989000	0.674209000	2.832626000

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TS7-3, E(SCRF) = -1276.26404 a.u., IF = *i*267.82 cm⁻¹

Y	-0.065551000	0.383897000	0.146479000
C	2.352853000	-0.085882000	0.566930000
C	1.527653000	0.342864000	2.449728000
C	0.149012000	0.718894000	2.528118000
C	-0.944949000	2.859000000	-0.123657000
C	1.941283000	2.076739000	-2.408644000
H	1.964185000	1.216507000	-3.085263000
H	2.810871000	2.000119000	-1.747382000
H	2.085381000	2.973294000	-3.026515000
C	-0.901325000	0.959457000	-3.371455000
H	-1.179825000	1.675474000	-4.156749000
H	-1.734070000	0.251940000	-3.282855000
H	-0.030773000	0.408330000	-3.743634000
C	-3.089111000	1.963060000	-1.320251000
H	-3.377065000	0.983485000	-1.718565000
H	-3.460987000	2.715640000	-2.028727000
H	-3.635223000	2.116743000	-0.384036000
C	-1.618123000	3.643510000	0.966636000
H	-1.925955000	4.631310000	0.597830000
H	-0.955749000	3.816750000	1.820838000
H	-2.521244000	3.151995000	1.345404000
C	1.495583000	3.681546000	0.298108000

H	1. 288272000	3. 755036000	1. 371444000
H	2. 494090000	3. 247481000	0. 180816000
H	1. 545825000	4. 709237000	-0. 086508000
C	2. 672974000	-1. 434596000	-1. 345825000
C	4. 048472000	-1. 248184000	-1. 266427000
C	4. 578525000	-0. 439280000	-0. 258719000
C	3. 727906000	0. 135102000	0. 676560000
C	0. 649940000	2. 163063000	-1. 646366000
N	1. 863260000	-0. 839763000	-0. 434497000
H	5. 650429000	-0. 264240000	-0. 209853000
H	4. 698163000	-1. 718882000	-1. 998276000
H	4. 128644000	0. 740922000	1. 483977000
C	2. 046411000	-2. 304799000	-2. 399887000
H	1. 095474000	-1. 856014000	-2. 714481000
H	2. 691342000	-2. 316108000	-3. 285757000
C	1. 820579000	-3. 744594000	-1. 917511000
H	1. 172749000	-3. 774507000	-1. 034178000
H	1. 355689000	-4. 345605000	-2. 706059000
H	2. 769380000	-4. 220481000	-1. 648834000
C	0. 448335000	2. 888949000	-0. 431931000
C	3. 075473000	-0. 899897000	3. 878895000
H	3. 661318000	0. 003720000	4. 028920000
H	3. 399873000	-1. 783278000	4. 422412000
C	1. 987614000	-0. 921325000	3. 096444000
C	-0. 615956000	1. 670270000	-2. 078189000
C	-1. 603296000	2. 100355000	-1. 138739000
H	-0. 516698000	0. 034419000	3. 054713000
H	-0. 051033000	1. 769869000	2. 732597000
C	-1. 742798000	-2. 199355000	-1. 034043000
C	-2. 674724000	-3. 165964000	-1. 380305000
C	-3. 883535000	-3. 180272000	-0. 689533000
C	-4. 100985000	-2. 237088000	0. 309191000
C	-3. 116469000	-1. 292523000	0. 608146000
N	-1. 944776000	-1. 279567000	-0. 071523000
H	-4. 647904000	-3. 915623000	-0. 924432000
H	-0. 786821000	-2. 151728000	-1. 549392000
H	-2. 457080000	-3. 879667000	-2. 167790000
H	-5. 035825000	-2. 230049000	0. 857931000
C	-3. 285896000	-0. 273505000	1. 707699000
H	-2. 747630000	-0. 638749000	2. 594016000
H	-2. 769685000	0. 648043000	1. 405926000
C	-4. 724727000	0. 058110000	2. 099739000
H	-5. 233010000	-0. 796157000	2. 558587000
H	-4. 729765000	0. 866089000	2. 837438000

H	-5.313664000	0.386111000	1.236538000
C	1.167529000	-2.167922000	2.907600000
H	1.625121000	-3.018683000	3.419644000
H	0.150979000	-2.053903000	3.304472000
H	1.078485000	-2.430087000	1.844003000
H	2.241330000	1.160167000	2.537373000

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N, E(SCRF) = -1276.331936 a.u.

Y	-0.007693000	-0.352637000	-0.086137000
C	3.031957000	-0.702881000	-1.235221000
C	0.024364000	-1.956227000	-2.234661000
C	-0.008377000	-0.697936000	-2.809412000
C	0.952305000	-2.345882000	-1.212766000
C	2.451337000	-2.094890000	-1.333115000
H	2.409704000	1.377571000	2.623898000
H	3.156311000	-0.154194000	2.157494000
H	2.571869000	0.082742000	3.803986000
C	-0.448821000	1.861731000	2.917602000
H	-0.706477000	1.881282000	3.985496000
H	-1.267747000	2.363778000	2.389042000
H	0.451207000	2.475074000	2.803425000
C	-2.752069000	-0.212668000	2.459985000
H	-3.070448000	0.744187000	2.032074000
H	-2.965062000	-0.166229000	3.536724000
H	-3.396308000	-0.995766000	2.048202000
C	-1.426407000	-3.083354000	1.882384000
H	-1.521558000	-3.572996000	2.861109000
H	-0.899516000	-3.784217000	1.225695000
H	-2.442906000	-2.962451000	1.491905000
C	1.711047000	-2.748359000	2.160976000
H	1.426471000	-3.586942000	1.517796000
H	2.715293000	-2.425058000	1.868195000
H	1.790708000	-3.140969000	3.184230000
C	2.852338000	1.547818000	-0.618393000
C	4.164591000	1.793680000	-1.000979000
C	4.927084000	0.751471000	-1.525393000
C	4.351637000	-0.501298000	-1.654294000
C	0.999175000	-0.253450000	2.380048000
N	2.302687000	0.310033000	-0.719728000
H	5.953992000	0.923425000	-1.835749000
H	4.584917000	2.787577000	-0.900785000
H	4.910467000	-1.334306000	-2.070007000
C	1.943894000	2.645177000	-0.123822000
H	1.309023000	2.957304000	-0.967332000

H	1. 275624000	2. 214333000	0. 637582000
C	2. 626883000	3. 880318000	0. 461423000
H	3. 189192000	4. 432651000	-0. 297967000
H	1. 878400000	4. 566771000	0. 869340000
H	3. 314690000	3. 612706000	1. 270341000
C	0. 716468000	-1. 625714000	2. 107582000
C	2. 349746000	0. 291662000	2. 748790000
H	2. 947128000	-2. 684153000	-0. 549330000
C	-0. 700197000	-1. 773481000	2. 011218000
C	-0. 242875000	0. 447589000	2. 451635000
C	-1. 293683000	-0. 494030000	2. 234256000
H	-0. 771502000	-0. 444599000	-3. 540235000
C	-1. 760757000	2. 514490000	-0. 529123000
C	-2. 740423000	3. 472800000	-0. 745436000
C	-4. 021235000	3. 035122000	-1. 068588000
C	-4. 257072000	1. 667793000	-1. 161455000
C	-3. 217582000	0. 762036000	-0. 940892000
N	-1. 972619000	1. 189906000	-0. 624812000
H	-4. 824992000	3. 744995000	-1. 241969000
H	-0. 756207000	2. 822952000	-0. 257314000
H	-2. 502047000	4. 527374000	-0. 654266000
H	-5. 247152000	1. 299641000	-1. 404875000
C	-3. 401769000	-0. 726512000	-1. 070975000
H	-2. 893771000	-1. 037637000	-1. 992161000
H	-2. 858286000	-1. 210947000	-0. 245238000
C	-4. 839519000	-1. 239010000	-1. 085761000
H	-5. 387723000	-0. 887746000	-1. 966166000
H	-4. 844552000	-2. 332592000	-1. 119804000
H	-5. 390120000	-0. 929352000	-0. 190925000
H	0. 771464000	-3. 353030000	-0. 835496000
H	2. 824087000	-2. 518145000	-2. 280225000
H	0. 864240000	-0. 045065000	-2. 805160000
C	-1. 083723000	-2. 939692000	-2. 544776000
H	-0. 650198000	-3. 784208000	-3. 094778000
H	-1. 538670000	-3. 359192000	-1. 639015000
H	-1. 869916000	-2. 509136000	-3. 171612000

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TS8, E(SCRF) = -1276.282934 a.u., IF = *i*1287.89 cm⁻¹

Y	-0. 556095000	-0. 099417000	-0. 256108000
C	-1. 588066000	0. 666046000	-2. 664781000
C	-0. 949027000	2. 313846000	-0. 431654000
H	-1. 441126000	1. 406443000	-1. 454820000
C	2. 245829000	-1. 022653000	-1. 696314000
H	-1. 181052000	5. 661901000	0. 030599000

H	-2.562278000	3.719524000	-0.737247000
H	1.183142000	5.282774000	0.709668000
C	2.541829000	2.897113000	0.700795000
H	2.804193000	3.464706000	1.602103000
H	2.649640000	1.834730000	0.939618000
C	3.505384000	3.271378000	-0.434506000
H	3.433548000	4.335179000	-0.684444000
H	4.539643000	3.064680000	-0.140875000
H	3.287961000	2.697366000	-1.341970000
C	1.202689000	-0.526678000	-2.661845000
C	-1.531888000	3.580099000	-0.422795000
C	0.565124000	4.451851000	0.381648000
C	-0.759095000	4.660309000	-0.000450000
C	1.105658000	3.164502000	0.344552000
N	0.334654000	2.133184000	-0.058124000
H	-3.570905000	1.967112000	1.263233000
H	-2.230193000	2.162373000	2.396334000
H	-3.686416000	1.296099000	2.891050000
C	-4.288545000	-0.409876000	-0.120547000
H	-4.568291000	-1.218326000	-0.801007000
H	-4.258268000	0.520227000	-0.700670000
H	-5.110628000	-0.306889000	0.599503000
C	-2.651713000	-3.221713000	-0.058144000
H	-3.411813000	-3.080082000	-0.829445000
H	-3.066627000	-3.930085000	0.672071000
H	-1.791367000	-3.717295000	-0.523399000
C	-0.449198000	-3.010841000	2.087345000
H	-1.112224000	-3.826083000	2.405139000
H	0.175535000	-2.760267000	2.948627000
H	0.206217000	-3.423643000	1.309989000
C	-0.648669000	-0.040894000	3.449445000
H	-1.373468000	0.128549000	4.256072000
H	0.080036000	-0.763045000	3.827683000
H	-0.123633000	0.910090000	3.293893000
C	2.832268000	-1.294791000	0.541059000
C	4.076895000	-1.809846000	0.165798000
C	4.396554000	-1.933997000	-1.178948000
C	3.469157000	-1.518886000	-2.130123000
C	-2.422585000	0.160625000	1.581328000
N	1.917381000	-0.935094000	-0.387011000
H	5.358271000	-2.337793000	-1.482944000
H	4.788366000	-2.105213000	0.928562000
H	3.685259000	-1.578831000	-3.192221000
C	2.485323000	-1.059755000	1.986816000

H	2.801555000	-0.038691000	2.247995000
C	-1.356536000	-0.539260000	2.217971000
C	-2.999651000	1.465137000	2.049489000
H	-2.619296000	0.935077000	-2.905046000
C	-1.265170000	-1.836401000	1.619993000
C	-3.001759000	-0.701131000	0.601678000
C	-2.283742000	-1.934756000	0.624463000
H	1.609689000	-0.544183000	-3.682701000
C	-0.082918000	-1.324084000	-2.634760000
H	0.030234000	-2.401716000	-2.741310000
C	-1.328095000	-0.772835000	-2.809089000
H	1.395507000	-1.061730000	2.072933000
C	3.093817000	-2.038256000	2.991242000
H	2.701844000	-1.835960000	3.993118000
H	2.855708000	-3.076642000	2.737978000
H	4.182683000	-1.943698000	3.053185000
H	-0.902474000	1.302121000	-3.235167000
H	1.021885000	0.542170000	-2.456842000
C	-2.492240000	-1.660816000	-3.155917000
H	-3.402080000	-1.379033000	-2.620350000
H	-2.703911000	-1.533311000	-4.226162000
H	-2.281193000	-2.718618000	-2.981087000

72

TSS', E(SCRF) = -1276.261424 a.u., IF = *i*1347.48 cm⁻¹

Y	0.236962000	-0.432669000	-0.163318000
N	1.393809000	1.527326000	0.403509000
C	-1.369128000	-0.096032000	3.294598000
C	-1.679865000	1.200009000	3.148109000
C	-0.888962000	-0.946041000	2.136407000
C	-2.109981000	-1.492848000	1.332438000
C	1.340237000	0.860697000	1.578410000
H	0.271782000	-0.072154000	1.848139000
N	-2.132964000	0.121143000	-0.483086000
C	0.786239000	-1.376201000	-3.641029000
H	1.311988000	-2.024367000	-4.355216000
H	1.083176000	-0.347502000	-3.876843000
H	-0.283429000	-1.475828000	-3.856028000
C	3.384194000	-0.478968000	-2.020830000
H	3.023230000	0.237135000	-2.766930000
H	4.164300000	-1.078700000	-2.508718000
H	3.870920000	0.090266000	-1.222002000
C	3.410483000	-2.049997000	0.746414000
H	3.929054000	-1.086393000	0.774123000
H	4.160813000	-2.813571000	0.500633000

