

Electronic Supplementary Information

Is it Possible to Achieve a Complete Desaturation of Cycloalkanes Promoted by *o*-Benzyne?

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Computational Details

All computations have been carried out with the G09 program package.¹ All geometries have been optimized at the DFT level using the M06-2X² functional in conjunction with the 6-311+G(d,p) basis set.³ The vibrational frequencies of the optimized structures have been computed in order to establish the nature of the stationary points.

- 1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Wallingford CT, **2009**.
- 2 Y. Zhao, and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
- 3 a) A. D. McLean, and G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639; (b) K. Raghavachari, J. S. Binkley, R. Seeger, and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650.

Cartesian Coordinates and free energies (in hartrees)

1 G = -235.673167 a.u.

C	-1.262540000	0.728928000	0.233499000
C	0.000000000	1.457855000	-0.233499000
C	1.262540000	0.728928000	0.233499000
C	1.262540000	-0.728928000	-0.233499000
C	0.000000000	-1.457855000	0.233499000
C	-1.262540000	-0.728928000	-0.233499000
H	-2.155470000	1.244461000	-0.130443000
H	-1.305709000	0.753851000	1.329436000
H	0.000000000	2.488922000	0.130443000
H	0.000000000	1.507702000	-1.329436000
H	2.155470000	1.244461000	-0.130443000
H	1.305709000	0.753851000	1.329436000
H	2.155470000	-1.244461000	0.130443000
H	1.305709000	-0.753851000	-1.329436000
H	0.000000000	-2.488922000	-0.130443000
H	0.000000000	-1.507702000	1.329436000
H	-2.155470000	-1.244461000	0.130443000
H	-1.305709000	-0.753851000	-1.329436000

1 boat conformation G = -235.662002 a.u.

C	-0.654976000	-1.214132000	0.394306000
C	-1.519998000	-0.000021000	-0.000032000
C	-0.655006000	1.214034000	-0.394467000
C	0.654846000	1.214064000	0.394535000
H	-1.209340000	-2.141208000	0.231625000
H	-2.173388000	0.268277000	0.835096000
H	-1.209471000	2.141126000	-0.232231000
H	-2.173641000	-0.268241000	-0.834961000
H	-0.420786000	1.175555000	-1.463959000
H	0.420639000	1.175435000	1.464035000
H	1.209213000	2.141236000	0.232427000
H	-0.421193000	-1.175960000	1.463907000
C	0.655143000	-1.214100000	-0.394240000
C	1.519990000	0.000196000	-0.000095000
H	1.209601000	-2.141088000	-0.231382000
H	0.421334000	-1.176163000	-1.463843000
H	2.173082000	0.268676000	-0.835403000
H	2.173950000	-0.267891000	0.834645000

2 G = -230.817789 a.u.

C	0.000000000	1.458755000	-0.132311000
C	0.000000000	0.702168000	1.051953000
C	0.000000000	0.619719000	-1.230769000
H	0.000000000	1.225405000	2.002001000
C	0.000000000	-0.702168000	1.051953000
C	0.000000000	-0.619719000	-1.230769000
H	0.000000000	-1.225405000	2.002001000
C	0.000000000	-1.458755000	-0.132311000
H	0.000000000	-2.540085000	-0.135247000
H	0.000000000	2.540085000	-0.135247000

3 G = -232.122388 a.u.

C	0.000000000	1.391593000	0.000000000
C	1.205155000	0.695796000	0.000000000
C	-1.205155000	0.695796000	0.000000000
H	2.143602000	1.237609000	0.000000000
H	-2.143602000	1.237609000	0.000000000
C	1.205155000	-0.695796000	0.000000000
C	-1.205155000	-0.695796000	0.000000000
H	2.143602000	-1.237609000	0.000000000
H	-2.143602000	-1.237609000	0.000000000
C	0.000000000	-1.391593000	0.000000000
H	0.000000000	-2.475218000	0.000000000
H	0.000000000	2.475218000	0.000000000

4 G = -234.471217 a.u.

C	0.007075000	1.497289000	0.042286000
C	-0.007075000	0.665769000	1.298955000
C	0.007075000	-0.665769000	1.298955000
C	-0.007075000	-1.497289000	0.042286000
C	-0.383081000	-0.661739000	-1.183190000
C	0.383081000	0.661739000	-1.183190000
H	0.707055000	2.329301000	0.164455000
H	-0.981039000	1.952231000	-0.101939000
H	-0.023793000	1.196644000	2.246621000
H	0.023793000	-1.196644000	2.246621000
H	-0.707055000	-2.329301000	0.164455000
H	0.981039000	-1.952231000	-0.101939000
H	-0.185745000	-1.224151000	-2.098956000
H	-1.458026000	-0.450655000	-1.158486000
H	0.185745000	1.224151000	-2.098956000
H	1.458026000	0.450655000	-1.158486000

5 G = -233.270602 a.u.

C	-0.326347000	0.691794000	-1.185577000
C	-0.055688000	1.418125000	0.108181000
C	0.055688000	0.732384000	1.250519000
C	-0.055688000	-0.732384000	1.250519000
C	0.055688000	-1.418125000	0.108181000
C	0.326347000	-0.691794000	-1.185577000
H	0.021769000	1.275778000	-2.039878000
H	-1.414799000	0.583644000	-1.299308000
H	-0.012667000	2.501958000	0.106817000
H	0.207154000	1.245354000	2.193633000
H	-0.207154000	-1.245354000	2.193633000
H	0.012667000	-2.501958000	0.106817000
H	-0.021769000	-1.275778000	-2.039878000
H	1.414799000	-0.583644000	-1.299308000

6 G = -233.271523 a.u.

C	1.496969000	-0.000850000	-0.000033000
C	0.665278000	1.251179000	-0.000017000
C	-0.663789000	1.251803000	0.000116000

C	-1.496895000	0.000732000	-0.000046000
C	-0.665335000	-1.251057000	0.000109000
C	0.663795000	-1.251818000	0.000006000
H	2.164646000	-0.001201000	0.870843000
H	2.164442000	-0.001184000	-0.871028000
H	1.199956000	2.196333000	0.000054000
H	-1.197572000	2.197486000	0.000217000
H	-2.164044000	0.001382000	-0.871412000
H	-2.165111000	0.001200000	0.870379000
H	-1.199828000	-2.196335000	0.000096000
H	1.197364000	-2.197611000	0.000042000

TS₁₋₄ G = -466.454227 a.u.

C	-2.438739000	1.431751000	-0.018208000
C	-1.385297000	0.582680000	0.283594000
C	-3.618350000	0.753553000	-0.340911000
H	-4.506008000	1.322992000	-0.594292000
C	-1.429503000	-0.697929000	0.283316000
C	-3.680777000	-0.647546000	-0.343623000
H	-4.616827000	-1.133010000	-0.598388000
C	-2.567418000	-1.432012000	-0.024839000
H	-2.623871000	-2.514216000	-0.027356000
H	-2.389095000	2.514005000	-0.013347000
C	2.003238000	-1.357069000	-0.333736000
C	1.231280000	-0.767938000	0.840967000
C	1.198103000	0.698658000	0.849596000
C	1.962092000	1.359397000	-0.288571000
H	2.065000000	-2.443862000	-0.244703000
H	1.490596000	-1.211990000	1.803141000
H	1.375554000	1.153737000	1.824608000
H	0.085108000	-1.104496000	0.687122000
H	0.008571000	0.980204000	0.654274000
H	1.448558000	1.165216000	-1.235874000
H	1.983073000	2.443516000	-0.159229000
H	1.454939000	-1.151852000	-1.258886000
C	3.412132000	-0.748999000	-0.424028000
C	3.392358000	0.799384000	-0.352005000
H	4.016605000	-1.148184000	0.395091000
H	3.888297000	-1.081467000	-1.349710000
H	3.913646000	1.230238000	-1.210201000
H	3.931136000	1.135591000	0.538444000

TS₄₋₅ G = -465.258159 a.u.

C	1.535499000	-0.649339000	-1.171017000
C	2.583325000	-1.251645000	-0.233746000
C	2.449249000	-0.687152000	1.181690000
C	2.461137000	0.819086000	1.143977000
C	2.002143000	1.495551000	0.088811000
C	1.376181000	0.814529000	-1.071123000
H	0.506560000	-1.095565000	-0.857213000
H	1.428975000	1.368082000	-2.007212000
H	2.488097000	-2.339677000	-0.219739000
H	1.513738000	-1.035937000	1.635060000
H	2.860383000	1.358039000	1.997206000
H	2.027960000	2.580412000	0.080649000

H	1.668318000	-0.977521000	-2.202554000
H	0.136016000	0.951083000	-0.835603000
C	-2.169086000	1.374654000	-0.099994000
C	-1.141820000	0.497570000	-0.412791000
C	-3.324670000	0.723393000	0.340137000
H	-4.193732000	1.311851000	0.613127000
C	-1.175346000	-0.779889000	-0.330396000
C	-3.385404000	-0.674453000	0.436707000
H	-4.302577000	-1.137968000	0.785106000
C	-2.295789000	-1.483111000	0.096523000
H	-2.355269000	-2.562575000	0.173233000
H	-2.114409000	2.453795000	-0.177909000
H	3.259822000	-1.053863000	1.816015000
H	3.583603000	-1.015317000	-0.612839000

TS₄₋₆ G = -465.254294 a.u.

C	-1.519317000	0.756941000	-1.108354000
C	-2.388102000	1.397387000	-0.018949000
C	-2.276071000	0.633000000	1.273980000
C	-2.219807000	-0.695708000	1.262509000
C	-2.268142000	-1.442743000	-0.044430000
C	-1.469003000	-0.706387000	-1.121595000
H	-0.397819000	1.088064000	-0.838791000
H	-1.667847000	1.206007000	-2.090326000
H	-2.104326000	2.442461000	0.121619000
H	-2.140679000	-1.257114000	2.187135000
H	-3.311655000	-1.531138000	-0.376296000
H	-1.548631000	-1.160901000	-2.108585000
H	-0.295435000	-0.958608000	-0.838543000
C	2.127308000	-1.420016000	-0.060630000
C	1.085783000	-0.569942000	-0.395804000
C	3.283239000	-0.739014000	0.335634000
H	4.161352000	-1.307325000	0.622683000
C	1.119072000	0.708930000	-0.370132000
C	3.334384000	0.662003000	0.368443000
H	4.252391000	1.148196000	0.681160000
C	2.233397000	1.446274000	0.006889000
H	2.282607000	2.528477000	0.030638000
H	2.087374000	-2.502157000	-0.090826000
H	-2.243516000	1.181563000	2.209160000
H	-3.435745000	1.400360000	-0.348313000
H	-1.894521000	-2.462241000	0.073927000

TS₅₋₃ G = -464.066396 a.u.