H	3.057035000	-2.262741000	1.760525000
C	0.850019000	-3.938803000	0.832620000
H	1.251580000	-3.658803000	1.811813000
H	-0.221621000	-4.130194000	0.956601000
H	1.312218000	-4.897110000	0.560446000
C	-2.717773000	1.005617000	-1.322101000
C	-4.069171000	1.315213000	-1.196357000
C	-4.815679000	0.705003000	-0.190411000
C	-4.204167000	-0.207337000	0.662196000
C	0.411959000	-2.718655000	-1.435057000
H	-1.343177000	-3.933362000	-1.043441000
H	-5.869934000	0.941209000	-0.075025000
H	-4.532453000	2.023911000	-1.872903000
H	-4.760786000	-0.698012000	1.453588000
C	-1.817946000	1.604709000	-2.377837000
H	-0.967209000	2.082558000	-1.866769000
H	-1.396744000	0.778088000	-2.968954000
C	-2.461480000	2.615785000	-3.322246000
H	-2.853971000	3.483405000	-2.781304000
H	-1.720724000	2.981163000	-4.039629000
H	-3.279381000	2.167169000	-3.895799000
C	1.136447000	-2.900589000	-0.215266000
C	-0.778677000	-3.519662000	-1.885639000
H	-1.782644000	-2.311610000	0.669381000
C	2.294645000	-2.063861000	-0.259977000
C	1.120740000	-1.765275000	-2.227395000
C	2.284628000	-1.362196000	-1.501697000
H	-2.067545000	1.791131000	3.974102000
H	-0.458778000	-4.372923000	-2.498764000
C	2.060239000	1.305910000	2.684912000
C	2.843450000	2.449991000	2.548851000
C	2.880186000	3.121090000	1.326606000
C	2.139250000	2.641275000	0.246125000
C	-2.851031000	-0.486943000	0.488555000
H	3.426250000	2.822188000	3.387681000
H	-1.476280000	-2.934551000	-2.495558000
H	2.008212000	0.771888000	3.628653000
H	3.487898000	4.013146000	1.204776000
C	2.118878000	3.340883000	-1.085086000
H	3.140950000	3.632399000	-1.355880000
H	1.777882000	2.632540000	-1.849106000
C	1.220535000	4.585873000	-1.082661000
H	1.568287000	5.325117000	-0.353530000
H	1.223677000	5.060878000	-2.068959000

H	0.185664000	4.330320000	-0.828382000
H	-0.384861000	-1.836384000	2.538968000
H	-2.824891000	-1.959997000	2.023885000
H	-1.565739000	1.719950000	2.198701000
C	-1.505894000	-0.795235000	4.621719000
H	-2.171713000	-1.665952000	4.547013000
H	-0.534420000	-1.178034000	4.963498000
H	-1.900311000	-0.131951000	5.397415000

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O, E(SCRF) = -2439.052152 a.u.

Sc	-1.967370000	-0.506030000	-0.026727000
C	-4.059221000	-0.502964000	-0.708095000
N	-3.033767000	-0.577000000	1.955213000
C	0.217715000	0.772743000	0.025158000
C	-0.866421000	1.672368000	0.192225000
H	-1.006453000	2.306019000	1.062957000
C	-1.673885000	1.703730000	-0.988397000
C	-1.078035000	0.756706000	-1.873247000
H	-1.435359000	0.515921000	-2.870714000
C	0.069837000	0.179723000	-1.264371000
C	1.399892000	0.628343000	0.964729000
H	1.440169000	-0.368536000	1.416535000
H	1.265367000	1.342269000	1.781417000
C	2.716876000	0.906592000	0.250669000
C	3.384927000	-0.131205000	-0.395179000
C	4.567162000	0.115286000	-1.158676000
C	5.065244000	1.451267000	-1.239413000
C	4.381929000	2.478988000	-0.548464000
H	4.783321000	3.489257000	-0.585634000
C	3.240312000	2.237206000	0.188648000
C	5.252749000	-0.909418000	-1.863411000
H	4.875754000	-1.927088000	-1.817934000
C	6.380606000	-0.624058000	-2.598311000
H	6.893986000	-1.419834000	-3.131320000
C	6.878599000	0.697335000	-2.667278000
H	7.771517000	0.907272000	-3.249611000
C	6.232806000	1.712328000	-2.001965000
H	6.607292000	2.732052000	-2.052090000
C	1.036341000	-0.783075000	-1.901631000
H	0.540648000	-1.291543000	-2.734533000
H	1.857202000	-0.206220000	-2.345068000
C	2.811849000	-1.505091000	-0.277334000
C	1.619348000	-1.787374000	-0.929129000
C	3.393767000	-2.452070000	0.626221000

C	2. 708752000	-3. 681062000	0. 879009000
C	1. 440828000	-3. 888105000	0. 286925000
H	0. 891087000	-4. 795940000	0. 527805000
C	0. 896397000	-2. 970464000	-0. 588791000
C	3. 283524000	-4. 635790000	1. 756742000
H	2. 757112000	-5. 571337000	1. 931558000
C	4. 483556000	-4. 382323000	2. 377294000
H	4. 919755000	-5. 119397000	3. 045756000
C	5. 150573000	-3. 156747000	2. 151818000
H	6. 094333000	-2. 959694000	2. 652952000
C	4. 618270000	-2. 212334000	1. 303851000
H	5. 140922000	-1. 276278000	1. 137008000
C	2. 608453000	3. 378709000	0. 910403000
C	2. 594424000	3. 428408000	2. 312705000
C	2. 074575000	4. 459910000	0. 197214000
C	2. 049857000	4. 522821000	2. 981706000
H	3. 043006000	2. 615700000	2. 880233000
C	1. 531363000	5. 556670000	0. 866290000
H	2. 087133000	4. 436898000	-0. 889575000
C	1. 513672000	5. 589675000	2. 259952000
H	2. 061731000	4. 551070000	4. 068396000
H	1. 127656000	6. 389276000	0. 295966000
H	1. 097002000	6. 447386000	2. 781278000
C	-0. 494485000	-3. 191966000	-1. 067402000
C	-0. 805556000	-3. 495037000	-2. 400898000
C	-1. 549139000	-3. 179824000	-0. 125564000
C	-2. 113579000	-3. 801022000	-2. 775775000
H	-0. 006991000	-3. 544869000	-3. 135909000
C	-2. 863384000	-3. 496047000	-0. 506088000
H	-1. 302658000	-3. 068130000	0. 932906000
C	-3. 144718000	-3. 805225000	-1. 834880000
H	-2. 325745000	-4. 060230000	-3. 809654000
H	-3. 652541000	-3. 521792000	0. 239906000
H	-4. 157912000	-4. 055587000	-2. 133145000
Si	-2. 929792000	3. 070226000	-1. 388732000
C	-1. 932794000	4. 674359000	-1. 423114000
H	-1. 421334000	4. 856717000	-0. 471225000
H	-1. 169500000	4. 647828000	-2. 209520000
H	-2. 587303000	5. 531788000	-1. 622606000
C	-3. 695946000	2. 793135000	-3. 087899000
H	-2. 929227000	2. 658448000	-3. 860124000
H	-4. 366014000	1. 928757000	-3. 111281000
H	-4. 285300000	3. 674504000	-3. 369137000
C	-4. 251618000	3. 195689000	-0. 047556000

H	-4.881768000	4.076573000	-0.221200000
H	-4.903406000	2.316157000	-0.031980000
H	-3.804619000	3.309221000	0.947814000
C	-4.695704000	-0.525722000	-1.953649000
C	-4.911644000	-0.553124000	0.428550000
C	-6.313249000	-0.605781000	0.320531000
C	-6.901815000	-0.626155000	-0.938166000
C	-6.088909000	-0.591640000	-2.074254000
H	-4.102347000	-0.496759000	-2.866207000
H	-6.933319000	-0.632867000	1.215118000
H	-7.982596000	-0.667891000	-1.037581000
H	-6.546663000	-0.610232000	-3.060837000
C	-4.315575000	-0.564935000	1.751236000
H	-5.000975000	-0.574466000	2.605056000
C	-2.532317000	-0.600453000	3.364425000
C	-2.921180000	0.706783000	4.068484000
H	-2.503809000	0.726868000	5.080594000
H	-2.534945000	1.574068000	3.522276000
H	-4.007835000	0.813920000	4.155900000
C	-3.099072000	-1.814601000	4.114117000
H	-2.853045000	-2.748193000	3.595198000
H	-2.666788000	-1.863533000	5.118754000
H	-4.186600000	-1.763379000	4.231018000
C	-1.009562000	-0.711721000	3.298801000
H	-0.693252000	-1.633000000	2.791734000
H	-0.576229000	0.147985000	2.777618000
H	-0.580602000	-0.737360000	4.305561000

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TS9, E(SCRF) = -2634.247009 a.u., IF = $i247.85 \text{ cm}^{-1}$

Sc	-1.993880000	-0.421159000	0.591225000
C	-3.462422000	-1.922410000	-0.364601000
C	-1.053663000	-2.500732000	1.393022000
C	-2.417311000	-2.794354000	1.308213000
C	-0.436189000	-1.535411000	2.258042000
C	-1.062987000	-0.603628000	3.035884000
C	-1.868290000	1.021538000	-1.335024000
C	-1.105860000	-0.138482000	-1.668983000
H	-1.360709000	-0.844569000	-2.451819000
C	0.082215000	-0.199479000	-0.893909000
C	1.147192000	1.390782000	0.915673000
H	1.425072000	0.616412000	1.635420000
H	0.786022000	2.251556000	1.482967000
C	2.361209000	1.751531000	0.085494000
C	3.243611000	0.738752000	-0.258615000

C	4. 327788000	0. 990984000	-1. 161847000
C	4. 479902000	2. 305306000	-1. 700875000
C	3. 573255000	3. 318029000	-1. 309395000
H	3. 716640000	4. 324774000	-1. 695748000
C	2. 535333000	3. 073788000	-0. 434644000
C	5. 250657000	-0. 011983000	-1. 561012000
H	5. 148544000	-1. 016682000	-1. 163094000
C	6. 268214000	0. 275080000	-2. 442340000
H	6. 964613000	-0. 506339000	-2. 734718000
C	6. 418587000	1. 577453000	-2. 969372000
H	7. 228242000	1. 790161000	-3. 662046000
C	5. 541180000	2. 570529000	-2. 604040000
H	5. 647844000	3. 576756000	-3. 002716000
C	1. 231068000	-1. 115790000	-1. 286655000
H	0. 791245000	-1. 986742000	-1. 777254000
H	1. 778664000	-0. 575066000	-2. 073743000
C	3. 109543000	-0. 638760000	0. 316719000
C	2. 232501000	-1. 567577000	-0. 237831000
C	3. 961531000	-0. 995013000	1. 412471000
C	3. 944283000	-2. 338654000	1. 895252000
C	3. 146030000	-3. 289444000	1. 220996000
H	3. 231715000	-4. 334579000	1. 509621000
C	2. 320480000	-2. 947208000	0. 165718000
C	4. 768319000	-2. 699033000	2. 992855000
H	4. 751720000	-3. 728224000	3. 344149000
C	5. 577085000	-1. 766549000	3. 597577000
H	6. 205360000	-2. 050066000	4. 437523000
C	5. 598442000	-0. 435401000	3. 122057000
H	6. 243399000	0. 295669000	3. 602156000
C	4. 815431000	-0. 058797000	2. 054637000
H	4. 841747000	0. 965255000	1. 696047000
C	1. 642919000	4. 204726000	-0. 055533000
C	1. 555921000	4. 650923000	1. 272067000
C	0. 915486000	4. 890486000	-1. 038247000
C	0. 753525000	5. 739603000	1. 608510000
H	2. 149110000	4. 159429000	2. 040247000
C	0. 113669000	5. 981248000	-0. 703002000
H	0. 980886000	4. 560333000	-2. 071905000
C	0. 025909000	6. 406292000	0. 622121000
H	0. 712760000	6. 080800000	2. 639969000
H	-0. 436823000	6. 504614000	-1. 480828000
H	-0. 592214000	7. 261389000	0. 882734000
C	1. 657569000	-4. 064620000	-0. 566879000
C	1. 789148000	-4. 197493000	-1. 959588000

C	0.981010000	-5.080569000	0.128304000
C	1.238305000	-5.285831000	-2.632408000
H	2.363301000	-3.460477000	-2.515405000
C	0.429767000	-6.170768000	-0.543697000
H	0.892179000	-5.017296000	1.210697000
C	0.549426000	-6.273954000	-1.928709000
H	1.366165000	-5.371848000	-3.708368000
H	-0.085194000	-6.945243000	0.019161000
H	0.126682000	-7.126364000	-2.453523000
Si	-3.182727000	1.793909000	-2.458060000
C	-2.326799000	3.211934000	-3.363801000
H	-1.957516000	3.968321000	-2.661817000
H	-1.469763000	2.849740000	-3.943240000
H	-3.016888000	3.705726000	-4.058849000
C	-3.775518000	0.505349000	-3.699109000
H	-2.952643000	0.141666000	-4.325466000
H	-4.239029000	-0.359824000	-3.212945000
H	-4.521060000	0.948803000	-4.370401000
C	-4.656607000	2.494826000	-1.505807000
H	-4.344182000	3.184689000	-0.713153000
H	-5.301427000	3.059729000	-2.190262000
H	-5.267768000	1.704573000	-1.057214000
C	-3.280174000	-2.813635000	-1.429271000
C	-4.774944000	-1.445022000	-0.134928000
C	-5.851683000	-1.865389000	-0.935142000
C	-5.637197000	-2.749168000	-1.987113000
C	-4.343325000	-3.211834000	-2.241642000
H	-2.292758000	-3.234070000	-1.616415000
H	-6.852534000	-1.485028000	-0.738983000
H	-6.469001000	-3.078127000	-2.602898000
H	-4.167265000	-3.902695000	-3.062304000
C	-5.030784000	-0.443461000	0.889085000
H	-6.081235000	-0.213360000	1.083997000
C	-4.490881000	1.200957000	2.550413000
C	-4.578218000	0.505716000	3.919358000
H	-4.897905000	1.227805000	4.678223000
H	-5.312173000	-0.307537000	3.897723000
H	-3.618824000	0.094660000	4.245796000
C	-3.404477000	2.278657000	2.558513000
H	-3.408136000	2.845093000	1.622151000
H	-3.572376000	2.982427000	3.380306000
H	-2.408049000	1.843965000	2.692276000
C	-5.842087000	1.871990000	2.258363000
H	-5.886269000	2.263350000	1.236905000

H	-6.696960000	1.206938000	2.422120000
H	-5.969044000	2.715241000	2.944500000
N	-4.097110000	0.183468000	1.521708000
H	-0.385527000	-3.058810000	0.745971000
C	0.050288000	0.921978000	-0.007110000
H	-3.109686000	-2.431897000	2.070563000
H	-2.710086000	-3.740323000	0.871612000
C	-1.131460000	1.655339000	-0.288768000
H	0.651499000	-1.511493000	2.211789000
H	-1.392105000	2.589658000	0.198406000
H	-2.150073000	-0.658648000	3.147176000
C	-0.351108000	0.303515000	3.994199000
H	-0.624411000	1.357323000	3.868233000
H	-0.607346000	0.033282000	5.027543000
H	0.734139000	0.219344000	3.890408000

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TS9-1, E(SCRF) = -2634.251128 a.u., IF = $i275.00 \text{ cm}^{-1}$

Sc	-2.047064000	-0.181063000	0.525186000
C	-3.083138000	-2.002286000	-0.481318000
C	-1.312631000	-1.830550000	1.928520000
C	-2.280375000	-2.623056000	1.273493000
C	-0.898077000	1.846916000	-0.136138000
H	-1.056200000	2.765367000	0.420957000
C	-1.680346000	1.394451000	-1.241637000
C	-1.055393000	0.177098000	-1.660824000
H	-1.369760000	-0.428195000	-2.504267000
C	0.102160000	-0.083093000	-0.878572000
C	1.351329000	1.249768000	1.007980000
H	1.579269000	0.401478000	1.659879000
H	1.096525000	2.100683000	1.644058000
C	2.569003000	1.541090000	0.153046000
C	3.346198000	0.469170000	-0.261251000
C	4.419827000	0.660539000	-1.189621000
C	4.674701000	1.977484000	-1.681128000
C	3.875059000	3.049564000	-1.220119000
H	4.097262000	4.054811000	-1.571566000
C	2.845154000	2.862884000	-0.321454000
C	5.233394000	-0.404754000	-1.658318000
H	5.050025000	-1.411366000	-1.295443000
C	6.245940000	-0.174264000	-2.561689000
H	6.858648000	-1.002263000	-2.908198000
C	6.499135000	1.130542000	-3.041738000
H	7.303738000	1.298017000	-3.752489000
C	5.728279000	2.183123000	-2.608545000

H	5.915331000	3.191259000	-2.971172000
C	1.135395000	-1.117839000	-1.290637000
H	0.603559000	-1.921501000	-1.804329000
H	1.750221000	-0.629114000	-2.061536000
C	3.089248000	-0.904521000	0.276761000
C	2.071512000	-1.699394000	-0.244133000
C	3.932063000	-1.380070000	1.333161000
C	3.742555000	-2.706158000	1.825507000
C	2.766147000	-3.521605000	1.213559000
H	2.692259000	-4.561307000	1.524223000
C	1.952313000	-3.064120000	0.193300000
C	4.561653000	-3.186939000	2.879740000
H	4.410883000	-4.202613000	3.238269000
C	5.529829000	-2.385229000	3.435243000
H	6.153684000	-2.759816000	4.242151000
C	5.718657000	-1.069513000	2.953788000
H	6.486761000	-0.441203000	3.396695000
C	4.942887000	-0.578707000	1.928478000
H	5.098455000	0.432664000	1.567184000
C	2.066540000	4.050890000	0.126699000
C	2.044575000	4.443605000	1.473704000
C	1.384666000	4.841538000	-0.808925000
C	1.347991000	5.582139000	1.874511000
H	2.606980000	3.868855000	2.206390000
C	0.689150000	5.982488000	-0.409467000
H	1.403035000	4.553940000	-1.857270000
C	0.663813000	6.353520000	0.934536000
H	1.356678000	5.879036000	2.920310000
H	0.173760000	6.587151000	-1.151584000
H	0.128411000	7.246619000	1.245693000
C	1.065928000	-4.072454000	-0.454413000
C	1.118774000	-4.312045000	-1.837955000
C	0.250549000	-4.908149000	0.326271000
C	0.366224000	-5.331435000	-2.419762000
H	1.790836000	-3.723925000	-2.457828000
C	-0.500888000	-5.930189000	-0.253832000
H	0.218324000	-4.759411000	1.403414000
C	-0.450898000	-6.142063000	-1.631347000
H	0.440473000	-5.508448000	-3.489748000
H	-1.116472000	-6.569396000	0.374214000
H	-1.026652000	-6.945181000	-2.083290000
Si	-2.872397000	2.418315000	-2.296502000
C	-1.929832000	2.865102000	-3.870107000
H	-1.015181000	3.422592000	-3.638754000

H	-1.638426000	1.970125000	-4.432060000
H	-2.544671000	3.487793000	-4.531471000
C	-4.415928000	1.439983000	-2.775899000
H	-5.068694000	1.242212000	-1.918699000
H	-5.002298000	2.002150000	-3.513089000
H	-4.157875000	0.475854000	-3.229285000
C	-3.342547000	4.004080000	-1.386909000
H	-3.971740000	3.829825000	-0.507178000
H	-2.454089000	4.557892000	-1.061865000
H	-3.906335000	4.660806000	-2.060818000
C	-2.623871000	-2.860236000	-1.490908000
C	-4.459244000	-1.649417000	-0.517891000
C	-5.320662000	-2.171691000	-1.497531000
C	-4.827653000	-3.015387000	-2.486045000
C	-3.470204000	-3.344607000	-2.488551000
H	-1.587314000	-3.191775000	-1.483680000
H	-6.372600000	-1.892780000	-1.494553000
H	-5.493376000	-3.416799000	-3.244368000
H	-3.072563000	-4.006114000	-3.253617000
C	-5.003632000	-0.655587000	0.393787000
H	-6.094157000	-0.579327000	0.437766000
C	-4.925305000	1.151418000	1.975379000
C	-5.434246000	0.440302000	3.237583000
H	-5.907098000	1.164921000	3.908858000
H	-6.179704000	-0.323671000	2.989335000
H	-4.619569000	-0.042579000	3.785978000
C	-3.863853000	2.190756000	2.338453000
H	-3.523536000	2.732311000	1.449598000
H	-4.270384000	2.924833000	3.041599000
H	-2.995786000	1.721211000	2.812445000
C	-6.094451000	1.855238000	1.270128000
H	-5.782031000	2.277052000	0.309297000
H	-6.951384000	1.195197000	1.099595000
H	-6.450416000	2.677386000	1.899147000
N	-4.263589000	0.143336000	1.086089000
H	-0.259940000	-1.970210000	1.680941000
C	0.189453000	0.959516000	0.089827000
H	-1.928603000	-3.529473000	0.794777000
H	-3.255104000	-2.725749000	1.751064000
C	-1.663199000	-0.896414000	2.977909000
H	-2.673600000	-0.983104000	3.384903000
C	-0.847608000	0.061734000	3.493223000
C	-1.177983000	0.939800000	4.654872000
H	-2.212702000	0.816780000	4.990271000

H	-0.522078000	0.699388000	5.502971000
H	-1.006245000	1.999355000	4.425592000
H	0.169700000	0.132520000	3.113335000

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TS9-2, E(SCRF) = -2634.236997 a.u., IF = $i295.01 \text{ cm}^{-1}$

Sc	-1.904835000	0.263633000	0.062638000
C	-3.582871000	-1.141468000	-0.504495000
C	-2.501830000	-2.117266000	0.981930000
C	-1.372177000	-1.394404000	1.465354000
C	-0.437422000	2.134639000	-0.339159000
H	-0.503318000	3.029198000	0.272663000
C	-1.165203000	1.892210000	-1.544022000
C	-0.690393000	0.626776000	-2.012746000
H	-1.003016000	0.140485000	-2.932679000
C	0.324856000	0.128085000	-1.153149000
C	1.486104000	1.030875000	1.025349000
H	1.403746000	0.113662000	1.618048000
H	1.301380000	1.872078000	1.698088000
C	2.870583000	1.118695000	0.413920000
C	3.484880000	-0.050911000	-0.009788000
C	4.721605000	-0.005726000	-0.732870000
C	5.311236000	1.266115000	-1.007108000
C	4.668398000	2.435905000	-0.539097000
H	5.140140000	3.399159000	-0.720736000
C	3.480514000	2.388990000	0.160054000
C	5.380303000	-1.170602000	-1.208357000
H	4.943608000	-2.144761000	-1.012052000
C	6.559843000	-1.077460000	-1.911586000
H	7.048715000	-1.980842000	-2.266544000
C	7.143635000	0.182095000	-2.175039000
H	8.076641000	0.240212000	-2.728888000
C	6.529892000	1.328945000	-1.730467000
H	6.970177000	2.303719000	-1.927479000
C	1.221866000	-1.027544000	-1.556149000
H	0.654226000	-1.643180000	-2.256372000
H	2.035347000	-0.577580000	-2.144997000
C	2.883130000	-1.388368000	0.293971000
C	1.846281000	-1.900513000	-0.481387000
C	3.434005000	-2.142353000	1.380337000
C	2.937399000	-3.456398000	1.632380000
C	1.951172000	-3.984508000	0.771195000
H	1.641989000	-5.017833000	0.911286000
C	1.410890000	-3.255130000	-0.271901000
C	3.469043000	-4.212253000	2.709224000

H	3.086629000	-5.215423000	2.883466000
C	4.450765000	-3.687839000	3.515381000
H	4.853227000	-4.272279000	4.338262000
C	4.942503000	-2.384875000	3.272472000
H	5.719180000	-1.976287000	3.913382000
C	4.450421000	-1.631586000	2.231219000
H	4.836699000	-0.633035000	2.054141000
C	2.885166000	3.669615000	0.634516000
C	2.728796000	3.937084000	2.003135000
C	2.526328000	4.665108000	-0.284932000
C	2.215801000	5.157753000	2.437845000
H	3.042739000	3.192526000	2.731542000
C	2.014698000	5.887733000	0.149116000
H	2.651207000	4.473045000	-1.347792000
C	1.853283000	6.136347000	1.511630000
H	2.118285000	5.352652000	3.502984000
H	1.748951000	6.650135000	-0.578909000
H	1.462330000	7.092059000	1.850710000
C	0.451792000	-3.966759000	-1.164061000
C	0.647119000	-4.036881000	-2.553577000
C	-0.617053000	-4.693934000	-0.614812000
C	-0.214161000	-4.774012000	-3.364094000
H	1.507475000	-3.544360000	-2.999515000
C	-1.477421000	-5.436775000	-1.423721000
H	-0.759953000	-4.689039000	0.463513000
C	-1.285187000	-5.471361000	-2.804497000
H	-0.032287000	-4.822803000	-4.434600000
H	-2.290279000	-5.999582000	-0.971240000
H	-1.948098000	-6.056328000	-3.436404000
Si	-2.244023000	3.103652000	-2.521557000
C	-1.726070000	2.977242000	-4.330606000
H	-0.659795000	3.197417000	-4.455089000
H	-1.909400000	1.976699000	-4.740066000
H	-2.289262000	3.690332000	-4.944679000
C	-4.086526000	2.693698000	-2.382456000
H	-4.453097000	2.798924000	-1.354492000
H	-4.672486000	3.377759000	-3.009019000
H	-4.304630000	1.673408000	-2.719471000
C	-1.930900000	4.844511000	-1.867450000
H	-2.286827000	4.978960000	-0.839519000
H	-0.863551000	5.091231000	-1.885068000
H	-2.453658000	5.580853000	-2.489868000
C	-3.668992000	-1.958551000	-1.639998000
C	-4.720528000	-0.351089000	-0.178765000