C	-1.439065000	0.721628000	0.989841000
C	-2.380289000	1.409525000	0.068974000
C	-3.112129000	0.744366000	-0.835133000
C	-3.084399000	-0.712254000	-0.894917000
C	-2.342891000	-1.423136000	-0.034571000
C	-1.444739000	-0.784199000	0.962720000
H	-1.486009000	1.132115000	2.000338000
H	-0.367088000	1.041494000	0.653644000
H	-2.438359000	2.491270000	0.131830000
H	-3.767019000	1.282641000	-1.510613000
H	-3.710426000	-1.216732000	-1.621875000

H	-2.368693000	-2.507665000	-0.057660000
H	-0.361200000	-1.101376000	0.678940000
H	-1.556401000	-1.232845000	1.952360000
C	2.315360000	1.450487000	-0.081722000
C	1.254985000	0.615800000	0.231522000
C	3.477660000	0.731872000	-0.390009000
H	4.378356000	1.275933000	-0.653268000
C	1.281842000	-0.647768000	0.251297000
C	3.511503000	-0.671003000	-0.368713000
H	4.437963000	-1.178387000	-0.615212000
C	2.384944000	-1.435540000	-0.038597000
H	2.413043000	-2.517793000	-0.023520000
H	2.289139000	2.532671000	-0.099113000

TS₄₋₇ G = -465.267411 a.u.

H	4.285343000	1.084194000	0.099052000
C	3.276955000	0.684808000	0.055857000
C	3.099088000	-0.703926000	-0.013882000
H	3.957631000	-1.365021000	-0.035524000
C	1.814171000	-1.240557000	-0.059223000
H	1.636215000	-2.307904000	-0.126669000
C	0.832772000	-0.265682000	-0.028292000
C	-0.957860000	-1.149611000	-0.610539000
H	-0.506190000	-2.008742000	-1.096533000
C	-1.701835000	-0.193101000	-1.504048000
H	-1.016738000	0.189143000	-2.265542000
H	-2.456494000	-0.788579000	-2.033480000
C	-2.363866000	0.966211000	-0.750696000
H	-1.611700000	1.736014000	-0.569700000
H	-3.147260000	1.401995000	-1.375237000
C	-2.933162000	0.515394000	0.594171000
H	-3.398747000	1.360060000	1.106751000
H	-3.711243000	-0.241641000	0.445688000
C	-1.812306000	-0.064166000	1.464359000
H	-1.087282000	0.736345000	1.685090000
H	-2.187909000	-0.443052000	2.417151000
C	-1.067274000	-1.139772000	0.748235000
H	-0.614475000	-1.939901000	1.324996000
C	0.876530000	1.031010000	0.068655000
C	2.185307000	1.553353000	0.082984000
H	2.367725000	2.623312000	0.138481000

7 G = -465.279538 a.u.

C	-0.614190000	0.336794000	-0.033180000
C	-0.690109000	-1.058773000	0.242432000
C	-2.032386000	-1.528044000	0.288385000
C	-1.753454000	1.201397000	-0.209465000
C	0.679519000	0.820282000	-0.896093000
C	0.708106000	1.125740000	0.508020000
H	0.360392000	1.605505000	-1.572154000
H	0.412674000	2.124555000	0.805349000
C	-3.005881000	0.680351000	-0.097748000
H	-3.885454000	1.301870000	-0.210481000
C	-3.135257000	-0.709837000	0.159235000
H	-4.134796000	-1.127457000	0.252776000

H	-1.608435000	2.256104000	-0.433719000
H	-2.209897000	-2.586388000	0.465061000
C	1.668710000	0.402780000	1.436437000
H	1.988678000	1.106145000	2.208739000
H	1.153977000	-0.425287000	1.924789000
C	1.613958000	-0.201856000	-1.510919000
H	1.055567000	-0.859365000	-2.180044000
H	2.302158000	0.381751000	-2.135593000
C	2.880169000	-0.137203000	0.668212000
H	3.481598000	0.700683000	0.294066000
H	3.516104000	-0.709429000	1.347834000
C	2.426424000	-1.014225000	-0.496678000
H	1.803673000	-1.822672000	-0.112777000
H	3.290101000	-1.450454000	-1.005666000

TS₇₋₈ G = -465.262239 a.u.

C	-0.663571000	0.588182000	-0.111712000
C	-0.594993000	-0.714118000	-0.662358000
C	-1.875215000	-1.385993000	-0.656287000
C	-1.877261000	1.218472000	0.359051000
C	0.666589000	1.219897000	0.246140000
C	0.501136000	-0.010347000	1.059073000
H	0.513202000	2.147599000	0.793313000
H	-0.058738000	0.106172000	1.981335000
C	-3.051608000	0.551547000	0.223840000
H	-3.988753000	1.012805000	0.514148000
C	-3.044940000	-0.782509000	-0.288360000
H	-3.990719000	-1.309952000	-0.374698000
H	-1.844819000	2.219416000	0.779741000
H	-1.920241000	-2.409470000	-1.020789000
C	1.539601000	-1.125670000	1.082428000
H	1.785925000	-1.283109000	2.139422000
H	1.122713000	-2.054975000	0.704731000
C	1.801851000	1.277090000	-0.773064000
H	1.414441000	1.684177000	-1.710247000
H	2.541600000	1.990559000	-0.393695000
C	2.811472000	-0.742232000	0.316420000
H	3.409675000	-0.058664000	0.931350000
H	3.416773000	-1.638602000	0.163572000
C	2.503373000	-0.063670000	-1.016173000
H	1.867329000	-0.709425000	-1.620298000
H	3.433020000	0.119578000	-1.561877000

8 G = -465.389406 a.u.

H	-3.658095000	1.220815000	0.834549000
C	-2.789290000	0.698573000	0.450175000
C	-2.789046000	-0.699238000	0.450267000
H	-3.657633000	-1.221781000	0.834700000
C	-1.700521000	-1.434492000	-0.030743000
H	-1.714761000	-2.518605000	-0.023233000
C	-0.629634000	-0.694498000	-0.502885000
C	0.767226000	-0.791371000	-1.098934000
H	0.790476000	-1.224077000	-2.102238000
C	1.861739000	-1.391353000	-0.220150000
H	1.728962000	-2.474870000	-0.145200000

H	2.827180000	-1.229437000	-0.712993000
C	1.874096000	-0.776202000	1.184488000
H	0.992808000	-1.134292000	1.723041000
H	2.742834000	-1.154110000	1.728359000
C	1.873155000	0.775948000	1.184965000
H	0.991154000	1.132659000	1.723243000
H	2.741129000	1.154564000	1.729581000
C	1.860863000	1.392001000	-0.219274000
H	1.727141000	2.475362000	-0.143597000
H	2.826557000	1.231214000	-0.711845000
C	0.766954000	0.791902000	-1.098799000
H	0.790560000	1.224959000	-2.101949000
C	-0.629917000	0.694461000	-0.502959000
C	-1.701059000	1.434158000	-0.030935000
H	-1.715717000	2.518268000	-0.023711000

TS₄₋₉ G = -465.265424 a.u.

C	1.397249000	-0.257459000	1.397982000
C	1.785743000	1.083218000	0.955772000
C	1.094144000	-1.223109000	0.491320000
H	2.295723000	1.648372000	1.736088000
H	0.718063000	-2.176086000	0.851229000
H	1.138280000	-0.403727000	2.442545000
H	0.763534000	1.561276000	0.814278000
C	-1.021046000	0.968791000	0.025068000
C	-0.913162000	-0.282908000	0.249883000
C	-2.271530000	1.485468000	-0.325483000
H	-2.448119000	2.533244000	-0.544960000
C	-1.860641000	-1.285191000	0.237964000
H	-1.686374000	-2.334192000	0.443518000
C	-3.127387000	-0.790937000	-0.095207000
H	-3.966354000	-1.476422000	-0.140447000
C	-3.326594000	0.568407000	-0.370628000
H	-4.324241000	0.913366000	-0.621363000
C	1.653961000	-1.165972000	-0.915980000
H	0.896376000	-0.815972000	-1.623492000
H	1.936014000	-2.175547000	-1.225600000
C	2.487969000	1.151231000	-0.419258000
H	1.811899000	1.626222000	-1.135837000
H	3.376794000	1.781935000	-0.352147000
C	2.864724000	-0.230820000	-0.953166000
H	3.244914000	-0.146094000	-1.973892000
H	3.662910000	-0.660692000	-0.339526000

9 G = -465.412295 a.u.

C	1.337589000	0.757226000	1.045847000
C	2.553115000	1.136520000	0.656344000
C	0.619018000	-0.457360000	0.503099000
H	2.987294000	2.036079000	1.083795000
H	0.673548000	-1.249656000	1.261789000
H	0.804945000	1.341175000	1.791938000
H	-0.490107000	1.724084000	-0.681365000
C	-1.243740000	0.994070000	-0.401429000
C	-0.848131000	-0.179248000	0.244741000
C	-2.583802000	1.235131000	-0.680256000

H	-2.874055000	2.151884000	-1.180412000
C	-1.826444000	-1.104777000	0.604161000
H	-1.533266000	-2.019101000	1.110722000
C	-3.169969000	-0.867764000	0.326667000
H	-3.917238000	-1.596992000	0.617594000
C	-3.552402000	0.303858000	-0.316498000
H	-4.597781000	0.492509000	-0.530465000
C	1.307891000	-0.966856000	-0.773815000
H	1.067325000	-0.282931000	-1.596327000
H	0.900983000	-1.945529000	-1.041587000
C	3.382389000	0.377843000	-0.346340000
H	3.414382000	0.939547000	-1.288538000
H	4.416823000	0.321968000	0.005598000
C	2.822974000	-1.024528000	-0.589504000
H	3.299072000	-1.477360000	-1.462518000
H	3.057154000	-1.660367000	0.271670000

10a G = -306.325581 a.u.

C	0.661400000	1.183424000	0.080524000
H	1.233045000	2.094949000	0.170439000
O	1.419042000	0.046955000	0.141652000
C	0.697055000	-1.089255000	-0.304679000
H	0.616947000	-1.059578000	-1.397329000
H	1.265611000	-1.968004000	-0.002261000
C	-0.696272000	-1.089761000	0.304646000
H	-1.264235000	-1.968869000	0.002152000
H	-0.616212000	-1.060124000	1.397301000
O	-1.419079000	0.045978000	-0.141584000
C	-0.662249000	1.182933000	-0.080554000
H	-1.234465000	2.094114000	-0.170470000

TS₁₀₋₁₁ (a) G = -537.097057 a.u.