C	-5.898880000	-0.437730000	-0.934136000
C	-5.946763000	-1.253998000	-2.061274000
C	-4.823931000	-1.998793000	-2.425678000
H	-2.833275000	-2.604608000	-1.905394000
H	-6.770067000	0.149615000	-0.650758000
H	-6.857004000	-1.312071000	-2.651043000
H	-4.857271000	-2.634930000	-3.306289000
C	-4.678978000	0.606518000	0.927626000
H	-5.638741000	0.914259000	1.350924000
C	-3.558616000	2.095297000	2.473811000
C	-4.769954000	1.972913000	3.404805000
H	-4.621384000	2.628003000	4.268761000
H	-5.705987000	2.287281000	2.930458000
H	-4.888190000	0.948868000	3.776611000
C	-2.274111000	1.850606000	3.273313000
H	-1.386871000	1.904917000	2.629832000
H	-2.162427000	2.614391000	4.049574000
H	-2.292081000	0.871590000	3.763135000
C	-3.523319000	3.492702000	1.839120000
H	-2.661155000	3.604458000	1.174889000
H	-4.433127000	3.684144000	1.259732000
H	-3.450254000	4.255310000	2.621549000
N	-3.572289000	1.100185000	1.363737000
H	-2.261957000	-2.874087000	0.236300000
C	0.461190000	1.060625000	-0.082475000
H	-0.389327000	-1.762167000	1.172470000
H	-1.421533000	-0.968940000	2.468691000
C	-3.660134000	-2.487742000	1.828159000
H	-4.515358000	-2.917865000	1.308246000
C	-3.679459000	-2.431869000	3.168459000
C	-4.808748000	-2.912353000	4.021829000
H	-5.647671000	-3.281731000	3.423878000
H	-4.476115000	-3.722324000	4.683859000
H	-5.177355000	-2.112104000	4.677196000
H	-2.805232000	-2.052075000	3.697228000

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TS9-3, E(SCRF) = -2634.238631 a.u., IF = *i*306.06 cm⁻¹

Sc	-1.844505000	0.458564000	0.203874000
C	-3.570216000	-0.826554000	-0.486415000
C	-2.634411000	-1.912029000	1.004648000
C	-1.454695000	-1.290318000	1.530760000
C	-0.266088000	2.203187000	-0.279030000
H	-0.263957000	3.103328000	0.327148000
C	-1.046325000	1.989660000	-1.456449000

C	-0.666242000	0.691528000	-1.921468000
H	-1.046037000	0.211807000	-2.818703000
C	0.339614000	0.139980000	-1.083816000
C	1.613591000	0.993090000	1.052202000
H	1.489317000	0.087402000	1.655274000
H	1.498277000	1.850091000	1.720434000
C	2.983908000	0.988945000	0.404324000
C	3.513434000	-0.220706000	-0.020843000
C	4.731335000	-0.259340000	-0.775533000
C	5.390516000	0.970864000	-1.079917000
C	4.832199000	2.183230000	-0.611531000
H	5.356022000	3.113867000	-0.818685000
C	3.662135000	2.216762000	0.117625000
C	5.305151000	-1.467566000	-1.252883000
H	4.814784000	-2.410869000	-1.033766000
C	6.470017000	-1.454762000	-1.986001000
H	6.893573000	-2.390285000	-2.341675000
C	7.122976000	-0.236410000	-2.279185000
H	8.043504000	-0.241729000	-2.856452000
C	6.591964000	0.950746000	-1.833871000
H	7.085907000	1.894422000	-2.053768000
C	1.150086000	-1.075816000	-1.493874000
H	0.524018000	-1.664783000	-2.166877000
H	1.971612000	-0.686398000	-2.113984000
C	2.839039000	-1.514974000	0.315726000
C	1.752159000	-1.971767000	-0.425052000
C	3.371666000	-2.288056000	1.397874000
C	2.802520000	-3.565716000	1.681497000
C	1.765106000	-4.043915000	0.852020000
H	1.399222000	-5.055449000	1.012939000
C	1.243707000	-3.296032000	-0.187580000
C	3.314690000	-4.338869000	2.755452000
H	2.876014000	-5.314095000	2.954030000
C	4.347426000	-3.865584000	3.528813000
H	4.734463000	-4.462840000	4.349880000
C	4.911688000	-2.598789000	3.254369000
H	5.728456000	-2.230543000	3.869364000
C	4.439602000	-1.830139000	2.215073000
H	4.881589000	-0.859663000	2.013921000
C	3.153989000	3.536455000	0.586817000
C	3.055296000	3.834686000	1.954387000
C	2.819145000	4.533840000	-0.339540000
C	2.621285000	5.088051000	2.382018000
H	3.351305000	3.086352000	2.686417000

C	2.385768000	5.788830000	0.087373000
H	2.899455000	4.317443000	-1.401943000
C	2.281118000	6.068647000	1.449413000
H	2.567659000	5.305687000	3.445855000
H	2.137403000	6.551768000	-0.646298000
H	1.951931000	7.049346000	1.782794000
C	0.228790000	-3.963564000	-1.051630000
C	0.393312000	-4.059558000	-2.443621000
C	-0.865901000	-4.627066000	-0.473624000
C	-0.519857000	-4.760623000	-3.229001000
H	1.269039000	-3.616923000	-2.911388000
C	-1.777328000	-5.334998000	-1.257417000
H	-0.989949000	-4.598340000	0.606637000
C	-1.613661000	-5.396316000	-2.640922000
H	-0.361176000	-4.830923000	-4.302008000
H	-2.607898000	-5.852618000	-0.783378000
H	-2.317112000	-5.954664000	-3.252762000
Si	-2.066378000	3.264604000	-2.406718000
C	-0.866949000	4.382953000	-3.338474000
H	-0.186690000	4.896046000	-2.649183000
H	-0.254691000	3.807116000	-4.041939000
H	-1.405547000	5.147830000	-3.911076000
C	-3.200316000	2.374744000	-3.624508000
H	-3.906474000	1.702108000	-3.123844000
H	-3.786006000	3.103308000	-4.198171000
H	-2.626701000	1.781972000	-4.346812000
C	-3.086490000	4.310204000	-1.205200000
H	-3.829886000	3.710373000	-0.666733000
H	-2.450012000	4.810379000	-0.465223000
H	-3.628267000	5.094810000	-1.747209000
C	-3.660354000	-1.608412000	-1.645267000
C	-4.638738000	0.077612000	-0.222221000
C	-5.763615000	0.126530000	-1.061763000
C	-5.822194000	-0.669296000	-2.201356000
C	-4.759051000	-1.522755000	-2.502991000
H	-2.873264000	-2.325255000	-1.874080000
H	-6.586443000	0.798365000	-0.824680000
H	-6.691202000	-0.625390000	-2.851319000
H	-4.795837000	-2.139355000	-3.397310000
C	-4.597702000	0.997223000	0.914693000
H	-5.550845000	1.435017000	1.224511000
C	-3.503294000	2.183275000	2.721693000
C	-3.623753000	1.269260000	3.950990000
H	-3.584854000	1.871827000	4.864563000

H	-4.574035000	0.723954000	3.944623000
H	-2.805006000	0.543666000	3.991840000
C	-2.159923000	2.915507000	2.751815000
H	-2.059326000	3.593834000	1.898824000
H	-2.073974000	3.509746000	3.667088000
H	-1.319749000	2.208998000	2.741693000
C	-4.645084000	3.206752000	2.717582000
H	-4.646560000	3.802870000	1.798295000
H	-5.631122000	2.746716000	2.844120000
H	-4.510082000	3.892824000	3.559369000
N	-3.499238000	1.305732000	1.514809000
H	-2.455420000	-2.697615000	0.273985000
C	0.567294000	1.077378000	-0.032378000
H	-0.499317000	-1.718721000	1.228309000
H	-1.492196000	-0.958351000	2.570721000
C	-3.786843000	-2.165098000	1.888209000
H	-3.900974000	-1.502449000	2.745415000
C	-4.611523000	-3.212749000	1.742039000
C	-5.711776000	-3.580480000	2.682013000
H	-5.792707000	-2.875281000	3.515191000
H	-6.677162000	-3.613122000	2.159882000
H	-5.551058000	-4.583472000	3.098282000
H	-4.472625000	-3.868646000	0.880488000

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P, E(SCRF) = -2634.287811 a.u.

Sc	-1.917500000	-0.273034000	0.583780000
C	-4.997509000	0.177585000	1.328355000
C	-2.370617000	-2.492507000	0.184389000
N	-3.790744000	0.369754000	1.741815000
C	-1.209949000	-2.528142000	0.996152000
C	-1.090301000	-1.935025000	2.244836000
C	-3.766723000	-2.614432000	0.790372000
C	-0.999467000	-0.069648000	-1.685801000
H	-1.277156000	-0.763297000	-2.473047000
C	0.192547000	-0.170016000	-0.921526000
C	1.291351000	1.304814000	0.955803000
H	1.528995000	0.475543000	1.629579000
H	0.953076000	2.143020000	1.569831000
C	2.521652000	1.678400000	0.155280000
C	3.379171000	0.666607000	-0.248711000
C	4.461326000	0.945886000	-1.147346000
C	4.639318000	2.284231000	-1.614591000
C	3.759662000	3.294153000	-1.159195000
H	3.923613000	4.317609000	-1.489471000

C	2. 722392000	3. 023560000	-0. 292022000
C	5. 356913000	-0. 053804000	-1. 611579000
H	5. 234890000	-1. 076547000	-1. 269389000
C	6. 372536000	0. 258643000	-2. 486495000
H	7. 047232000	-0. 521189000	-2. 829574000
C	6. 548957000	1. 584611000	-2. 941498000
H	7. 357072000	1. 817137000	-3. 629596000
C	5. 698392000	2. 575450000	-2. 512224000
H	5. 824903000	3. 599763000	-2. 855187000
C	1. 309705000	-1. 114319000	-1. 334818000
H	0. 839816000	-1. 962957000	-1. 837319000
H	1. 859494000	-0. 573082000	-2. 120710000
C	3. 227056000	-0. 735419000	0. 258472000
C	2. 318912000	-1. 620066000	-0. 317923000
C	4. 103839000	-1. 162891000	1. 308419000
C	4. 082771000	-2. 531008000	1. 716007000
C	3. 245957000	-3. 431141000	1. 020260000
H	3. 315936000	-4. 491191000	1. 253427000
C	2. 391022000	-3. 018694000	0. 015213000
C	4. 936344000	-2. 963432000	2. 763942000
H	4. 915056000	-4. 010473000	3. 057476000
C	5. 777372000	-2. 077299000	3. 393333000
H	6. 427871000	-2. 415685000	4. 195213000
C	5. 801627000	-0. 721533000	2. 993512000
H	6. 470613000	-0. 026408000	3. 493728000
C	4. 990491000	-0. 275448000	1. 975268000
H	5. 019227000	0. 767465000	1. 676429000
C	1. 856280000	4. 149224000	0. 157750000
C	1. 794764000	4. 525088000	1. 508542000
C	1. 125195000	4. 896585000	-0. 775976000
C	1. 014471000	5. 606200000	1. 914145000
H	2. 389659000	3. 982956000	2. 240481000
C	0. 344225000	5. 979008000	-0. 371426000
H	1. 171460000	4. 621247000	-1. 826666000
C	0. 282667000	6. 334774000	0. 975427000
H	0. 994541000	5. 893210000	2. 962618000
H	-0. 210558000	6. 549741000	-1. 111951000
H	-0. 317783000	7. 184308000	1. 290137000
C	1. 670252000	-4. 085022000	-0. 738707000
C	1. 788340000	-4. 191694000	-2. 134551000
C	0. 947097000	-5. 078695000	-0. 060506000
C	1. 183918000	-5. 238280000	-2. 827047000
H	2. 391025000	-3. 467575000	-2. 677403000
C	0. 342158000	-6. 126897000	-0. 752309000

H	0.860486000	-5.027764000	1.022523000
C	0.453235000	-6.207446000	-2.139453000
H	1.300474000	-5.306653000	-3.905548000
H	-0.210972000	-6.885075000	-0.203780000
H	-0.012459000	-7.027207000	-2.679773000
Si	-3.029907000	1.940686000	-2.423744000
C	-2.120852000	3.066849000	-3.651746000
H	-1.037211000	3.041623000	-3.496184000
H	-2.313313000	2.757596000	-4.685591000
H	-2.446745000	4.108804000	-3.553772000
C	-3.978995000	0.612177000	-3.367249000
H	-4.726444000	1.075828000	-4.022729000
H	-3.307660000	0.028603000	-4.008725000
H	-4.504044000	-0.085048000	-2.705792000
C	-4.196871000	2.993055000	-1.373743000
H	-4.787255000	2.393460000	-0.672528000
H	-3.645171000	3.747434000	-0.799411000
H	-4.900309000	3.532406000	-2.019951000
C	-5.430873000	-2.723217000	-1.075051000
C	-5.439721000	-0.716568000	0.259707000
C	-6.574892000	-0.280238000	-0.454556000
C	-7.098513000	-1.027115000	-1.498573000
C	-6.514180000	-2.254563000	-1.814337000
H	-5.022391000	-3.707418000	-1.292237000
H	-7.036433000	0.667669000	-0.186804000
H	-7.962419000	-0.667706000	-2.049136000
H	-6.922647000	-2.862739000	-2.616617000
C	-4.869794000	-1.980981000	-0.030785000
H	-5.808833000	0.742558000	1.799427000
C	-3.598893000	1.250568000	2.948484000
C	-4.174278000	0.528112000	4.174383000
H	-3.997913000	1.123251000	5.076387000
H	-5.255098000	0.375839000	4.080575000
H	-3.702545000	-0.450497000	4.317062000
C	-2.090621000	1.441760000	3.123835000
H	-1.658963000	2.017025000	2.296820000
H	-1.874825000	1.997628000	4.041656000
H	-1.567985000	0.479116000	3.216279000
C	-4.259909000	2.621815000	2.760905000
H	-3.903937000	3.109494000	1.847662000
H	-5.352343000	2.562851000	2.719092000
H	-4.007935000	3.264775000	3.610407000
C	-1.721448000	1.113545000	-1.336822000
H	-2.273170000	-2.923708000	-0.809814000

C	0.195757000	0.928318000	-0.011613000
H	-3.793564000	-2.213706000	1.809251000
H	-4.004433000	-3.684115000	0.896107000
C	-0.956816000	1.715691000	-0.287931000
H	-0.281903000	-2.800709000	0.496089000
H	-1.175731000	2.666365000	0.188815000
H	-2.004514000	-1.787809000	2.830599000
C	0.187505000	-1.902472000	3.039257000
H	1.061163000	-2.047426000	2.397573000
H	0.318719000	-0.957028000	3.580621000
H	0.197017000	-2.697642000	3.797535000

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P', E(SCRF) = -2634.290628 a.u.

Sc	-1.868930000	0.242191000	0.848862000
C	-4.236657000	-2.157419000	-0.478074000
C	-2.217877000	-2.024341000	1.072582000
C	-3.576725000	-2.623662000	0.804573000
C	-0.540039000	2.125420000	0.091676000
H	-0.504583000	3.050388000	0.659980000
C	-1.475746000	1.819911000	-0.944243000
C	-1.072974000	0.533830000	-1.427679000
H	-1.550116000	-0.011998000	-2.237770000
C	0.096557000	0.088992000	-0.752882000
C	1.657778000	1.188229000	1.075876000
H	1.771429000	0.329715000	1.744532000
H	1.573925000	2.078709000	1.703407000
C	2.863749000	1.272359000	0.163046000
C	3.415729000	0.087246000	-0.298790000
C	4.463683000	0.101193000	-1.275434000
C	4.926512000	1.360442000	-1.766560000
C	4.350411000	2.549266000	-1.260649000
H	4.729669000	3.505064000	-1.615635000
C	3.345838000	2.532322000	-0.315363000
C	5.054378000	-1.082917000	-1.790791000
H	4.712618000	-2.047456000	-1.428453000
C	6.051262000	-1.019638000	-2.737724000
H	6.492061000	-1.936933000	-3.118962000
C	6.510426000	0.227725000	-3.217548000
H	7.300178000	0.262387000	-3.963004000
C	5.958060000	1.392377000	-2.739882000
H	6.304791000	2.357671000	-3.101579000
C	0.920393000	-1.085662000	-1.255949000
H	0.233586000	-1.775359000	-1.752683000
H	1.560322000	-0.676075000	-2.052155000

C	2. 945621000	-1. 232677000	0. 230439000
C	1. 803345000	-1. 845624000	-0. 279081000
C	3. 731861000	-1. 865922000	1. 246797000
C	3. 354949000	-3. 164206000	1. 704303000
C	2. 261545000	-3. 808134000	1. 085141000
H	2. 049150000	-4. 840166000	1. 354529000
C	1. 502510000	-3. 199777000	0. 102653000
C	4. 114358000	-3. 796086000	2. 722786000
H	3. 820251000	-4. 789052000	3. 055096000
C	5. 203991000	-3. 167184000	3. 276157000
H	5. 780768000	-3. 657082000	4. 055897000
C	5. 580559000	-1. 880820000	2. 826824000
H	6. 444704000	-1. 390329000	3. 266805000
C	4. 866679000	-1. 246700000	1. 835683000
H	5. 166247000	-0. 259814000	1. 497884000
C	2. 806028000	3. 831393000	0. 174322000
C	2. 915388000	4. 207130000	1. 521978000
C	2. 224768000	4. 736715000	-0. 724623000
C	2. 442861000	5. 442999000	1. 959455000
H	3. 404166000	3. 536366000	2. 225237000
C	1. 753879000	5. 975036000	-0. 288545000
H	2. 144541000	4. 461970000	-1. 773571000
C	1. 856359000	6. 329981000	1. 056145000
H	2. 550781000	5. 721758000	3. 004667000
H	1. 314715000	6. 666947000	-1. 002987000
H	1. 496451000	7. 297606000	1. 395673000
C	0. 492478000	-4. 054184000	-0. 584973000
C	0. 508793000	-4. 215380000	-1. 980517000
C	-0. 410874000	-4. 831641000	0. 157463000
C	-0. 356272000	-5. 107627000	-2. 610446000
H	1. 238326000	-3. 669704000	-2. 573886000
C	-1. 271328000	-5. 731307000	-0. 470613000
H	-0. 430341000	-4. 731606000	1. 239881000
C	-1. 250453000	-5. 870290000	-1. 858652000
H	-0. 311317000	-5. 227039000	-3. 689888000
H	-1. 948119000	-6. 336173000	0. 128143000
H	-1. 909159000	-6. 582753000	-2. 348459000
Si	-2. 503149000	3. 124637000	-1. 851042000
C	-1. 580996000	3. 513298000	-3. 450975000
H	-0. 555694000	3. 841549000	-3. 246897000
H	-1. 523577000	2. 634441000	-4. 103775000
H	-2. 084679000	4. 310976000	-4. 010540000
C	-4. 243542000	2. 541017000	-2. 291572000
H	-4. 871597000	2. 392568000	-1. 406441000

H	-4.735779000	3.291624000	-2.922219000
H	-4.224145000	1.601123000	-2.854366000
C	-2.584858000	4.678266000	-0.779529000
H	-3.087068000	4.518059000	0.181974000
H	-1.583438000	5.072739000	-0.571817000
H	-3.140354000	5.463891000	-1.306102000
C	-4.206363000	-2.993217000	-1.598035000
C	-4.983351000	-0.958550000	-0.569858000
C	-5.743538000	-0.692651000	-1.723463000
C	-5.685213000	-1.532186000	-2.828344000
C	-4.896228000	-2.679949000	-2.768264000
H	-3.642175000	-3.920823000	-1.539345000
H	-6.367520000	0.197211000	-1.756288000
H	-6.261344000	-1.301870000	-3.719522000
H	-4.847040000	-3.353534000	-3.619436000
C	-5.086214000	0.043127000	0.497444000
H	-6.093775000	0.445732000	0.650558000
C	-4.430300000	1.481605000	2.308519000
C	-5.076441000	0.719231000	3.472623000
H	-5.249851000	1.395818000	4.316163000
H	-6.042197000	0.294844000	3.177270000
H	-4.435811000	-0.098683000	3.818633000
C	-3.076699000	2.054650000	2.742281000
H	-2.593626000	2.607606000	1.923497000
H	-3.186795000	2.762986000	3.569128000
H	-2.402290000	1.266496000	3.119133000
C	-5.340798000	2.623976000	1.843381000
H	-4.927788000	3.129792000	0.965067000
H	-6.353479000	2.283712000	1.604891000
H	-5.436368000	3.361909000	2.646495000
N	-4.119346000	0.507759000	1.209724000
H	-1.424709000	-2.313964000	0.376303000
C	0.417538000	1.086404000	0.222413000
H	-3.504153000	-3.718993000	0.756254000
H	-4.237157000	-2.398796000	1.652611000
C	-1.831927000	-1.633163000	2.368388000
H	-2.608187000	-1.635813000	3.141315000
C	-0.666967000	-0.924977000	2.647102000
C	-0.300427000	-0.430152000	4.021450000
H	-1.181036000	-0.348400000	4.670336000
H	0.402000000	-1.116224000	4.513316000
H	0.189883000	0.550496000	3.990948000
H	0.168865000	-1.067344000	1.955939000

TS10, E(SCRF) = -2634.243656 a.u., IF = *i*192.24 cm⁻¹

Sc	-1.876743000	0.372022000	0.554867000
C	-4.166352000	-0.283828000	1.270224000
C	-2.585888000	-1.801391000	0.430865000
N	-3.649517000	0.918598000	1.526055000
C	-1.501193000	-2.012281000	1.404003000
C	-1.620971000	-2.299609000	2.725955000
C	-3.794394000	-2.715583000	0.266159000
C	-0.993782000	0.605018000	-1.711372000
H	-1.435711000	0.067645000	-2.545950000
C	0.157303000	0.171612000	-1.001693000
C	1.570674000	1.184725000	0.976931000
H	1.576057000	0.288229000	1.607893000
H	1.453285000	2.048130000	1.636396000
C	2.873453000	1.262960000	0.207900000
C	3.450707000	0.084827000	-0.241014000
C	4.603026000	0.117966000	-1.093620000
C	5.142317000	1.386291000	-1.470179000
C	4.535930000	2.565620000	-0.977446000
H	4.970000000	3.526807000	-1.243807000
C	3.430849000	2.530936000	-0.153651000
C	5.224033000	-1.055085000	-1.598761000
H	4.825149000	-2.027201000	-1.326832000
C	6.321388000	-0.972882000	-2.425567000
H	6.782674000	-1.882424000	-2.800980000
C	6.856252000	0.283102000	-2.790008000
H	7.724555000	0.332440000	-3.441251000
C	6.276574000	1.437663000	-2.320490000
H	6.679458000	2.409832000	-2.594834000
C	1.030966000	-0.964858000	-1.502119000
H	0.399260000	-1.609220000	-2.117456000
H	1.746569000	-0.496714000	-2.195017000
C	2.902052000	-1.251175000	0.157832000
C	1.809940000	-1.804926000	-0.505495000
C	3.573672000	-1.975310000	1.195715000
C	3.143481000	-3.301541000	1.505466000
C	2.111698000	-3.878208000	0.731339000
H	1.863572000	-4.924730000	0.893636000
C	1.457591000	-3.179043000	-0.265888000
C	3.793706000	-4.024023000	2.539792000
H	3.463758000	-5.037330000	2.757440000
C	4.826462000	-3.457599000	3.248146000
H	5.320078000	-4.017840000	4.037519000
C	5.254246000	-2.144517000	2.945706000

H	6. 073178000	-1. 703987000	3. 507929000
C	4. 647630000	-1. 422522000	1. 943407000
H	4. 986028000	-0. 416320000	1. 717636000
C	2. 861523000	3. 818428000	0. 334779000
C	2. 860036000	4. 142396000	1. 700191000
C	2. 362838000	4. 760516000	-0. 575589000
C	2. 360014000	5. 365661000	2. 142800000
H	3. 283870000	3. 440849000	2. 415698000
C	1. 863532000	5. 985535000	-0. 133586000
H	2. 367444000	4. 525318000	-1. 637025000
C	1. 855835000	6. 289987000	1. 227123000
H	2. 382616000	5. 605644000	3. 202892000
H	1. 487035000	6. 706145000	-0. 855252000
H	1. 473983000	7. 247504000	1. 571234000
C	0. 491448000	-3. 938885000	-1. 110268000
C	0. 646115000	-4. 001640000	-2. 505222000
C	-0. 522061000	-4. 711789000	-0. 523923000
C	-0. 198421000	-4. 787333000	-3. 286191000
H	1. 461182000	-3. 459155000	-2. 978274000
C	-1. 363273000	-5. 504837000	-1. 304045000
H	-0. 645348000	-4. 694936000	0. 555928000
C	-1. 209956000	-5. 539577000	-2. 689278000
H	-0. 051081000	-4. 828400000	-4. 362201000
H	-2. 131817000	-6. 107120000	-0. 825489000
H	-1. 860951000	-6. 161533000	-3. 297639000
Si	-2. 619948000	3. 060663000	-2. 130610000
C	-1. 554534000	4. 223129000	-3. 167476000
H	-0. 867678000	4. 801444000	-2. 539000000
H	-0. 953016000	3. 668600000	-3. 896875000
H	-2. 180242000	4. 933509000	-3. 721515000
C	-3. 747125000	2. 050079000	-3. 253166000
H	-3. 172916000	1. 488751000	-3. 999907000
H	-4. 369035000	1. 339278000	-2. 697855000
H	-4. 421448000	2. 717639000	-3. 803484000
C	-3. 614812000	4. 062623000	-0. 880230000
H	-2. 959618000	4. 648003000	-0. 223299000
H	-4. 271333000	4. 773491000	-1. 396528000
H	-4. 241135000	3. 420516000	-0. 251892000
C	-5. 728144000	-2. 336162000	-1. 410833000
C	-4. 998969000	-0. 590583000	0. 086005000
C	-5. 929857000	0. 295242000	-0. 455632000
C	-6. 764692000	-0. 143143000	-1. 487446000
C	-6. 665674000	-1. 450440000	-1. 958139000
H	-5. 645781000	-3. 349302000	-1. 796991000