C	1.378713000	-0.569966000	-1.001156000
O	2.175154000	-1.368546000	-0.200193000
C	3.001585000	-0.702717000	0.671924000
C	2.885143000	0.594154000	0.922524000
O	1.914721000	1.371922000	0.359745000
C	1.409736000	0.880418000	-0.867590000
H	0.148250000	-0.844314000	-0.620358000
H	1.851176000	1.399252000	-1.720465000
H	3.530852000	1.119651000	1.610272000
H	1.359983000	-0.944860000	-2.022786000
H	0.261410000	1.199186000	-0.842834000
C	-2.500358000	1.376677000	-0.045867000
C	-1.284603000	0.773073000	-0.353934000
C	-3.509859000	0.497764000	0.353902000
H	-4.487314000	0.892168000	0.611117000
C	-1.111392000	-0.502598000	-0.266849000
C	-3.293044000	-0.885516000	0.432957000
H	-4.102950000	-1.532991000	0.749539000
C	-2.054502000	-1.445564000	0.115324000
H	-1.874584000	-2.511607000	0.175887000
H	-2.680914000	2.443565000	-0.102705000
H	3.746576000	-1.341412000	1.118505000

11a G = -305.117834 a.u.

C	-0.664221000	-1.143856000	-0.000651000
H	-1.249979000	-2.049559000	-0.001952000
O	-1.431262000	0.002035000	0.001494000
C	-0.660740000	1.145956000	-0.000618000
H	-1.244055000	2.053197000	-0.002385000
C	0.664183000	1.143877000	-0.000597000
H	1.249895000	2.049553000	-0.002094000
O	1.431342000	-0.001970000	0.001486000
C	0.660656000	-1.146078000	-0.000675000
H	1.244230000	-2.053101000	-0.002160000

TS₁₀₋₁₂ (a) G = -537.119849 a.u.

H	-4.268377000	1.016424000	-0.189977000
C	-3.253523000	0.638941000	-0.114119000
C	-3.051031000	-0.741642000	0.022687000
H	-3.896168000	-1.418917000	0.061762000
C	-1.755934000	-1.245816000	0.113842000
H	-1.558454000	-2.306127000	0.233354000
C	-0.794762000	-0.252803000	0.052474000
C	1.031565000	-0.995172000	0.736813000
H	0.625812000	-1.785278000	1.351500000
O	1.681985000	-0.051357000	1.435743000
C	2.235636000	1.012450000	0.646082000
H	1.444342000	1.732547000	0.446599000
H	3.027769000	1.453378000	1.251109000
C	2.796562000	0.471226000	-0.653488000
H	3.112233000	1.285265000	-1.303004000
H	3.639641000	-0.200424000	-0.467898000
O	1.800837000	-0.258624000	-1.379834000
C	1.114589000	-1.116457000	-0.624895000
H	0.648289000	-1.930180000	-1.160690000
C	-0.853303000	1.043690000	-0.090394000
C	-2.178670000	1.526301000	-0.157441000
H	-2.384436000	2.588862000	-0.259392000

12a G = -537.124534 a.u.

H	-4.085505000	1.182189000	-0.184768000
C	-3.102083000	0.737091000	-0.062594000
C	-2.981391000	-0.664959000	-0.072332000
H	-3.862299000	-1.291487000	-0.147622000
C	-1.733461000	-1.227700000	0.061416000
H	-1.624090000	-2.307083000	0.143804000
C	-0.619901000	-0.356398000	0.165695000
C	0.774586000	-1.108880000	0.422122000
H	0.560725000	-2.136630000	0.695657000
O	1.679259000	-0.564285000	1.309078000
C	2.200584000	0.703127000	0.917375000
H	1.425552000	1.460855000	1.032270000
H	3.053741000	0.893051000	1.569996000
C	2.669194000	0.667726000	-0.523455000
H	2.867853000	1.671188000	-0.893184000
H	3.556855000	0.042334000	-0.640175000
O	1.672497000	0.123566000	-1.423772000

C	0.945746000	-0.855482000	-0.977092000
H	0.438563000	-1.435717000	-1.736152000
C	-0.667629000	1.033238000	0.120122000
C	-1.986377000	1.543550000	0.103330000
H	-2.141039000	2.619181000	0.150204000

13a G = -537.237518 a.u.

H	-3.673656000	1.221322000	0.756408000
C	-2.788269000	0.700387000	0.410049000
C	-2.788211000	-0.700534000	0.410062000
H	-3.673555000	-1.221535000	0.756433000
C	-1.684641000	-1.436023000	-0.024464000
H	-1.697601000	-2.519512000	-0.021754000
C	-0.588668000	-0.694680000	-0.441479000
C	0.820312000	-0.787985000	-1.023194000
H	0.901023000	-1.261212000	-2.001667000
O	1.848042000	-1.321268000	-0.233945000
C	1.884413000	-0.775508000	1.073506000
H	1.030030000	-1.148238000	1.651121000
H	2.799278000	-1.163100000	1.519605000
C	1.884159000	0.775463000	1.073620000
H	1.029523000	1.147839000	1.651083000
H	2.798795000	1.163278000	1.519992000
O	1.847912000	1.321379000	-0.233766000
C	0.820268000	0.788118000	-1.023154000
H	0.901043000	1.261434000	-2.001579000
C	-0.588724000	0.694700000	-0.441489000
C	-1.684757000	1.435959000	-0.024485000
H	-1.697807000	2.519447000	-0.021797000

10b G = -940.684070 a.u.

C	-0.649631000	1.207130000	-0.471911000
H	-1.256780000	2.100321000	-0.474102000
N	-1.340424000	-0.021324000	-0.437923000
C	-0.507672000	-1.171970000	-0.082338000
H	-0.231012000	-1.138404000	0.977877000
H	-1.062454000	-2.086648000	-0.287009000
C	0.750128000	-1.108578000	-0.945861000
H	1.395810000	-1.961042000	-0.741080000
H	0.469687000	-1.131346000	-2.000249000
N	1.494033000	0.130014000	-0.706640000
C	0.678907000	1.282151000	-0.558986000
H	1.183012000	2.235728000	-0.604853000
C	2.582254000	0.029227000	0.170724000
F	3.222473000	1.193303000	0.268318000
F	2.238764000	-0.334206000	1.430981000
F	3.447333000	-0.898304000	-0.252014000
C	-2.623676000	0.001061000	0.123643000
F	-3.344028000	1.007793000	-0.373219000
F	-3.263958000	-1.143944000	-0.127103000
F	-2.628959000	0.151629000	1.467451000

TS₁₀₋₁₁ (b) G = -1171.460597 a.u.

C	0.839553000	-0.493320000	1.187776000
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N	1.667898000	-1.224898000	0.261248000
C	1.022477000	-1.861883000	-0.825931000
C	-0.287484000	-2.070782000	-0.832911000
N	-1.124020000	-1.679547000	0.230654000
C	-0.584197000	-0.802794000	1.265003000
H	0.829580000	0.719194000	0.777320000
H	-0.899846000	-1.124669000	2.254914000
H	-0.762536000	-2.617419000	-1.633522000
H	1.313917000	-0.405703000	2.161501000
H	-1.106847000	0.276542000	1.115581000
C	-1.999018000	2.755380000	0.173213000
C	-1.066204000	1.781456000	0.509208000
C	-1.431193000	3.909662000	-0.371893000
H	-2.078343000	4.728448000	-0.667555000
C	0.196197000	1.913916000	0.331456000
C	-0.045350000	4.039458000	-0.556011000
H	0.346532000	4.953093000	-0.989012000
C	0.841387000	3.019711000	-0.203685000
H	1.910067000	3.105402000	-0.351809000
H	-3.069183000	2.656112000	0.305917000
H	1.660999000	-2.232955000	-1.611761000
C	2.910586000	-0.634596000	-0.018373000
F	2.830980000	0.471280000	-0.792923000
F	3.510103000	-0.257485000	1.113083000
F	3.705797000	-1.489289000	-0.660908000
C	-2.477453000	-1.491349000	-0.084080000
F	-2.725355000	-0.433182000	-0.884389000
F	-2.965205000	-2.560121000	-0.722306000
F	-3.186020000	-1.299657000	1.031051000

11b G = -939.477908 a.u.

C	-0.662684000	1.196399000	-0.333289000
H	-1.227242000	2.113955000	-0.271746000
N	-1.418209000	-0.000006000	-0.495004000
C	-0.662669000	-1.196410000	-0.333290000
H	-1.227236000	-2.113954000	-0.271677000
C	0.662665000	-1.196386000	-0.333302000
H	1.227198000	-2.113953000	-0.271666000
N	1.418181000	0.000025000	-0.494878000
C	0.662653000	1.196422000	-0.333214000
H	1.227188000	2.113993000	-0.271676000
C	2.701726000	-0.000017000	0.082062000
F	3.378458000	1.084161000	-0.297483000
F	2.696530000	-0.000236000	1.430259000
F	3.378565000	-1.083945000	-0.297842000
C	-2.701712000	0.000013000	0.082041000
F	-3.378602000	1.083951000	-0.297744000
F	-3.378488000	-1.084135000	-0.297444000
F	-2.696417000	0.000171000	1.430242000

TS₁₀₋₁₂ (b) G = -1171.479533 a.u.

H	-1.848477000	4.536880000	1.082423000
C	-1.517751000	3.588811000	0.670430000
C	-1.957839000	3.213525000	-0.605576000
H	-2.632028000	3.857626000	-1.158540000

C	-1.545824000	2.006538000	-1.173230000
H	-1.897024000	1.679938000	-2.145354000
C	-0.699840000	1.302207000	-0.336897000
C	-0.400034000	-0.605011000	-1.123179000
H	-1.008092000	-0.518520000	-2.011255000
N	-0.862697000	-1.527103000	-0.158104000
C	-0.093701000	-1.612906000	1.091079000
H	-0.317373000	-0.760655000	1.735090000
H	-0.359614000	-2.544913000	1.590679000
C	1.393034000	-1.629274000	0.769714000
H	1.956493000	-1.516901000	1.694786000
H	1.674613000	-2.568881000	0.286660000
N	1.730113000	-0.509077000	-0.117262000
C	0.924018000	-0.269495000	-1.187766000
H	1.303316000	0.331809000	-1.999482000
C	-0.218078000	1.574026000	0.830234000
C	-0.663536000	2.771254000	1.413885000
H	-0.348932000	3.087953000	2.403785000
C	3.064577000	-0.055525000	-0.106045000
F	3.454637000	0.249415000	1.129698000
F	3.921123000	-0.999568000	-0.549153000
F	3.212224000	1.009700000	-0.882614000
C	-2.254962000	-1.634472000	0.005211000
F	-2.800294000	-0.674888000	0.771024000
F	-2.872638000	-1.589688000	-1.177987000
F	-2.556737000	-2.798209000	0.593657000

12b G = -1171.484768 a.u.