H	-6.012693000	1.304072000	-0.060839000
H	-7.492009000	0.537797000	-1.920283000
H	-7.312548000	-1.785088000	-2.764403000
C	-4.891455000	-1.908254000	-0.389950000
H	-4.330301000	-0.966837000	2.110051000
C	-3.394062000	1.399484000	2.915406000
C	-3.965773000	0.504794000	4.016005000
H	-3.807719000	0.985338000	4.986961000
H	-5.044565000	0.356964000	3.894281000
H	-3.479316000	-0.475997000	4.056791000
C	-1.872257000	1.535010000	3.092406000
H	-1.428910000	2.182111000	2.318327000
H	-1.617298000	2.008014000	4.046563000
H	-1.371530000	0.550623000	3.101953000
C	-4.038993000	2.790659000	2.997190000
H	-3.643060000	3.451374000	2.220292000
H	-5.122593000	2.716549000	2.861039000
H	-3.845739000	3.246039000	3.974953000
C	-1.423464000	1.888038000	-1.239300000
H	-2.156190000	-1.655713000	-0.580048000
C	0.421216000	1.160750000	-0.002343000
H	-4.131534000	-3.089986000	1.244828000
H	-3.538030000	-3.598193000	-0.332424000
C	-0.520381000	2.212207000	-0.185456000
H	-0.474899000	-1.933025000	1.022805000
H	-0.523093000	3.133932000	0.389511000
H	-2.616889000	-2.467394000	3.140841000
C	-0.478707000	-2.511998000	3.663157000
H	-0.564769000	-1.871875000	4.551615000
H	-0.477193000	-3.545440000	4.036093000
H	0.487833000	-2.326152000	3.185413000

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TS10', E(SCRF) = -2634.245288 a.u., IF = *i*159.08 cm⁻¹

C	-3.583050000	-0.851812000	1.818262000
C	-3.299247000	-3.083164000	-0.787363000
C	-5.184570000	-1.775046000	-0.051760000
C	-4.618412000	-3.174713000	-0.069419000
C	-2.166038000	-2.736239000	-0.130685000
C	-2.156221000	-2.415207000	1.293802000
C	-1.641672000	1.368452000	-1.481677000
C	-0.952521000	0.192097000	-1.910464000
H	-1.210053000	-0.402005000	-2.783394000
C	0.165558000	-0.063780000	-1.074988000
C	1.243624000	1.207866000	0.962942000

H	1. 406251000	0. 336599000	1. 606203000
H	0. 929253000	2. 034557000	1. 602049000
C	2. 531081000	1. 541549000	0. 236426000
C	3. 354932000	0. 499676000	-0. 161885000
C	4. 509815000	0. 749973000	-0. 972945000
C	4. 794878000	2. 094029000	-1. 364026000
C	3. 942246000	3. 133234000	-0. 923538000
H	4. 183146000	4. 157837000	-1. 198260000
C	2. 834972000	2. 889668000	-0. 138210000
C	5. 376432000	-0. 281392000	-1. 422508000
H	5. 172751000	-1. 308691000	-1. 137212000
C	6. 466943000	0. 006845000	-2. 211344000
H	7. 118865000	-0. 796366000	-2. 544334000
C	6. 749399000	1. 338286000	-2. 590969000
H	7. 615431000	1. 551155000	-3. 211642000
C	5. 928619000	2. 359233000	-2. 174323000
H	6. 136640000	3. 387670000	-2. 460345000
C	1. 261741000	-1. 035786000	-1. 485338000
H	0. 796456000	-1. 805249000	-2. 106032000
H	1. 914362000	-0. 464321000	-2. 162566000
C	3. 070835000	-0. 909680000	0. 256966000
C	2. 135937000	-1. 683984000	-0. 424818000
C	3. 825447000	-1. 454707000	1. 345842000
C	3. 646069000	-2. 827430000	1. 694271000
C	2. 777044000	-3. 616624000	0. 909410000
H	2. 726657000	-4. 685059000	1. 106855000
C	2. 043455000	-3. 091249000	-0. 138820000
C	4. 377504000	-3. 376242000	2. 779337000
H	4. 238162000	-4. 426081000	3. 027036000
C	5. 250045000	-2. 597046000	3. 500810000
H	5. 807000000	-3. 024045000	4. 330317000
C	5. 429242000	-1. 236600000	3. 160721000
H	6. 122207000	-0. 626955000	3. 734278000
C	4. 738848000	-0. 679180000	2. 108779000
H	4. 885705000	0. 365906000	1. 855796000
C	2. 001934000	4. 046451000	0. 294875000
C	1. 866686000	4. 381489000	1. 650708000
C	1. 382344000	4. 865171000	-0. 659639000
C	1. 121047000	5. 492547000	2. 040296000
H	2. 377441000	3. 783275000	2. 402190000
C	0. 636598000	5. 977671000	-0. 270864000
H	1. 489420000	4. 622146000	-1. 713976000
C	0. 499509000	6. 292195000	1. 080633000
H	1. 041231000	5. 745204000	3. 094611000

H	0.168860000	6.604122000	-1.026307000
H	-0.074970000	7.163376000	1.384136000
C	1.272194000	-4.057160000	-0.972599000
C	1.465188000	-4.135695000	-2.362334000
C	0.421042000	-4.998194000	-0.372140000
C	0.810905000	-5.101514000	-3.123806000
H	2.167294000	-3.459842000	-2.844369000
C	-0.230729000	-5.968236000	-1.132248000
H	0.273862000	-4.970588000	0.705220000
C	-0.043722000	-6.019398000	-2.512667000
H	0.987480000	-5.150748000	-4.195129000
H	-0.880085000	-6.689448000	-0.642444000
H	-0.545356000	-6.779035000	-3.106047000
Si	-2.841284000	2.376859000	-2.544601000
C	-1.789199000	3.293511000	-3.816121000
H	-1.065576000	3.956429000	-3.328520000
H	-1.228414000	2.596628000	-4.449654000
H	-2.417825000	3.908332000	-4.472008000
C	-4.024198000	1.215637000	-3.446068000
H	-3.474616000	0.514079000	-4.085687000
H	-4.645422000	0.632639000	-2.758052000
H	-4.695945000	1.785588000	-4.099519000
C	-3.744381000	3.642021000	-1.474733000
H	-3.034523000	4.324289000	-0.992010000
H	-4.410449000	4.254697000	-2.094344000
H	-4.352832000	3.179837000	-0.690972000
C	-6.269539000	-1.496819000	-0.886080000
C	-4.592800000	-0.710596000	0.692753000
C	-5.111731000	0.590490000	0.504000000
C	-6.199758000	0.840524000	-0.327051000
C	-6.792287000	-0.211999000	-1.015436000
H	-6.717624000	-2.313507000	-1.446466000
H	-4.682486000	1.398298000	1.083667000
H	-6.594920000	1.848442000	-0.410935000
H	-7.654985000	-0.039935000	-1.652914000
Sc	-1.995761000	-0.247136000	0.257443000
H	-3.927560000	-1.457343000	2.655086000
C	-2.709205000	0.834542000	3.428948000
C	-2.646941000	-0.240191000	4.525482000
H	-2.483709000	0.243624000	5.494039000
H	-3.578885000	-0.810189000	4.613301000
H	-1.820509000	-0.939668000	4.365591000
C	-1.435380000	1.678048000	3.477284000
H	-1.440750000	2.435382000	2.687231000

H	-1.357261000	2.194314000	4.439938000
H	-0.540309000	1.057776000	3.357752000
C	-3.923411000	1.742511000	3.694874000
H	-3.961225000	2.567555000	2.974861000
H	-4.862375000	1.180239000	3.631516000
H	-3.861091000	2.177799000	4.698612000
N	-2.846756000	0.274717000	2.061649000
H	-3.275152000	-3.289211000	-1.854417000
C	0.165934000	0.952013000	-0.063040000
H	-4.496611000	-3.585818000	0.939963000
H	-5.302157000	-3.841113000	-0.602257000
C	-0.925244000	1.818869000	-0.329164000
H	-1.226289000	-2.689180000	-0.685689000
H	-1.153111000	2.707790000	0.248627000
H	-2.751406000	-3.073737000	1.917029000
C	-0.847606000	-1.982424000	1.884182000
H	-0.777886000	-0.863450000	1.997804000
H	-0.722064000	-2.326913000	2.913270000
H	0.021104000	-2.301219000	1.299863000

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Q, E(SCRF) = -2634.27836 a.u.

Sc	-1.735796000	0.643126000	0.560614000
C	-4.197823000	-0.524107000	1.082684000
C	-3.173957000	-1.471455000	0.384633000
N	-3.578159000	0.779240000	1.256636000
C	-1.909661000	-1.809459000	1.135278000
C	-1.655140000	-1.506377000	2.428243000
C	-4.022994000	-2.674779000	-0.087932000
C	-0.767675000	0.702311000	-1.666123000
H	-1.228544000	0.186029000	-2.504724000
C	0.328748000	0.183590000	-0.916548000
C	1.793078000	1.126792000	1.054943000
H	1.734916000	0.236506000	1.690832000
H	1.727467000	2.002688000	1.705108000
C	3.099349000	1.112317000	0.288075000
C	3.595628000	-0.106596000	-0.147803000
C	4.743995000	-0.160090000	-1.004881000
C	5.362879000	1.065588000	-1.400013000
C	4.836556000	2.288362000	-0.921192000
H	5.330716000	3.215627000	-1.202659000
C	3.735017000	2.336911000	-0.093382000
C	5.285727000	-1.377368000	-1.496374000
H	4.826604000	-2.318146000	-1.209668000
C	6.382358000	-1.377253000	-2.328255000

H	6.782291000	-2.319625000	-2.692906000
C	6.995766000	-0.163500000	-2.711424000
H	7.862564000	-0.179054000	-3.366321000
C	6.494237000	1.032192000	-2.255045000
H	6.958120000	1.972536000	-2.543552000
C	1.108755000	-1.033454000	-1.383689000
H	0.421132000	-1.647348000	-1.969326000
H	1.845883000	-0.644003000	-2.102760000
C	2.967913000	-1.400030000	0.275106000
C	1.842868000	-1.901652000	-0.375067000
C	3.605762000	-2.143611000	1.320923000
C	3.113102000	-3.443183000	1.647700000
C	2.054995000	-3.977890000	0.879486000
H	1.765474000	-5.012852000	1.047118000
C	1.428508000	-3.257065000	-0.121425000
C	3.729518000	-4.185193000	2.688538000
H	3.350846000	-5.178414000	2.918933000
C	4.789792000	-3.661104000	3.388667000
H	5.257110000	-4.234969000	4.184175000
C	5.279893000	-2.373970000	3.069824000
H	6.120066000	-1.966893000	3.625845000
C	4.707399000	-1.635227000	2.059618000
H	5.093956000	-0.649428000	1.821854000
C	3.247791000	3.664830000	0.374691000
C	3.259564000	4.008129000	1.735285000
C	2.812735000	4.622575000	-0.551906000
C	2.833632000	5.266085000	2.157433000
H	3.635119000	3.292359000	2.463513000
C	2.387657000	5.882326000	-0.130471000
H	2.807912000	4.371676000	-1.609816000
C	2.391943000	6.206280000	1.225793000
H	2.864510000	5.519155000	3.214195000
H	2.059950000	6.614177000	-0.864535000
H	2.067623000	7.190132000	1.554211000
C	0.436416000	-3.990711000	-0.959578000
C	0.556219000	-4.032125000	-2.359452000
C	-0.570972000	-4.767321000	-0.364589000
C	-0.316621000	-4.793458000	-3.133002000
H	1.368830000	-3.496254000	-2.843453000
C	-1.442164000	-5.534699000	-1.137276000
H	-0.663342000	-4.780613000	0.719336000
C	-1.324278000	-5.543567000	-2.526193000
H	-0.194405000	-4.818009000	-4.212631000
H	-2.206543000	-6.135157000	-0.650447000

H	-1.997897000	-6.145350000	-3.130060000
Si	-2.205640000	3.265097000	-2.149179000
C	-1.326634000	3.724413000	-3.754292000
H	-0.346055000	4.172856000	-3.558346000
H	-1.170323000	2.847392000	-4.393045000
H	-1.918029000	4.449730000	-4.326334000
C	-3.866731000	2.462583000	-2.539588000
H	-3.743326000	1.586261000	-3.188066000
H	-4.394323000	2.136538000	-1.636236000
H	-4.517206000	3.166697000	-3.072762000
C	-2.402792000	4.803971000	-1.075362000
H	-1.431907000	5.264128000	-0.856357000
H	-3.004343000	5.553821000	-1.603250000
H	-2.903283000	4.601396000	-0.121757000
C	-6.355832000	-2.477626000	-1.232182000
C	-5.427256000	-0.749296000	0.203178000
C	-6.563809000	0.031351000	0.019591000
C	-7.593281000	-0.443458000	-0.796609000
C	-7.492955000	-1.689037000	-1.416521000
H	-6.273112000	-3.445941000	-1.720040000
H	-6.659588000	1.003324000	0.489619000
H	-8.479130000	0.166578000	-0.951067000
H	-8.299931000	-2.044566000	-2.051221000
C	-5.329579000	-1.999258000	-0.424953000
H	-4.419499000	-0.970907000	2.068966000
C	-3.968035000	1.736484000	2.312065000
C	-4.583966000	1.070958000	3.549136000
H	-4.798952000	1.830455000	4.308598000
H	-5.529855000	0.572488000	3.311007000
H	-3.911148000	0.334903000	4.006134000
C	-2.649172000	2.425472000	2.712227000
H	-2.180381000	2.921049000	1.844607000
H	-2.795800000	3.215036000	3.457098000
H	-1.939506000	1.706852000	3.156438000
C	-4.932764000	2.815884000	1.793228000
H	-4.573405000	3.236749000	0.849466000
H	-5.934100000	2.411609000	1.626085000
H	-5.030302000	3.629187000	2.522146000
C	-1.088443000	2.030032000	-1.240620000
H	-2.888360000	-0.987876000	-0.586964000
C	0.658896000	1.169293000	0.060285000
H	-4.136791000	-3.386639000	0.742487000
H	-3.564590000	-3.213702000	-0.922422000
C	-0.193708000	2.290040000	-0.156945000

H	-1.168059000	-2.379073000	0.574111000
H	-0.128311000	3.219309000	0.402270000
H	-2.420049000	-0.979426000	3.000780000
C	-0.427360000	-1.907765000	3.180068000
H	0.030454000	-1.050123000	3.688570000
H	-0.701285000	-2.617647000	3.972345000
H	0.319354000	-2.379449000	2.535996000

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Q', E(SCRF) = -2634.277809 a.u.