H	-0.675523000	4.657866000	1.058381000
C	-0.658489000	3.651574000	0.651819000
C	-1.474499000	3.332386000	-0.433928000
H	-2.154180000	4.071629000	-0.841327000
C	-1.436235000	2.054705000	-0.976097000
H	-2.126389000	1.771984000	-1.766977000
C	-0.534145000	1.131109000	-0.432951000
C	-0.559047000	-0.337662000	-1.042713000
H	-1.123874000	-0.341487000	-1.970301000
N	-1.111955000	-1.338592000	-0.125663000
C	-0.407513000	-1.404253000	1.156447000
H	-0.578576000	-0.498806000	1.745681000
H	-0.767365000	-2.274736000	1.706245000
C	1.083270000	-1.567543000	0.918629000
H	1.620519000	-1.327655000	1.833791000
H	1.319563000	-2.586113000	0.600318000
N	1.568474000	-0.653143000	-0.140358000
C	0.868759000	-0.501501000	-1.256440000
H	1.345603000	-0.029556000	-2.102890000
C	0.308464000	1.442072000	0.598528000
C	0.187145000	2.688203000	1.207835000
H	0.787677000	2.952511000	2.073706000
C	2.986360000	-0.416921000	-0.144494000
F	3.401382000	-0.030897000	1.050157000
F	3.644908000	-1.545699000	-0.447612000
F	3.306522000	0.498517000	-1.041005000
C	-2.508590000	-1.306097000	0.018487000
F	-2.976630000	-0.280552000	0.757900000

F	-3.106194000	-1.224835000	-1.173637000
F	-2.933985000	-2.422081000	0.624730000

13b G = -1171.597142 a.u.

H	-0.864381000	4.609083000	-0.805382000
C	-0.419435000	3.693313000	-0.433759000
C	0.973074000	3.627033000	-0.302050000
H	1.563736000	4.493631000	-0.575603000
C	1.617663000	2.477658000	0.161473000
H	2.696613000	2.429459000	0.243639000
C	0.788594000	1.414964000	0.480668000
C	0.767749000	-0.035216000	0.967440000
H	1.169399000	-0.225226000	1.960969000
N	1.245092000	-1.070421000	0.053103000
C	0.686469000	-0.918010000	-1.294270000
H	0.937463000	0.067826000	-1.699883000
H	1.131598000	-1.673349000	-1.938181000
C	-0.841855000	-1.111142000	-1.276365000
H	-1.295033000	-0.384181000	-1.961037000
H	-1.095181000	-2.112628000	-1.618814000
N	-1.392160000	-0.968975000	0.081517000
C	-0.798319000	0.071003000	0.902451000
H	-1.261445000	0.038970000	1.887686000
C	-0.591839000	1.483629000	0.356900000
C	-1.244550000	2.616196000	-0.101852000
H	-2.320865000	2.672685000	-0.209835000
C	2.632140000	-1.248062000	0.077449000
F	3.334683000	-0.175244000	-0.378442000
F	3.066067000	-1.470282000	1.320713000
F	3.000835000	-2.280552000	-0.684961000
C	-2.787360000	-0.990833000	0.119657000
F	-3.241397000	-1.091582000	1.372114000
F	-3.368886000	0.129577000	-0.394781000
F	-3.272015000	-2.014549000	-0.587124000

10c G = -722.249982 a.u.

C	0.667527000	1.422863000	-0.001491000
H	1.246863000	2.332655000	0.014866000
N	1.406158000	0.228731000	-0.048046000
C	0.663726000	-0.981139000	-0.377317000
H	0.472101000	-1.013012000	-1.455023000
H	1.252403000	-1.850407000	-0.096594000
C	-0.663666000	-0.981320000	0.376663000
H	-1.252344000	-1.850453000	0.095519000
H	-0.472004000	-1.013874000	1.454342000
N	-1.406123000	0.228745000	0.048085000
C	-0.667461000	1.422812000	0.000842000
H	-1.246818000	2.332580000	-0.016026000
C	2.771283000	0.290389000	0.043630000
O	3.400877000	1.297265000	0.256709000
O	3.332147000	-0.921525000	-0.135458000
C	4.756847000	-0.935702000	-0.035537000
H	5.195122000	-0.263719000	-0.773052000
H	5.070916000	-0.626101000	0.961296000
H	5.051935000	-1.963871000	-0.228806000

C	-2.771300000	0.290378000	-0.043417000
O	-3.400948000	1.297304000	-0.256057000
O	-3.332156000	-0.921588000	0.135381000
C	-4.756896000	-0.935660000	0.036003000
H	-5.194826000	-0.263337000	0.773409000
H	-5.071307000	-0.626445000	-0.960843000
H	-5.051996000	-1.963728000	0.229783000

TS₁₀₋₁₁ (c) G = -953.032579 a.u.

C	0.730779000	-0.389584000	1.364677000
N	1.386284000	-1.216813000	0.377904000
C	0.665380000	-2.226718000	-0.281503000
C	-0.664601000	-2.226924000	-0.281486000
N	-1.385800000	-1.217256000	0.377958000
C	-0.730543000	-0.389864000	1.364765000
H	1.023640000	0.754191000	1.050002000
H	-1.178501000	-0.501001000	2.352063000
H	-1.242188000	-2.995204000	-0.768421000
H	1.178910000	-0.500410000	2.351932000
H	-1.023947000	0.753790000	1.050204000
C	-1.441674000	3.075184000	-0.160370000
C	-0.639430000	2.078019000	0.373888000
C	-0.703004000	4.119927000	-0.725006000
H	-1.227762000	4.954684000	-1.177191000
C	0.638505000	2.078207000	0.373787000
C	0.701361000	4.120115000	-0.725128000
H	1.225819000	4.955009000	-1.177407000
C	1.440404000	3.075572000	-0.160614000
H	2.523041000	3.069254000	-0.153432000
H	-2.524308000	3.068591000	-0.153009000
H	1.243185000	-2.994844000	-0.768418000
C	2.725223000	-0.996454000	0.186542000
O	3.357706000	-0.151639000	0.773966000
O	3.247018000	-1.835929000	-0.723760000
C	4.643320000	-1.657078000	-0.965929000
H	4.834834000	-0.655967000	-1.352169000
H	5.209904000	-1.802239000	-0.046243000
H	4.908827000	-2.409316000	-1.704163000
C	-2.724777000	-0.997216000	0.186538000
O	-3.357518000	-0.152669000	0.774072000
O	-3.246290000	-1.836666000	-0.723946000
C	-4.642684000	-1.658358000	-0.965970000
H	-5.209236000	-1.805253000	-0.046531000
H	-4.834851000	-0.656820000	-1.350758000
H	-4.907636000	-2.409721000	-1.705296000

11c G = -721.049711 a.u.

C	-0.663947000	1.414633000	-0.000158000
H	-1.250030000	2.319724000	-0.000270000
N	-1.405507000	0.210202000	-0.000329000
C	-0.664904000	-0.993536000	-0.000219000
H	-1.235221000	-1.906932000	-0.000394000
C	0.664904000	-0.993540000	0.000073000
H	1.235230000	-1.906930000	0.000152000
N	1.405510000	0.210202000	0.000294000

C	0.663951000	1.414634000	0.000128000
H	1.250036000	2.319724000	0.000241000
C	-2.775951000	0.272343000	-0.000112000
O	-3.409227000	1.299473000	-0.000061000
O	-3.321574000	-0.955977000	-0.000013000
C	-4.750617000	-0.971449000	0.000262000
H	-5.134372000	-0.470801000	0.888925000
H	-5.134697000	-0.471395000	-0.888598000
H	-5.029454000	-2.021892000	0.000653000
C	2.775949000	0.272340000	0.000129000
O	3.409231000	1.299470000	0.000086000
O	3.321569000	-0.955981000	0.000037000
C	4.750613000	-0.971447000	-0.000148000
H	5.134414000	-0.470932000	-0.888867000
H	5.134638000	-0.471257000	0.888658000
H	5.029449000	-2.021891000	-0.000370000

TS₁₀₋₁₂ (c) G = -953.048805 a.u.

H	-4.044018000	1.428976000	-0.760964000
C	-3.073941000	0.964117000	-0.615460000
C	-2.987007000	-0.434992000	-0.602276000
H	-3.876485000	-1.041503000	-0.727629000
C	-1.749501000	-1.049964000	-0.422858000
H	-1.638287000	-2.129115000	-0.402393000
C	-0.723068000	-0.136091000	-0.275913000
C	0.972663000	-1.106086000	0.585415000
H	0.460827000	-1.952779000	1.014747000
N	1.576209000	-0.241687000	1.474390000
C	2.353378000	0.901357000	0.970502000
H	1.685953000	1.753451000	0.846718000
H	3.120080000	1.135099000	1.708916000
C	2.989462000	0.530428000	-0.359506000
H	3.414246000	1.414363000	-0.829751000
H	3.779580000	-0.210451000	-0.211228000
N	1.997050000	-0.029960000	-1.273321000
C	1.156524000	-1.002043000	-0.770172000
H	0.750764000	-1.735856000	-1.449521000
C	-0.670074000	1.170000000	-0.277679000
C	-1.940932000	1.761511000	-0.446346000
H	-2.059118000	2.842285000	-0.457510000
C	1.247530000	-0.232357000	2.819301000
O	1.671237000	0.577641000	3.599830000
O	0.426691000	-1.241934000	3.138715000
C	0.029007000	-1.277305000	4.512511000
H	0.900872000	-1.398233000	5.154882000
H	-0.490440000	-0.356504000	4.775914000
H	-0.636164000	-2.132084000	4.599596000
C	1.741536000	0.604760000	-2.479338000
O	2.359062000	1.551348000	-2.888812000
O	0.744547000	-0.002418000	-3.129795000
C	0.301599000	0.673478000	-4.308972000
H	-0.048675000	1.672565000	-4.049590000
H	1.112053000	0.745441000	-5.033897000
H	-0.515306000	0.072297000	-4.698707000

12c G = -953.053792 a.u.

H	0.483207000	4.269245000	1.443807000
C	0.410847000	3.325357000	0.909812000
C	0.258562000	3.353930000	-0.496206000
H	0.213614000	4.297327000	-1.026210000
C	0.172787000	2.165115000	-1.165709000
H	0.059203000	2.144929000	-2.247860000
C	0.244690000	0.957186000	-0.409518000
C	-0.799815000	-0.281421000	-1.081594000
H	-1.418440000	0.209872000	-1.816301000
N	-1.462304000	-1.130053000	-0.216379000
C	-0.707203000	-2.110184000	0.579221000
H	-0.387810000	-1.632512000	1.506932000
H	-1.372782000	-2.946839000	0.789195000
C	0.498936000	-2.561650000	-0.222812000
H	1.132223000	-3.204362000	0.384552000
H	0.181549000	-3.111985000	-1.113452000
N	1.301978000	-1.417751000	-0.643108000
C	0.614162000	-0.361238000	-1.283082000
H	1.006599000	-0.042483000	-2.242242000
C	0.390095000	0.853839000	0.989627000
C	0.465621000	2.130539000	1.605604000
H	0.578382000	2.184106000	2.686233000
C	-2.747921000	-0.837134000	0.213407000
O	-3.326201000	-1.466078000	1.057546000
O	-3.261171000	0.211594000	-0.443214000
C	-4.586209000	0.574205000	-0.043729000
H	-5.276515000	-0.246913000	-0.235869000
H	-4.601896000	0.819785000	1.017582000
H	-4.843235000	1.443126000	-0.643252000
C	2.513050000	-1.191338000	-0.022787000
O	3.036131000	-1.948687000	0.753153000
O	3.049896000	-0.038665000	-0.443592000
C	4.238816000	0.351365000	0.244645000
H	4.024602000	0.483947000	1.305437000
H	5.015387000	-0.403165000	0.120452000
H	4.540442000	1.293829000	-0.205012000

13c G = -953.161460 a.u.

H	1.640001000	4.452104000	1.018594000
C	1.032340000	3.633642000	0.649731000
C	-0.359384000	3.715568000	0.788700000
H	-0.784706000	4.595114000	1.258477000
C	-1.208665000	2.704343000	0.332260000
H	-2.285318000	2.778859000	0.425915000
C	-0.576109000	1.616824000	-0.246586000
C	-0.814980000	0.293227000	-0.959123000
H	-1.279775000	0.410491000	-1.937244000
N	-1.506908000	-0.769437000	-0.253198000
C	-0.760471000	-1.509523000	0.755923000
H	-0.525031000	-0.862833000	1.610652000
H	-1.373409000	-2.338706000	1.099846000
C	0.524091000	-2.034696000	0.142291000
H	1.083970000	-2.603274000	0.880888000
H	0.282385000	-2.695652000	-0.698641000
N	1.353673000	-0.922153000	-0.300441000

C	0.758782000	0.174511000	-1.055800000
H	1.130517000	0.163518000	-2.083727000
C	0.799883000	1.533606000	-0.377082000
C	1.654945000	2.535242000	0.050941000
H	2.729617000	2.467737000	-0.059522000
C	-2.870179000	-0.698497000	-0.269244000
O	-3.505739000	0.084291000	-0.937554000
O	-3.438060000	-1.618796000	0.536094000
C	-4.865544000	-1.613114000	0.530165000
H	-5.243538000	-0.644080000	0.855421000
H	-5.242938000	-1.825763000	-0.469892000
H	-5.162967000	-2.393549000	1.225835000
C	2.709312000	-0.904406000	-0.216382000
O	3.404011000	-0.013196000	-0.653686000
O	3.202947000	-1.990544000	0.413999000
C	4.623156000	-1.999631000	0.555623000
H	5.103474000	-1.967911000	-0.422043000
H	4.952984000	-1.142912000	1.143173000
H	4.859040000	-2.928628000	1.068410000

14a G = -231.117869 a.u.

C	0.986314000	-0.646274000	0.107840000
O	-0.338459000	-1.171744000	-0.103524000
C	-1.191670000	-0.115230000	0.013519000
C	-0.607531000	1.076732000	0.062612000
C	0.884536000	0.876883000	-0.091527000
H	1.660130000	-1.147032000	-0.584991000
H	-2.239916000	-0.377346000	0.032695000
H	-1.115964000	2.025572000	0.125556000
H	1.475817000	1.417527000	0.649039000
H	1.224158000	1.190666000	-1.084002000
H	1.273561000	-0.888103000	1.135231000

TS₁₄₋₁₅ (a) G = -461.911061 a.u.

C	-1.810173000	-0.717983000	0.828122000
O	-2.639836000	-1.099106000	-0.266264000
C	-2.928434000	0.024259000	-0.958129000
C	-2.469937000	1.150454000	-0.398941000
C	-1.687646000	0.765803000	0.793892000
H	-0.755814000	-1.157330000	0.630876000
H	-1.823524000	1.316150000	1.722271000
H	-3.498394000	-0.126545000	-1.863280000
H	-2.604142000	2.148734000	-0.782462000
H	-2.184567000	-1.167055000	1.745760000
H	-0.487543000	0.967116000	0.563491000
C	1.928139000	1.411386000	0.064763000
C	0.892412000	0.514152000	0.272367000
C	3.135644000	0.774931000	-0.237185000
H	4.019431000	1.375748000	-0.421504000
C	0.953322000	-0.760217000	0.212633000
C	3.230292000	-0.622831000	-0.309526000
H	4.188362000	-1.072956000	-0.547504000
C	2.124667000	-1.448876000	-0.083758000
H	2.208879000	-2.527498000	-0.143868000
H	1.846290000	2.490011000	0.120896000

15a G = -229.944363 a.u.

C	0.000000000	0.717336000	-0.954927000
C	0.000000000	-0.717336000	-0.954927000
C	0.000000000	-1.088614000	0.347385000
O	0.000000000	0.000000000	1.151750000
C	0.000000000	1.088614000	0.347385000
H	0.000000000	1.374807000	-1.808494000
H	0.000000000	-1.374807000	-1.808494000
H	0.000000000	-2.042249000	0.846750000
H	0.000000000	2.042249000	0.846750000

TS₁₄₋₁₆ (a) G = -461.920110 a.u.

H	-4.143470000	0.817321000	-0.237382000
C	-3.108660000	0.509867000	-0.127531000
C	-2.816091000	-0.858066000	-0.032479000
H	-3.619618000	-1.585189000	-0.066230000
C	-1.495689000	-1.303294000	0.106229000
H	-1.235212000	-2.351932000	0.185153000
C	-0.628079000	-0.236738000	0.135774000
C	1.474237000	-0.891259000	0.765735000
H	1.131121000	-1.645525000	1.456309000
C	2.077618000	0.437553000	1.142667000
H	1.309812000	1.111941000	1.534540000
H	2.872984000	0.330786000	1.881695000
C	2.605574000	0.939161000	-0.216117000
H	2.165882000	1.886167000	-0.517820000
H	3.694241000	0.998651000	-0.255361000
O	2.203799000	-0.048035000	-1.206225000
C	1.642375000	-1.068322000	-0.561850000
H	1.353578000	-1.906291000	-1.182331000
C	-0.782200000	1.023674000	0.047330000
C	-2.102277000	1.480245000	-0.089434000
H	-2.360571000	2.531423000	-0.170709000

16a G = -461.930525 a.u.

H	-3.897995000	0.993047000	-0.280998000
C	-2.893718000	0.611058000	-0.119682000
C	-2.692822000	-0.781700000	-0.083523000
H	-3.527618000	-1.463486000	-0.193309000
C	-1.417747000	-1.258647000	0.113816000
H	-1.234579000	-2.329147000	0.185325000
C	-0.369977000	-0.317724000	0.271543000
C	1.051611000	-0.928574000	0.597751000
H	0.967839000	-1.905844000	1.059995000
C	2.067108000	0.066544000	1.154924000
H	1.587916000	0.736734000	1.867635000
H	2.896319000	-0.464326000	1.624565000
C	2.521030000	0.848245000	-0.085235000
H	2.075057000	1.836738000	-0.126155000
H	3.599682000	0.870021000	-0.238817000
O	1.969670000	0.119854000	-1.235403000
C	1.222647000	-0.849410000	-0.822076000
H	0.812438000	-1.504705000	-1.579459000

C	-0.486116000	1.073725000	0.193091000
C	-1.832220000	1.489482000	0.038763000
H	-2.055191000	2.554133000	0.008205000

TS₁₆₋₁₇ (a) G = -461.926619 a.u.

C	0.436224000	-0.434359000	-0.134018000
C	0.468709000	0.971548000	-0.197844000
C	1.790763000	1.481258000	-0.128793000
C	1.547248000	-1.284918000	0.033130000
C	-0.975276000	-1.052975000	-0.125519000
C	-1.345769000	-0.375702000	1.112784000
H	-0.950381000	-2.139688000	-0.045363000
H	-0.952291000	-0.574333000	2.103891000
C	2.804432000	-0.715018000	0.056225000
H	3.689181000	-1.336433000	0.135088000
C	2.920320000	0.682071000	-0.028996000
H	3.909473000	1.130715000	-0.006187000
H	1.429319000	-2.363473000	0.105456000
H	1.941797000	2.558890000	-0.156649000
O	-2.221046000	0.537912000	1.012568000
C	-1.977920000	-0.467818000	-1.134807000
H	-1.459927000	-0.147436000	-2.037750000
H	-2.748866000	-1.198690000	-1.382456000
C	-2.566706000	0.741591000	-0.404478000
H	-3.650908000	0.830564000	-0.433941000
H	-2.051183000	1.662521000	-0.668745000

17a G = -462.040642 a.u.

H	-3.537999000	-1.251734000	-0.625590000
C	-2.640682000	-0.716650000	-0.336523000
C	-2.663747000	0.681691000	-0.325117000
H	-3.578655000	1.190989000	-0.605973000
C	-1.542633000	1.435692000	0.035906000
H	-1.575854000	2.519097000	0.035145000
C	-0.414158000	0.711383000	0.383255000
C	1.039390000	0.840630000	0.809854000
H	1.231736000	1.368511000	1.743480000
C	2.109812000	-0.164241000	-1.081668000
H	1.275647000	-0.244388000	-1.789042000
H	3.046396000	-0.315689000	-1.616217000
O	2.008661000	-1.179141000	-0.089897000
C	1.056049000	-0.742957000	0.849266000
H	1.245770000	-1.239481000	1.799872000
C	-0.395856000	-0.676500000	0.382031000
C	-1.494975000	-1.435302000	0.018170000
H	-1.487225000	-2.518762000	0.005135000
C	2.040347000	1.157547000	-0.305616000
H	1.732922000	1.994745000	-0.934341000
H	3.016692000	1.382089000	0.129367000

TS₁₄₋₁₈ (a) G = -461.912852 a.u.