C	-3.976974000	-0.987658000	1.807297000
C	-1.329920000	-2.358670000	0.870770000
C	-3.511096000	-2.037875000	-0.568783000
C	-2.272441000	-2.867971000	-0.200287000
C	-1.762359000	-2.047136000	2.109348000
C	-3.216687000	-2.151073000	2.500945000
C	-1.569848000	1.459902000	-1.605348000
C	-0.905693000	0.251490000	-1.981986000
H	-1.153818000	-0.350836000	-2.851316000
C	0.184759000	-0.013643000	-1.110641000
C	1.192967000	1.239564000	0.977282000
H	1.290202000	0.357076000	1.619258000
H	0.856395000	2.066909000	1.606230000
C	2.529426000	1.548765000	0.333349000
C	3.339351000	0.490060000	-0.048326000
C	4.534100000	0.721177000	-0.806045000
C	4.873417000	2.063088000	-1.159425000
C	4.035977000	3.119344000	-0.730574000
H	4.320401000	4.141469000	-0.970667000
C	2.890119000	2.894481000	0.003208000
C	5.389402000	-0.326640000	-1.238973000
H	5.145690000	-1.352550000	-0.981454000
C	6.518912000	-0.056392000	-1.977736000
H	7.160974000	-0.872251000	-2.298939000
C	6.854244000	1.272682000	-2.320719000
H	7.750641000	1.471215000	-2.901751000
C	6.046435000	2.309471000	-1.918129000
H	6.295280000	3.336393000	-2.175526000
C	1.272392000	-1.013128000	-1.475231000
H	0.809577000	-1.775466000	-2.105812000
H	1.959259000	-0.460189000	-2.134097000
C	3.011033000	-0.917883000	0.343713000
C	2.100027000	-1.677363000	-0.386219000
C	3.714318000	-1.481259000	1.457737000
C	3.514211000	-2.857356000	1.780100000

C	2. 679448000	-3. 632270000	0. 946227000
H	2. 620262000	-4. 703471000	1. 124890000
C	1. 993337000	-3. 089850000	-0. 125353000
C	4. 194784000	-3. 424308000	2. 888729000
H	4. 039735000	-4. 476525000	3. 116091000
C	5. 038101000	-2. 659079000	3. 658093000
H	5. 555930000	-3. 099458000	4. 505732000
C	5. 238369000	-1. 295380000	3. 343694000
H	5. 908213000	-0. 696697000	3. 954998000
C	4. 597740000	-0. 720868000	2. 269736000
H	4. 760923000	0. 326500000	2. 037437000
C	2. 080416000	4. 067323000	0. 436652000
C	1. 900440000	4. 364040000	1. 796326000
C	1. 531558000	4. 938097000	-0. 514980000
C	1. 180836000	5. 489914000	2. 191912000
H	2. 356078000	3. 722646000	2. 547708000
C	0. 812329000	6. 065845000	-0. 119979000
H	1. 670622000	4. 723635000	-1. 571649000
C	0. 630707000	6. 342906000	1. 234526000
H	1. 065488000	5. 711499000	3. 249898000
H	0. 400275000	6. 733166000	-0. 872822000
H	0. 076855000	7. 225646000	1. 542871000
C	1. 257918000	-4. 044096000	-1. 004735000
C	1. 487150000	-4. 087881000	-2. 390485000
C	0. 403186000	-5. 010586000	-0. 449933000
C	0. 861525000	-5. 040492000	-3. 192119000
H	2. 195419000	-3. 395335000	-2. 838298000
C	-0. 219165000	-5. 968048000	-1. 249971000
H	0. 232907000	-5. 013909000	0. 624550000
C	0. 000625000	-5. 981322000	-2. 626672000
H	1. 066249000	-5. 061408000	-4. 259351000
H	-0. 869446000	-6. 710951000	-0. 794629000
H	-0. 478526000	-6. 730351000	-3. 251200000
Si	-2. 799263000	2. 439961000	-2. 665303000
C	-1. 929548000	4. 027769000	-3. 192628000
H	-1. 624163000	4. 625040000	-2. 325810000
H	-1. 029960000	3. 809092000	-3. 779305000
H	-2. 590212000	4. 648057000	-3. 810431000
C	-3. 237220000	1. 400489000	-4. 177003000
H	-2. 350706000	1. 172987000	-4. 780394000
H	-3. 714515000	0. 452906000	-3. 902345000
H	-3. 937018000	1. 947246000	-4. 820403000
C	-4. 363054000	2. 873405000	-1. 698656000
H	-4. 138382000	3. 477398000	-0. 811769000

H	-5.043064000	3.462373000	-2.326740000
H	-4.906567000	1.978400000	-1.373996000
C	-3.932826000	-2.158654000	-1.912935000
C	-4.341918000	-1.330495000	0.345468000
C	-5.564797000	-0.818515000	-0.133153000
C	-5.978053000	-0.992062000	-1.444366000
C	-5.147261000	-1.658420000	-2.350358000
H	-3.294923000	-2.700129000	-2.607423000
H	-6.208554000	-0.286569000	0.561078000
H	-6.943228000	-0.608764000	-1.763125000
H	-5.452531000	-1.793645000	-3.383797000
Sc	-2.040717000	-0.046102000	0.208469000
H	-4.931455000	-0.843219000	2.326209000
C	-3.706947000	1.410266000	2.634543000
C	-3.654526000	1.072711000	4.131850000
H	-3.960411000	1.944576000	4.721008000
H	-4.333618000	0.255410000	4.392955000
H	-2.638633000	0.800206000	4.438242000
C	-2.793864000	2.613463000	2.385124000
H	-2.885230000	2.966068000	1.352988000
H	-3.066871000	3.443793000	3.044816000
H	-1.745403000	2.359728000	2.580916000
C	-5.147481000	1.819966000	2.273877000
H	-5.231176000	2.065527000	1.210471000
H	-5.876883000	1.036936000	2.512458000
H	-5.439117000	2.704279000	2.851558000
N	-3.219765000	0.302176000	1.780142000
H	-0.264450000	-2.354094000	0.650541000
C	0.178879000	1.017958000	-0.119214000
H	-2.641118000	-3.852571000	0.129934000
H	-1.703197000	-3.063214000	-1.112022000
C	-0.870282000	1.918272000	-0.446801000
H	-1.042210000	-1.741010000	2.867411000
H	-1.067642000	2.835213000	0.095584000
H	-3.612683000	-3.081665000	2.064839000
C	-3.385451000	-2.273331000	4.014257000
H	-2.908531000	-1.452140000	4.553295000
H	-4.444581000	-2.299924000	4.292088000
H	-2.931641000	-3.208042000	4.362434000

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TS5-2, E(SCRF) = -2015.559818 a.u., IF = *i*1357.41 cm⁻¹

C	-0.786593000	1.024864000	1.609857000
C	-0.456736000	-2.231458000	-0.450767000
Y	-1.491161000	0.076463000	-0.725963000

H	-0.087213000	-1.052135000	0.323295000
N	4.339558000	-1.087143000	-0.798344000
N	-3.150659000	-1.293818000	0.478623000
C	3.719076000	2.905745000	1.235305000
C	4.930310000	0.934968000	0.507634000
C	6.109088000	1.521014000	1.002913000
C	6.133494000	2.774577000	1.601769000
C	4.917422000	3.451978000	1.700289000
H	7.042983000	0.970359000	0.902881000
H	4.897554000	4.439938000	2.157653000
C	5.164677000	-0.375912000	-0.134686000
H	6.207016000	-0.698145000	-0.012511000
C	4.810666000	-2.330107000	-1.437824000
C	3.778610000	-3.411830000	-1.091928000
H	4.010905000	-4.352486000	-1.603715000
H	3.767703000	-3.600689000	-0.011890000
H	2.777084000	-3.090195000	-1.397849000
C	4.798448000	-2.072969000	-2.953510000
H	5.522964000	-1.295197000	-3.218534000
H	5.059634000	-2.986279000	-3.500231000
H	3.809610000	-1.742147000	-3.285770000
C	6.204592000	-2.823121000	-1.022366000
H	7.001332000	-2.137320000	-1.331743000
H	6.277856000	-2.973072000	0.061504000
H	6.406496000	-3.785484000	-1.504285000
C	2.375609000	1.031326000	0.210561000
H	0.018627000	-0.820165000	2.093334000
H	2.234292000	-0.674763000	1.492142000
H	1.898339000	0.833554000	2.311193000
C	-0.121518000	0.353903000	-2.995627000
H	-1.574370000	0.749480000	2.315633000
H	-0.171937000	2.578082000	0.288784000
C	-1.909002000	3.286554000	1.369426000
C	-2.772823000	3.175937000	2.475602000
C	-1.976271000	4.462878000	0.601093000
C	-3.686125000	4.182247000	2.772093000
H	-2.711070000	2.314045000	3.134609000
C	-2.886639000	5.472078000	0.900752000
H	-1.290194000	4.592192000	-0.232377000
C	-3.753593000	5.332446000	1.983476000
H	-4.335620000	4.078343000	3.637266000
H	-2.912194000	6.372464000	0.292951000
H	-4.461171000	6.120527000	2.224716000
C	3.703068000	1.627239000	0.634942000

C	-0.691545000	1.635233000	-2.744399000
H	2.531716000	0.334727000	-0.615491000
H	1.726745000	1.840624000	-0.142162000
C	-2.415125000	0.170094000	-3.221451000
C	-1.187008000	-0.551912000	-3.288152000
C	7.410925000	3.386018000	2.111929000
H	8.247381000	2.684053000	2.041807000
H	7.679201000	4.281466000	1.537756000
H	7.316074000	3.691913000	3.160428000
C	2.462342000	3.727636000	1.385539000
H	2.038936000	4.005900000	0.410795000
H	1.679065000	3.199204000	1.941075000
H	2.671655000	4.658149000	1.921211000
C	1.337340000	0.050063000	-3.179897000
H	1.665539000	-0.842683000	-2.637183000
H	1.555116000	-0.121415000	-4.242720000
H	1.970855000	0.876711000	-2.850269000
C	0.064058000	2.928484000	-2.624932000
H	1.005847000	2.823988000	-2.076604000
H	0.320331000	3.311080000	-3.622487000
H	-0.529853000	3.705155000	-2.134112000
C	-3.073418000	2.679397000	-2.865078000
H	-2.924964000	3.353707000	-2.013732000
H	-2.957344000	3.281608000	-3.776144000
H	-4.115206000	2.345338000	-2.839350000
C	-3.744498000	-0.359837000	-3.684033000
H	-3.885790000	-1.415415000	-3.426468000
H	-4.592250000	0.199518000	-3.275261000
H	-3.820560000	-0.289386000	-4.777644000
C	-1.018323000	-1.944812000	-3.823661000
H	-1.858528000	-2.601203000	-3.569830000
H	-0.952792000	-1.924237000	-4.920201000
H	-0.102411000	-2.419855000	-3.458763000
C	-2.110647000	1.523821000	-2.874611000
C	-3.032249000	-2.409228000	1.141679000
H	-3.929167000	-2.757417000	1.653850000
C	-4.515537000	-0.660988000	0.534314000
C	-4.375955000	0.720632000	-0.105523000
H	-5.340361000	1.235758000	-0.157064000
H	-3.715283000	1.380107000	0.476672000
H	-4.028096000	0.648144000	-1.146985000
C	-5.511809000	-1.506714000	-0.268905000
H	-5.635511000	-2.502592000	0.170379000
H	-6.495676000	-1.025298000	-0.282680000

H	-5.177795000	-1.632407000	-1.303891000
C	-5.005137000	-0.474649000	1.978617000
H	-5.227506000	-1.422406000	2.478603000
H	-4.264655000	0.066143000	2.578104000
H	-5.930755000	0.110477000	1.978489000
C	0.195970000	-0.030411000	1.353008000
C	-0.665906000	-3.187116000	0.656054000
C	0.382810000	-4.040742000	1.016808000
C	-1.895087000	-3.270692000	1.369608000
C	0.257661000	-4.984651000	2.032131000
H	1.318232000	-3.972686000	0.467864000
C	-2.045399000	-4.261239000	2.392296000
C	-0.971465000	-5.081899000	2.701783000
H	-1.086188000	-5.825422000	3.487158000
C	1.708518000	0.280918000	1.380907000
H	-1.275135000	-2.332221000	-1.183279000
C	-0.929253000	2.252412000	1.005155000
H	0.476089000	-2.430840000	-0.983817000
C	-3.323537000	-4.446191000	3.176986000
H	-3.600731000	-3.550484000	3.745913000
H	-4.173276000	-4.711033000	2.535252000
H	-3.205156000	-5.259296000	3.897704000
C	1.395776000	-5.893244000	2.400168000
H	1.104395000	-6.945813000	2.301520000
H	2.271861000	-5.722979000	1.768544000
H	1.694744000	-5.741342000	3.444532000