C	-1.642670000	0.562109000	1.114882000
C	-2.066012000	-0.805587000	0.839559000
C	-1.371995000	1.129328000	-0.103227000

H	-2.709575000	-1.299427000	1.561957000
H	-1.070581000	2.144804000	-0.321667000
H	-1.350808000	0.975062000	2.068528000
H	-1.052096000	-1.364545000	0.755403000
C	0.647869000	-0.939105000	0.058197000
C	0.527745000	0.348654000	0.093484000
C	1.923506000	-1.487782000	-0.092751000
H	2.104659000	-2.555556000	-0.161625000
C	1.511139000	1.319621000	0.064161000
H	1.336443000	2.389883000	0.089044000
C	2.799262000	0.788705000	-0.043294000
H	3.650786000	1.458888000	-0.078391000
C	2.999353000	-0.595055000	-0.117992000
H	4.011800000	-0.978240000	-0.192110000
O	-1.931774000	0.462505000	-1.140434000
C	-2.581062000	-0.712617000	-0.600068000
H	-2.287508000	-1.563349000	-1.212898000
H	-3.661744000	-0.557186000	-0.662465000

18a G = -462.056213 a.u.

C	1.704578000	-0.833726000	0.943441000
C	2.766455000	-0.042124000	0.950113000
C	0.976076000	-0.709622000	-0.374464000
H	3.474012000	0.088073000	1.757901000
H	1.004858000	-1.658888000	-0.926811000
H	1.359976000	-1.479810000	1.739421000
H	0.007518000	1.772420000	0.103621000
C	-0.788088000	1.036462000	0.067659000
C	-0.469685000	-0.292786000	-0.203954000
C	-2.109756000	1.412317000	0.270737000
H	-2.350618000	2.449269000	0.474621000
C	-1.487834000	-1.239007000	-0.270251000
H	-1.245485000	-2.272891000	-0.496874000
C	-2.812654000	-0.866094000	-0.059874000
H	-3.599049000	-1.609460000	-0.118993000
C	-3.125576000	0.460871000	0.210503000
H	-4.156465000	0.755405000	0.367243000
O	1.715703000	0.272459000	-1.092632000
C	2.869809000	0.676025000	-0.365211000
H	2.865262000	1.766190000	-0.252638000
H	3.774418000	0.396116000	-0.918624000

14b G = -548.296666 a.u.

C	2.425650000	0.611898000	-0.044722000
C	0.986539000	1.153531000	0.004593000
N	0.172345000	-0.010893000	-0.416581000
C	0.935702000	-1.169634000	-0.111209000
C	2.211387000	-0.876269000	0.115364000
H	2.896170000	0.826658000	-1.010079000
H	0.808626000	1.998786000	-0.656679000
H	0.452105000	-2.135267000	-0.145551000
H	2.992715000	-1.600144000	0.289354000
H	0.719942000	1.429322000	1.031265000
H	3.049574000	1.052052000	0.733775000
C	-1.167958000	0.000277000	-0.026347000

F	-1.771473000	1.108434000	-0.464583000
F	-1.813581000	-1.063081000	-0.512931000
F	-1.356442000	-0.024683000	1.316171000

TS₁₄₋₁₅ (b) G = -779.089350 a.u.

C	-0.798329000	0.753256000	1.135128000
N	-1.889341000	0.531674000	0.193063000
C	-1.765451000	1.463694000	-0.850642000
C	-0.855853000	2.398302000	-0.553414000
C	-0.180915000	2.041272000	0.718192000
H	0.030734000	-0.070148000	0.954680000
H	-0.066953000	2.811945000	1.477572000
H	-2.405527000	1.373942000	-1.715763000
H	-0.627664000	3.262000000	-1.158179000
H	-1.112224000	0.656554000	2.171472000
H	0.985322000	1.755445000	0.464630000
C	3.380833000	0.983052000	-0.219514000
C	2.091462000	0.718646000	0.219686000
C	4.126934000	-0.179221000	-0.437389000
H	5.150700000	-0.092309000	-0.784513000
C	1.594477000	-0.439034000	0.418663000
C	3.585016000	-1.456010000	-0.223746000
H	4.202253000	-2.327515000	-0.414326000
C	2.271232000	-1.634483000	0.221583000
H	1.852479000	-2.620650000	0.380354000
H	3.797689000	1.968719000	-0.386510000
C	-2.285506000	-0.781940000	-0.075152000
F	-1.347716000	-1.524546000	-0.699981000
F	-2.570776000	-1.419259000	1.063841000
F	-3.366489000	-0.794518000	-0.859552000

15b G = -547.124424 a.u.

C	2.357852000	0.714496000	0.031437000
C	1.060834000	1.130698000	-0.043409000
N	0.265845000	-0.000132000	-0.110276000
C	1.061008000	-1.130808000	-0.043217000
C	2.357973000	-0.714357000	0.031476000
H	3.219840000	1.360728000	0.068136000
H	0.620992000	2.113358000	-0.073771000
H	0.621369000	-2.113558000	-0.073257000
H	3.220064000	-1.360442000	0.068162000
C	-1.139946000	-0.000103000	-0.001699000
F	-1.650207000	1.083066000	-0.584194000
F	-1.650308000	-1.084614000	-0.581627000
F	-1.558319000	0.001690000	1.269725000

TS₁₄₋₁₆ (b) G = -779.096325 a.u.

H	-4.686621000	-1.697111000	-0.635811000
C	-3.820087000	-1.089266000	-0.396231000
C	-3.782978000	-0.417478000	0.832970000
H	-4.616050000	-0.504348000	1.521353000
C	-2.681843000	0.371453000	1.188245000
H	-2.628525000	0.910259000	2.126746000
C	-1.733004000	0.367845000	0.190825000

C	-0.110996000	1.821138000	0.600721000
H	-0.688346000	2.450579000	1.260325000
C	0.297892000	2.203107000	-0.806428000
H	-0.549760000	2.128222000	-1.490071000
H	0.692791000	3.219137000	-0.845989000
C	1.379914000	1.159441000	-1.168755000
H	1.155470000	0.625455000	-2.088655000
H	2.378601000	1.602800000	-1.228148000
N	1.333371000	0.213938000	-0.030561000
C	0.613327000	0.749950000	1.006739000
H	0.602332000	0.251403000	1.965957000
C	-1.662434000	-0.221170000	-0.939421000
C	-2.767012000	-0.999811000	-1.313026000
H	-2.824797000	-1.533470000	-2.256515000
C	2.351347000	-0.723960000	0.152405000
F	3.540208000	-0.159288000	0.464895000
F	2.052015000	-1.562051000	1.143966000
F	2.555172000	-1.420660000	-0.964808000

16b G = -779.109301 a.u.

H	4.157948000	-2.008232000	0.700138000
C	3.410681000	-1.259280000	0.452963000
C	3.501160000	-0.586989000	-0.777242000
H	4.318680000	-0.790897000	-1.458696000
C	2.543305000	0.354010000	-1.090895000
H	2.614228000	0.924314000	-2.015177000
C	1.514640000	0.593541000	-0.152657000
C	0.476824000	1.711541000	-0.541159000
H	0.890272000	2.385104000	-1.285672000
C	-0.267925000	2.346885000	0.638846000
H	0.406378000	2.475900000	1.483889000
H	-0.686082000	3.309679000	0.341492000
C	-1.387254000	1.352131000	0.994508000
H	-1.142891000	0.777759000	1.884526000
H	-2.377008000	1.807659000	1.061811000
N	-1.371896000	0.419048000	-0.162770000
C	-0.393471000	0.664101000	-1.017745000
H	-0.278964000	0.078953000	-1.919680000
C	1.330274000	-0.075345000	1.058089000
C	2.378986000	-0.982374000	1.340969000
H	2.368454000	-1.529043000	2.281899000
C	-2.174935000	-0.755450000	-0.160012000
F	-3.461614000	-0.412500000	-0.054044000
F	-2.009292000	-1.429256000	-1.293737000
F	-1.891476000	-1.551707000	0.857878000

TS₁₆₋₁₇ (b) G = -779.106020 a.u.

C	1.651616000	0.543101000	-0.136980000
C	1.294892000	-0.473850000	0.771133000
C	2.340806000	-1.410405000	0.961655000
C	2.866881000	0.638059000	-0.838836000
C	0.550168000	1.576631000	-0.441619000
C	-0.428360000	0.603635000	-0.939880000
H	0.870835000	2.291872000	-1.199564000
H	-0.352018000	0.028355000	-1.853742000

C	3.847428000	-0.301803000	-0.581397000
H	4.811409000	-0.239939000	-1.073400000
C	3.575669000	-1.332400000	0.329551000
H	4.342212000	-2.075853000	0.529887000
H	3.050965000	1.444814000	-1.544475000
H	2.180307000	-2.246771000	1.640006000
N	-1.427475000	0.439692000	-0.119409000
C	-0.149650000	2.195101000	0.785382000
H	0.549331000	2.287619000	1.614729000
H	-0.559638000	3.175865000	0.538842000
C	-1.275207000	1.212327000	1.139524000
H	-2.227599000	1.681345000	1.388437000
H	-0.949725000	0.493196000	1.892468000
C	-2.385890000	-0.624933000	-0.201381000
F	-3.614283000	-0.107820000	-0.164121000
F	-2.241075000	-1.289987000	-1.338057000
F	-2.261738000	-1.454539000	0.815483000

17b G = -779.220779 a.u.

H	3.108400000	-2.747696000	0.518413000
C	2.704242000	-1.772146000	0.274041000
C	3.495526000	-0.639936000	0.495350000
H	4.491090000	-0.771335000	0.903855000
C	3.037191000	0.648566000	0.207465000
H	3.661314000	1.516150000	0.388069000
C	1.756081000	0.728308000	-0.313134000
C	0.689519000	1.700402000	-0.790110000
H	0.946927000	2.311853000	-1.654645000
C	-0.955031000	1.407831000	0.952036000
H	-0.388053000	0.798661000	1.666990000
H	-1.830603000	1.822561000	1.449322000
N	-1.367392000	0.609355000	-0.214051000
C	-0.197156000	0.428095000	-1.076547000
H	-0.498428000	0.234817000	-2.104620000
C	0.974232000	-0.394549000	-0.535418000
C	1.411708000	-1.676292000	-0.248326000
H	0.802341000	-2.558153000	-0.405787000
C	-0.059140000	2.467751000	0.308318000
H	0.615609000	2.929686000	1.030296000
H	-0.679702000	3.245319000	-0.141178000
C	-2.129132000	-0.524260000	0.050137000
F	-3.255410000	-0.203846000	0.698540000
F	-2.457664000	-1.149537000	-1.087296000
F	-1.511969000	-1.456613000	0.822619000

TS₁₄₋₁₈ (b) G = -779.089570 a.u.

C	0.524967000	2.094919000	1.101627000
C	0.806273000	2.442782000	-0.288417000
C	0.749365000	0.758561000	1.259853000
H	1.100585000	3.465347000	-0.508110000
H	0.641723000	0.170734000	2.160622000
H	-0.003126000	2.709978000	1.814722000
H	-0.209531000	2.218650000	-0.799378000
C	-1.501780000	0.841841000	-0.688363000
C	-1.230066000	0.404935000	0.487977000

C	-2.628504000	0.357236000	-1.354951000
H	-2.912184000	0.665049000	-2.355582000
C	-1.919250000	-0.497563000	1.274471000
H	-1.623737000	-0.834709000	2.261280000
C	-3.066404000	-0.983440000	0.639633000
H	-3.690591000	-1.705667000	1.153694000
C	-3.413244000	-0.560752000	-0.650190000
H	-4.312997000	-0.957389000	-1.108657000
N	1.609961000	0.290765000	0.249197000
C	1.764728000	1.345438000	-0.781803000
H	1.469115000	0.962805000	-1.760090000
H	2.807409000	1.667383000	-0.815213000
C	1.642997000	-1.050373000	-0.127801000
F	1.493853000	-1.835548000	0.944593000
F	0.699317000	-1.419366000	-1.014954000
F	2.816733000	-1.336091000	-0.709625000

18b G = -779.234918 a.u.

C	-0.356884000	2.096870000	-0.766811000
C	-1.393177000	2.503289000	-0.047114000
C	-0.173708000	0.599666000	-0.697398000
H	-1.726269000	3.525683000	0.069846000
H	-0.389590000	0.148120000	-1.675998000
H	0.316217000	2.719236000	-1.341086000
H	0.939929000	0.754482000	1.768710000
C	1.647489000	0.381449000	1.036101000
C	1.229587000	0.202669000	-0.281046000
C	2.949594000	0.070081000	1.405329000
H	3.266822000	0.205497000	2.432608000
C	2.126916000	-0.290267000	-1.223028000
H	1.800258000	-0.443435000	-2.246829000
C	3.434521000	-0.598581000	-0.856052000
H	4.125331000	-0.987662000	-1.594819000
C	3.847159000	-0.418792000	0.458494000
H	4.862122000	-0.664727000	0.747553000
N	-1.201484000	0.218434000	0.295998000
C	-2.096567000	1.349518000	0.606815000
H	-2.201052000	1.470171000	1.688331000
H	-3.098425000	1.201950000	0.184092000
C	-1.830534000	-0.999120000	0.072707000
F	-2.637692000	-1.313010000	1.093266000
F	-2.619688000	-1.021916000	-1.039497000
F	-0.941656000	-1.980522000	-0.092922000

14c G = -439.078993 a.u.

C	-2.729791000	0.337891000	-0.077351000
C	-1.400779000	1.116571000	0.059379000
N	-0.375031000	0.070307000	-0.053015000
C	-0.973527000	-1.198044000	0.031714000
C	-2.300664000	-1.108604000	0.048639000
H	-3.447180000	0.633532000	0.690004000
H	-1.308640000	1.604219000	1.033354000
H	-0.340063000	-2.070801000	0.064051000
H	-2.976929000	-1.948211000	0.095189000
H	-1.251795000	1.870209000	-0.712525000

H	-3.201235000	0.517080000	-1.048388000
C	0.947854000	0.372632000	-0.013076000
O	1.386738000	1.498486000	0.024304000
O	1.712026000	-0.739131000	-0.028109000
C	3.117518000	-0.493318000	-0.003610000
H	3.418100000	0.084481000	-0.877822000
H	3.393317000	0.054038000	0.897838000
H	3.585867000	-1.474310000	-0.014321000

TS₁₄₋₁₅ (c) G = -669.871570 a.u.

C	-0.671096000	0.686150000	1.079307000
N	-1.652689000	0.755871000	0.010152000
C	-1.459285000	1.911960000	-0.742229000
C	-0.479625000	2.661406000	-0.217151000
C	0.118726000	1.942967000	0.932217000
H	0.051218000	-0.204253000	0.875262000
H	0.344028000	2.501716000	1.837871000
H	-2.079399000	2.072557000	-1.611096000
H	-0.141313000	3.609628000	-0.603982000
H	-1.121989000	0.497276000	2.051608000
H	1.240196000	1.553148000	0.597760000
C	3.523699000	0.745184000	-0.156870000
C	2.224157000	0.475210000	0.242282000
C	4.236782000	-0.413356000	-0.480288000
H	5.266856000	-0.326041000	-0.807887000
C	1.671727000	-0.672634000	0.326428000
C	3.651291000	-1.685180000	-0.393929000
H	4.243443000	-2.555314000	-0.657482000
C	2.326603000	-1.859893000	0.019578000
H	1.882630000	-2.846148000	0.083050000
H	3.969390000	1.730031000	-0.224266000
C	-2.557972000	-0.215370000	-0.321468000
O	-3.326208000	-0.154054000	-1.248763000
O	-2.476882000	-1.244014000	0.538574000
C	-3.390326000	-2.310568000	0.278349000
H	-4.418117000	-1.951789000	0.334371000
H	-3.210946000	-2.730105000	-0.711550000
H	-3.200539000	-3.052513000	1.049434000

15c G = -437.904468 a.u.

C	0.083088000	2.697116000	0.000000000
C	-0.767185000	1.634199000	0.000000000
N	0.000000000	0.479546000	0.000000000
C	1.345705000	0.823790000	0.000000000
C	1.422396000	2.183094000	0.000000000
H	-0.210024000	3.734706000	0.000000000
H	-1.841461000	1.561261000	0.000000000
H	2.103770000	0.060264000	0.000000000
H	2.334457000	2.758280000	0.000000000
C	-0.552192000	-0.800632000	0.000000000
O	-1.731027000	-1.018165000	0.000000000
O	0.403895000	-1.730113000	0.000000000
C	-0.072076000	-3.079557000	0.000000000
H	-0.673496000	-3.266045000	0.889442000
H	-0.673496000	-3.266045000	-0.889442000

H	0.818889000	-3.701077000	0.000000000
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TS₁₄₋₁₆ (c) G = -669.881232 a.u.

H	4.145547000	-2.057838000	1.036419000
C	3.393510000	-1.367688000	0.667890000
C	3.481022000	-0.915989000	-0.656411000
H	4.296032000	-1.251511000	-1.287907000
C	2.529652000	-0.031870000	-1.181816000
H	2.572305000	0.338998000	-2.198484000
C	1.589218000	0.282547000	-0.228803000
C	0.222451000	1.980130000	-0.972508000
H	0.904097000	2.374593000	-1.711313000
C	-0.105271000	2.658937000	0.338152000
H	0.748965000	2.620670000	1.018451000
H	-0.377093000	3.704659000	0.185052000
C	-1.291797000	1.835669000	0.889162000
H	-1.087842000	1.393680000	1.861571000
H	-2.216289000	2.414032000	0.945309000
N	-1.456344000	0.755896000	-0.102893000
C	-0.622961000	0.945123000	-1.180186000
H	-0.674716000	0.265875000	-2.017835000
C	1.409100000	-0.079834000	0.977586000
C	2.361440000	-0.956555000	1.518222000
H	2.318528000	-1.325458000	2.538020000
C	-2.183343000	-0.371689000	0.186457000
O	-2.838703000	-0.506885000	1.186912000
O	-2.085370000	-1.280626000	-0.797440000
C	-2.803320000	-2.493172000	-0.561367000
H	-2.449077000	-2.967576000	0.353519000
H	-3.871006000	-2.291439000	-0.473430000
H	-2.600686000	-3.123514000	-1.423174000

16c G = -669.892252 a.u.

H	3.700821000	-2.412728000	1.083023000
C	3.096842000	-1.590559000	0.709537000
C	3.341054000	-1.094154000	-0.580056000
H	4.144342000	-1.499800000	-1.183910000
C	2.561320000	-0.058775000	-1.055538000
H	2.771732000	0.386009000	-2.025936000
C	1.543704000	0.446223000	-0.219129000
C	0.717802000	1.659706000	-0.809820000
H	1.248552000	2.100850000	-1.647850000
C	0.141917000	2.619063000	0.237816000
H	0.854573000	2.767659000	1.047535000
H	-0.092821000	3.578752000	-0.225318000
C	-1.132929000	1.928218000	0.751987000
H	-1.006630000	1.513084000	1.747107000
H	-2.024990000	2.555089000	0.703769000
N	-1.298294000	0.792670000	-0.187092000
C	-0.348275000	0.737348000	-1.108840000
H	-0.373115000	-0.012603000	-1.886470000
C	1.208782000	-0.044874000	1.038355000
C	2.091515000	-1.045463000	1.500194000
H	1.959419000	-1.454406000	2.500035000
C	-2.219706000	-0.227633000	0.104672000

O	-3.014711000	-0.138190000	0.992907000
O	-2.092479000	-1.242232000	-0.744251000
C	-2.960136000	-2.353536000	-0.485367000
H	-2.754293000	-2.758198000	0.504951000
H	-4.001383000	-2.037874000	-0.543980000
H	-2.731981000	-3.084534000	-1.255422000

TS₁₆₋₁₇ (c) G = -669.888063 a.u.

C	1.697025000	0.387519000	-0.243691000
C	1.218432000	-0.357187000	0.854135000
C	2.126975000	-1.369019000	1.251855000
C	2.899091000	0.155902000	-0.936065000
C	0.751565000	1.484109000	-0.774699000
C	-0.390168000	0.592268000	-0.997857000
H	1.142059000	1.931353000	-1.689303000
H	-0.456989000	-0.197154000	-1.734513000
C	3.743049000	-0.837607000	-0.474855000
H	4.696316000	-1.018012000	-0.958705000
C	3.348454000	-1.602267000	0.631923000
H	4.007930000	-2.385211000	0.995993000
H	3.181354000	0.760317000	-1.795049000
H	1.864123000	-2.010594000	2.091609000
N	-1.353294000	0.784168000	-0.136024000
C	0.225544000	2.486573000	0.271790000
H	0.975038000	2.662192000	1.041714000
H	-0.034131000	3.433437000	-0.204884000
C	-1.022106000	1.819356000	0.870304000
H	-1.878172000	2.480650000	0.998683000
H	-0.792560000	1.281447000	1.789854000
C	-2.411540000	-0.127580000	0.118307000
O	-3.159082000	0.017287000	1.035504000
O	-2.434844000	-1.090601000	-0.788087000
C	-3.433296000	-2.099355000	-0.568859000
H	-3.279236000	-2.561324000	0.405289000
H	-4.426528000	-1.653834000	-0.615014000
H	-3.292883000	-2.822195000	-1.366561000

17c G = -670.000610 a.u.