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TS5-3, E(SCRF) = -2015.557132 a.u., IF = *i*1329.09 cm⁻¹

C	0.021987000	-0.207617000	-1.058256000
C	-1.471296000	1.485641000	0.819768000
Y	-1.969440000	-0.978590000	0.483889000
H	-0.739329000	0.590177000	-0.080819000
N	4.551504000	1.702229000	0.924771000
N	-3.984053000	0.182414000	-0.226557000
C	0.491818000	1.032494000	-1.752233000
C	5.782700000	-0.152628000	-0.118742000
C	7.098217000	-0.644553000	-0.166519000
C	7.473312000	-1.698665000	-0.991351000
C	6.476208000	-2.272850000	-1.782460000
H	7.851806000	-0.173709000	0.462945000
H	6.735713000	-3.100509000	-2.440926000
C	5.602404000	0.991115000	0.797698000
H	6.511542000	1.207400000	1.375735000
C	4.531840000	2.852603000	1.839621000

C	4. 253161000	4. 083767000	0. 961752000
H	4. 124135000	4. 979188000	1. 580741000
H	5. 083878000	4. 262424000	0. 269938000
H	3. 344120000	3. 932340000	0. 369700000
C	3. 346887000	2. 627190000	2. 790908000
H	3. 516864000	1. 746569000	3. 420937000
H	3. 204738000	3. 494607000	3. 445743000
H	2. 427445000	2. 467404000	2. 217517000
C	5. 805026000	3. 089464000	2. 662568000
H	6. 041971000	2. 234332000	3. 306821000
H	6. 674336000	3. 295012000	2. 027119000
H	5. 663943000	3. 960044000	3. 311832000
C	3. 342668000	-0. 289646000	-0. 907135000
H	1. 760699000	2. 409232000	-2. 577852000
H	3. 757758000	1. 710924000	-1. 516573000
H	3. 491513000	0. 631352000	-2. 861777000
C	-0. 460472000	-1. 157572000	2. 662851000
H	-0. 309551000	1. 698068000	-2. 073997000
H	0. 822844000	-0. 728034000	-0. 530564000
C	-0. 770501000	-1. 152240000	-1. 884767000
C	-1. 614229000	-0. 730170000	-2. 942258000
C	-0. 796946000	-2. 534552000	-1. 561294000
C	-2. 368635000	-1. 643761000	-3. 670246000
H	-1. 626564000	0. 316887000	-3. 227715000
C	-1. 564749000	-3. 446904000	-2. 299073000
H	-0. 106177000	-2. 913589000	-0. 810230000
C	-2. 350503000	-3. 009013000	-3. 359424000
H	-2. 967614000	-1. 289783000	-4. 505801000
H	-1. 517427000	-4. 504370000	-2. 052230000
H	-2. 929204000	-3. 715393000	-3. 947099000
C	4. 782116000	-0. 754632000	-0. 917936000
C	-0. 281538000	-2. 407464000	2. 000432000
H	3. 065361000	0. 029660000	0. 102327000
H	2. 704984000	-1. 130534000	-1. 195872000
C	-2. 470929000	-2. 291289000	2. 728147000
C	-1. 813337000	-1. 087431000	3. 118392000
C	8. 893194000	-2. 196656000	-1. 044913000
H	9. 358147000	-1. 966146000	-2. 011674000
H	9. 508361000	-1. 738268000	-0. 264512000
H	8. 941092000	-3. 284148000	-0. 915502000
C	4. 146828000	-2. 524816000	-2. 642898000
H	3. 403974000	-3. 083352000	-2. 057460000
H	3. 594673000	-1. 825587000	-3. 281595000
H	4. 646038000	-3. 243642000	-3. 299397000

C	0.646487000	-0.205800000	3.011004000
H	0.268945000	0.776590000	3.308680000
H	1.226988000	-0.592446000	3.859709000
H	1.351192000	-0.056392000	2.186192000
C	1.046096000	-2.964215000	1.571292000
H	1.677365000	-2.224943000	1.065694000
H	1.611302000	-3.308897000	2.447918000
H	0.943484000	-3.830420000	0.909434000
C	-1.760906000	-4.519497000	1.576063000
H	-1.068538000	-4.824198000	0.784839000
H	-1.617581000	-5.218258000	2.411286000
H	-2.778272000	-4.678650000	1.200847000
C	-3.814304000	-2.744161000	3.230942000
H	-4.256514000	-3.527871000	2.607099000
H	-3.712584000	-3.166800000	4.239901000
H	-4.538213000	-1.925586000	3.305598000
C	-2.393257000	-0.039368000	4.026767000
H	-3.460355000	0.131066000	3.843166000
H	-2.296903000	-0.346433000	5.077024000
H	-1.883433000	0.924356000	3.929935000
C	-1.526571000	-3.103083000	2.021795000
C	-4.212082000	1.432751000	-0.523704000
H	-5.219839000	1.667023000	-0.864798000
C	-5.149656000	-0.749311000	-0.404694000
C	-4.581626000	-2.167921000	-0.300519000
H	-5.371506000	-2.920328000	-0.392531000
H	-3.863495000	-2.376288000	-1.107545000
H	-4.126923000	-2.356194000	0.686259000
C	-6.171790000	-0.509425000	0.713297000
H	-6.596841000	0.498206000	0.649301000
H	-6.997027000	-1.226133000	0.640279000
H	-5.710079000	-0.617863000	1.700447000
C	-5.812071000	-0.603635000	-1.783207000
H	-6.345060000	0.344687000	-1.901611000
H	-5.068294000	-0.687498000	-2.582516000
H	-6.551576000	-1.399970000	-1.919119000
C	1.732891000	1.455250000	-2.046524000
C	-2.031929000	2.601700000	0.038130000
C	-1.255264000	3.762036000	-0.108625000
C	-3.337120000	2.576847000	-0.534631000
C	-1.719679000	4.890874000	-0.769746000
H	-0.259240000	3.773876000	0.327398000
C	-3.836418000	3.750428000	-1.191739000
C	-3.021673000	4.863947000	-1.300123000

H	-3.401158000	5.747630000	-1.808017000
C	3.114215000	0.891388000	-1.859624000
H	-2.203015000	1.159525000	1.579966000
C	5.152825000	-1.826011000	-1.758406000
H	-0.579929000	1.802883000	1.367022000
C	-5.219277000	3.825310000	-1.796209000
H	-5.368322000	3.091601000	-2.597808000
H	-6.009790000	3.670695000	-1.051038000
H	-5.383318000	4.814045000	-2.232272000
C	-0.873952000	6.125269000	-0.901990000
H	0.117877000	5.986844000	-0.462902000
H	-0.745239000	6.401433000	-1.955497000
H	-1.349190000	6.979542000	-0.404381000

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TS5-1, E(SCRF) = -2015.532997 a.u., IF = $i1271.13 \text{ cm}^{-1}$

C	-0.462274000	-0.742592000	-1.476003000
C	0.357590000	1.936621000	-1.286973000
Y	-0.176673000	0.644628000	0.958309000
H	-0.139908000	0.574092000	-1.118573000
N	2.353951000	1.354660000	0.880905000
N	-2.180033000	2.347679000	0.077980000
C	3.991699000	-2.485749000	-1.353374000
C	3.958968000	-0.285043000	-0.310453000
C	5.353504000	-0.206628000	-0.537958000
C	6.077296000	-1.219009000	-1.151367000
C	5.368600000	-2.356972000	-1.544762000
H	5.889666000	0.682417000	-0.211832000
H	5.907283000	-3.177007000	-2.016240000
C	3.469178000	0.918664000	0.384485000
H	4.314775000	1.600941000	0.495456000
C	2.514460000	2.742996000	1.492948000
C	1.152441000	3.185495000	2.024455000
H	1.242797000	4.110653000	2.603100000
H	0.441406000	3.409230000	1.220421000
H	0.732498000	2.444145000	2.717146000
C	3.507169000	2.708493000	2.665178000
H	4.518859000	2.438897000	2.346626000
H	3.566193000	3.699289000	3.128027000
H	3.194443000	1.994333000	3.431210000
C	2.977626000	3.770529000	0.446796000
H	3.990028000	3.571429000	0.081207000
H	2.302036000	3.797173000	-0.413265000
H	2.990297000	4.768166000	0.899268000
C	1.781731000	-1.577871000	-0.585560000

H	-0.890606000	-0.243231000	-2.362399000
H	1.452047000	-0.387113000	-2.358264000
H	0.929647000	-2.048547000	-2.529858000
C	0.795820000	-0.767422000	3.063861000
H	-2.471681000	-1.363163000	-0.916342000
H	-0.336408000	-3.514726000	-1.350058000
C	-2.357075000	-4.123951000	-0.907914000
C	-3.733307000	-3.834741000	-0.857472000
C	-1.966044000	-5.466074000	-0.758769000
C	-4.669096000	-4.841338000	-0.646827000
H	-4.079140000	-2.814889000	-1.006076000
C	-2.901975000	-6.474847000	-0.549356000
H	-0.908316000	-5.718244000	-0.810014000
C	-4.259890000	-6.166810000	-0.488276000
H	-5.727050000	-4.592903000	-0.617913000
H	-2.569981000	-7.503714000	-0.437129000
H	-4.994295000	-6.951500000	-0.329094000
C	3.265848000	-1.442027000	-0.743901000
C	-0.103068000	-1.652928000	2.395355000
H	1.491915000	-0.956026000	0.273925000
H	1.529128000	-2.593657000	-0.274860000
C	-1.357397000	-0.010815000	3.418750000
C	0.017887000	0.241586000	3.705154000
C	7.560528000	-1.108394000	-1.379827000
H	7.801052000	-1.161740000	-2.448197000
H	7.958067000	-0.164819000	-0.994509000
H	8.099288000	-1.925650000	-0.886238000
C	3.318071000	-3.763037000	-1.791059000
H	2.842046000	-4.280359000	-0.948467000
H	2.543683000	-3.586802000	-2.545265000
H	4.045431000	-4.453853000	-2.226039000
C	2.253555000	-1.046518000	3.297904000
H	2.794761000	-0.160672000	3.638809000
H	2.373078000	-1.814805000	4.074289000
H	2.765146000	-1.414316000	2.402270000
C	0.231720000	-3.050713000	1.966500000
H	1.308988000	-3.193833000	1.844288000
H	-0.095388000	-3.753047000	2.745854000
H	-0.272110000	-3.345151000	1.042138000
C	-2.678875000	-1.947664000	2.289080000
H	-2.565893000	-2.587347000	1.411195000
H	-2.921855000	-2.603923000	3.137301000
H	-3.552591000	-1.307739000	2.128458000
C	-2.495192000	0.513487000	4.250202000

H	-3.455590000	0.497145000	3.730946000
H	-2.605859000	-0.125968000	5.137656000
H	-2.326425000	1.530222000	4.615060000
C	0.490721000	1.165448000	4.793500000
H	-0.056729000	2.114716000	4.819214000
H	0.341374000	0.690977000	5.773332000
H	1.556227000	1.398250000	4.717393000
C	-1.431220000	-1.167705000	2.586470000
C	-2.520434000	2.585572000	-1.155971000
H	-3.488766000	3.060944000	-1.303446000
C	-3.170854000	2.858950000	1.089175000
C	-4.158596000	1.723744000	1.376263000
H	-4.833679000	1.984895000	2.198569000
H	-4.767036000	1.519228000	0.487658000
H	-3.632648000	0.801757000	1.638380000
C	-2.367661000	3.256461000	2.327735000
H	-1.735392000	4.124832000	2.111611000
H	-3.033478000	3.521589000	3.155260000
H	-1.729182000	2.436033000	2.673776000
C	-3.955193000	4.112066000	0.655267000
H	-3.287962000	4.887279000	0.260974000
H	-4.735952000	3.910716000	-0.085407000
H	-4.464201000	4.525000000	1.532469000
C	-1.473883000	-1.764000000	-1.107897000
C	-0.434516000	2.171495000	-2.501764000
C	0.168011000	2.106326000	-3.765764000
C	-1.832476000	2.388451000	-2.416125000
C	-0.566583000	2.239163000	-4.939690000
H	1.244025000	1.953148000	-3.822881000
C	-2.595450000	2.540105000	-3.612607000
C	-1.951624000	2.447362000	-4.838466000
H	-2.537253000	2.547679000	-5.749645000
C	0.948147000	-1.204144000	-1.828609000
H	0.167282000	2.735781000	-0.559719000
C	-1.322693000	-3.106585000	-1.127321000
H	1.425636000	1.887293000	-1.502861000
C	-4.086580000	2.777893000	-3.602310000
H	-4.630113000	2.004623000	-3.046935000
H	-4.348474000	3.748622000	-3.160979000
H	-4.475821000	2.778502000	-4.623910000
C	0.092637000	2.169277000	-6.288732000
H	1.169499000	1.996642000	-6.205297000
H	-0.335129000	1.360840000	-6.893912000
H	-0.058353000	3.100764000	-6.847747000