H	-2.670386000	-3.115398000	-0.812141000
C	-2.432371000	-2.114143000	-0.471936000
C	-3.413270000	-1.121298000	-0.563545000
H	-4.382618000	-1.382612000	-0.972503000
C	-3.177710000	0.192116000	-0.144769000
H	-3.949208000	0.949269000	-0.226247000
C	-1.915881000	0.443527000	0.366916000
C	-1.017886000	1.527157000	0.948669000
H	-1.345265000	1.938480000	1.903742000
C	0.552639000	1.828929000	-0.867486000
H	0.070861000	1.311200000	-1.705407000
H	1.347885000	2.457441000	-1.264259000
N	1.107736000	0.859855000	0.078444000
C	0.096545000	0.413553000	1.026655000
H	0.531083000	0.173384000	1.994845000
C	-0.945461000	-0.544141000	0.458746000

C	-1.160655000	-1.846335000	0.044101000
H	-0.403817000	-2.618941000	0.111746000
C	-0.474069000	2.583873000	-0.018950000
H	-1.256206000	3.039198000	-0.628029000
H	0.026578000	3.371927000	0.548174000
C	2.181515000	0.106269000	-0.278738000
O	2.900205000	0.321341000	-1.226191000
O	2.364085000	-0.919456000	0.583893000
C	3.507057000	-1.728239000	0.312598000
H	3.421094000	-2.191200000	-0.670874000
H	4.416823000	-1.128421000	0.344306000
H	3.522002000	-2.486009000	1.092343000

TS₁₄₋₁₈ (c) G = -669.874239 a.u.

C	0.166260000	2.334842000	-0.859440000
C	-0.176290000	2.556292000	0.541798000
C	-0.302698000	1.101556000	-1.214627000
H	-0.239403000	3.579050000	0.902292000
H	-0.248340000	0.598226000	-2.169415000
H	0.882307000	2.902752000	-1.434540000
H	0.697729000	2.010006000	1.082644000
C	1.667164000	0.416597000	0.869682000
C	1.460106000	0.210343000	-0.380782000
C	2.621356000	-0.346123000	1.544490000
H	2.837600000	-0.239497000	2.602100000
C	2.075933000	-0.678996000	-1.238891000
H	1.831186000	-0.821704000	-2.284635000
C	3.057562000	-1.439939000	-0.595604000
H	3.610301000	-2.179876000	-1.163637000
C	3.325887000	-1.272829000	0.769024000
H	4.098008000	-1.878714000	1.231558000
N	-1.286320000	0.689227000	-0.304483000
C	-1.403747000	1.665924000	0.792575000
H	-1.361761000	1.156005000	1.754068000
H	-2.350367000	2.207431000	0.710374000
C	-1.839317000	-0.553773000	-0.361746000
O	-1.612805000	-1.366082000	-1.226637000
O	-2.686350000	-0.747100000	0.664427000
C	-3.310805000	-2.031210000	0.683739000
H	-3.886853000	-2.187367000	-0.228382000
H	-2.558990000	-2.815591000	0.771705000
H	-3.962415000	-2.025952000	1.553621000

18c G = -670.000610 a.u.

C	0.391406000	-2.297029000	-0.941117000
C	1.385800000	-2.743282000	-0.183443000
C	0.264661000	-0.792044000	-0.883395000
H	1.661053000	-3.780211000	-0.045671000
H	0.411064000	-0.340925000	-1.871541000
H	-0.294069000	-2.897490000	-1.524083000
H	-0.786928000	-1.260027000	1.570888000
C	-1.468405000	-0.687673000	0.948847000
C	-1.084079000	-0.344219000	-0.346737000
C	-2.707318000	-0.298039000	1.440460000
H	-2.996742000	-0.566194000	2.449847000

C	-1.954881000	0.390840000	-1.143388000
H	-1.650413000	0.675448000	-2.145295000
C	-3.200518000	0.777403000	-0.656336000
H	-3.870593000	1.353769000	-1.283489000
C	-3.578492000	0.433773000	0.636283000
H	-4.545440000	0.738086000	1.019002000
N	1.386203000	-0.456352000	-0.000859000
C	2.117372000	-1.618610000	0.493708000
H	2.075840000	-1.683304000	1.586771000
H	3.173646000	-1.562609000	0.210368000
C	1.848597000	0.794836000	0.230024000
O	2.803452000	1.059547000	0.925135000
O	1.108742000	1.715639000	-0.422588000
C	1.497642000	3.067560000	-0.189112000
H	1.422215000	3.307450000	0.871683000
H	2.523121000	3.232910000	-0.520434000
H	0.805558000	3.674982000	-0.767184000

14d G = -548.607949 a.u.

C	-2.409530000	-0.607432000	0.050511000
C	-0.997646000	-1.186758000	-0.091279000
N	-0.144870000	0.002517000	-0.547075000
C	-0.936861000	1.214688000	-0.186916000
C	-2.168158000	0.872273000	0.140060000
H	-3.039976000	-0.836264000	-0.812571000
H	-0.886574000	-1.988139000	-0.817316000
H	-0.442000000	2.170751000	-0.275219000
H	-2.932243000	1.589732000	0.409072000
H	-0.595195000	-1.499854000	0.871309000
H	-2.908683000	-0.999616000	0.936831000
C	1.233817000	-0.003829000	0.044031000
F	1.809905000	-1.133639000	-0.294428000
F	1.888009000	1.018249000	-0.455717000
F	1.134969000	0.097910000	1.344117000
H	-0.006917000	-0.030569000	-1.566786000

TS₁₄₋₁₅ (d) G = -779.399490 a.u.

C	-0.829281000	0.811257000	1.246122000
N	-1.988303000	0.465858000	0.321958000
C	-1.928204000	1.453620000	-0.789506000
C	-1.018734000	2.375134000	-0.505315000
C	-0.293368000	2.072297000	0.744845000
H	0.033387000	-0.020420000	1.049132000
H	-0.073243000	2.874930000	1.440951000
H	-2.602766000	1.311021000	-1.619963000
H	-0.808409000	3.225869000	-1.139346000
H	-1.127719000	0.718217000	2.284845000
H	0.912414000	1.734285000	0.363114000
C	3.157239000	1.059359000	-0.397330000
C	1.901088000	0.782365000	0.134375000
C	3.949851000	-0.083323000	-0.514297000
H	4.950779000	0.015462000	-0.918520000
C	1.489563000	-0.376434000	0.490632000
C	3.494750000	-1.352068000	-0.124131000
H	4.156090000	-2.204456000	-0.232981000

C	2.217210000	-1.555775000	0.404867000
H	1.870029000	-2.533256000	0.710688000
H	3.506911000	2.038596000	-0.694796000
C	-2.009561000	-0.957823000	-0.153478000
F	-1.010658000	-1.158173000	-0.968349000
F	-1.922252000	-1.738389000	0.899098000
F	-3.157343000	-1.146526000	-0.770095000
H	-2.870389000	0.594892000	0.836582000

15d G = -547.395702 a.u.

C	-2.196850000	-0.735561000	0.169507000
C	-1.031677000	-1.179256000	-0.290256000
N	-0.197018000	-0.000123000	-0.629297000
C	-1.031683000	1.179230000	-0.290268000
C	-2.196846000	0.735555000	0.169492000
H	-3.016821000	-1.360589000	0.492667000
H	-0.612184000	-2.160378000	-0.451516000
H	-0.611858000	2.160241000	-0.451345000
H	-3.016810000	1.360603000	0.492637000
C	1.143452000	-0.000020000	0.080577000
F	1.783885000	-1.079162000	-0.296462000
F	1.784818000	1.077692000	-0.299001000
F	0.932126000	0.001616000	1.365424000
H	0.010962000	-0.000020000	-1.641319000

TS₁₄₋₁₈ (d) G = -779.403030 a.u.

C	0.893412000	2.144593000	1.120361000
C	0.962931000	2.427385000	-0.307337000
C	0.966175000	0.817462000	1.336994000
H	1.317473000	3.406113000	-0.619417000
H	0.941059000	0.247105000	2.254318000
H	0.532836000	2.842427000	1.864170000
H	-0.140850000	2.306432000	-0.623846000
C	-1.464994000	0.969793000	-0.474756000
C	-1.139557000	0.357350000	0.583236000
C	-2.617720000	0.692775000	-1.203360000
H	-2.917942000	1.189281000	-2.116481000
C	-1.837192000	-0.633578000	1.253738000
H	-1.536810000	-1.136077000	2.164202000
C	-3.024116000	-0.945578000	0.580378000
H	-3.672043000	-1.709151000	0.995815000
C	-3.401343000	-0.302631000	-0.608952000
H	-4.339480000	-0.578032000	-1.077942000
N	1.733504000	0.196863000	0.201919000
C	1.711220000	1.244713000	-0.928130000
H	1.193101000	0.806240000	-1.778183000
H	2.744581000	1.463830000	-1.187428000
C	1.401631000	-1.216397000	-0.212387000
F	1.096276000	-1.891541000	0.872165000
F	0.434220000	-1.261275000	-1.082290000
F	2.506992000	-1.698727000	-0.751819000
H	2.703466000	0.112364000	0.530141000

18d G = -779.560314 a.u.

C	-0.450620000	2.037651000	-0.970554000
C	-1.460317000	2.474792000	-0.234877000
C	-0.138470000	0.581556000	-0.775277000
H	-1.856052000	3.481180000	-0.228489000
H	-0.445176000	-0.014884000	-1.638984000
H	0.131487000	2.624018000	-1.668943000
H	1.482684000	1.941699000	0.945926000
C	1.944037000	1.037332000	0.558865000
C	1.266296000	0.234988000	-0.363433000
C	3.229102000	0.693454000	0.959348000
H	3.758347000	1.316600000	1.669412000
C	1.881884000	-0.899300000	-0.889779000
H	1.357698000	-1.517643000	-1.610882000
C	3.171701000	-1.233509000	-0.493917000
H	3.652215000	-2.110509000	-0.909077000
C	3.841378000	-0.440669000	0.432027000
H	4.846859000	-0.701881000	0.738648000
N	-1.132775000	0.222826000	0.384804000
C	-2.078211000	1.399590000	0.606880000
H	-2.120273000	1.617108000	1.674130000
H	-3.075042000	1.113845000	0.264604000
C	-1.848474000	-1.059876000	0.166651000
F	-2.608769000	-1.293497000	1.214133000
F	-2.585065000	-0.950651000	-0.916829000
F	-0.962288000	-2.017542000	0.022061000
H	-0.548062000	0.089828000	1.220135000