

Supplementary Information

Ring-opening polymerization and epimerization of L-lactide catalyzed by indium(III) acetate: synthesis, characterization, and computational validation

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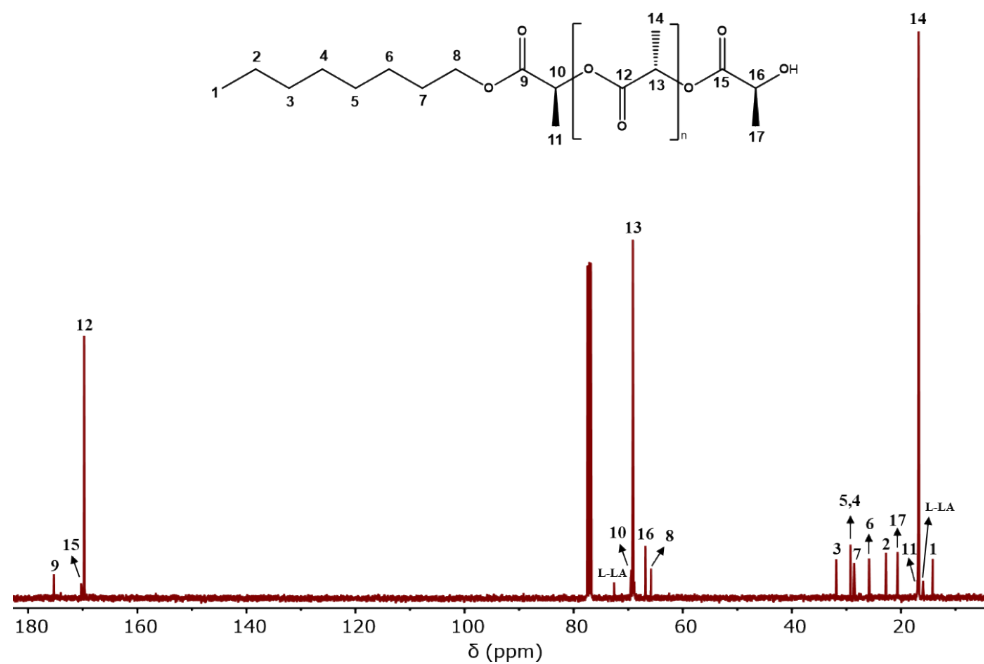


Figure S1. ^{13}C NMR spectrum of the oligomers obtained from ROP of L-lactide catalyzed by indium (III) acetate (Table 4, entry 5) in presence of 1-octanol as initiator.

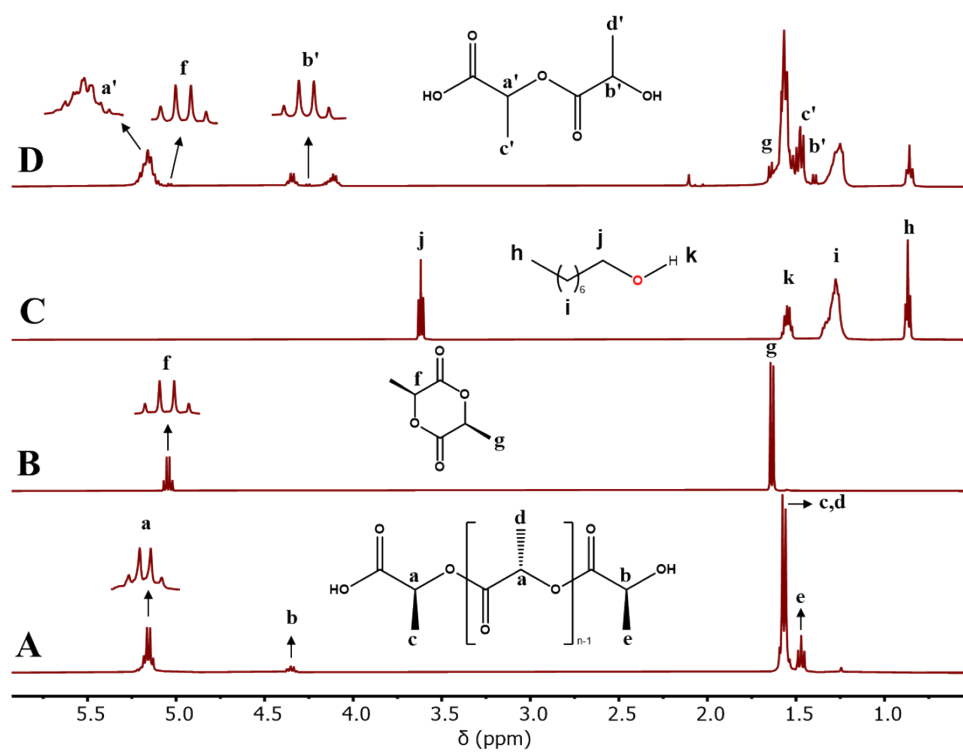
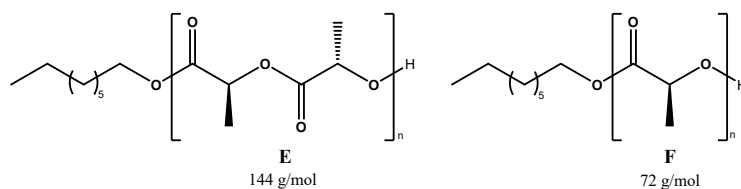


Figure S2. ^1H NMR analysis of the PLLA exposed to indium(III) acetate and 1-octanol under bulk conditions (140 °C) for 5 hours. A: PLLA; B: L-lactide; C: 1-octanol; D: reaction crude after exposition.



Scheme S1. Species observed [oligoesters obtained by ROP with 1-octanol as initiator] in MALDI-TOF analysis, where the numbers indicate the molecular mass of the repetitive unit.

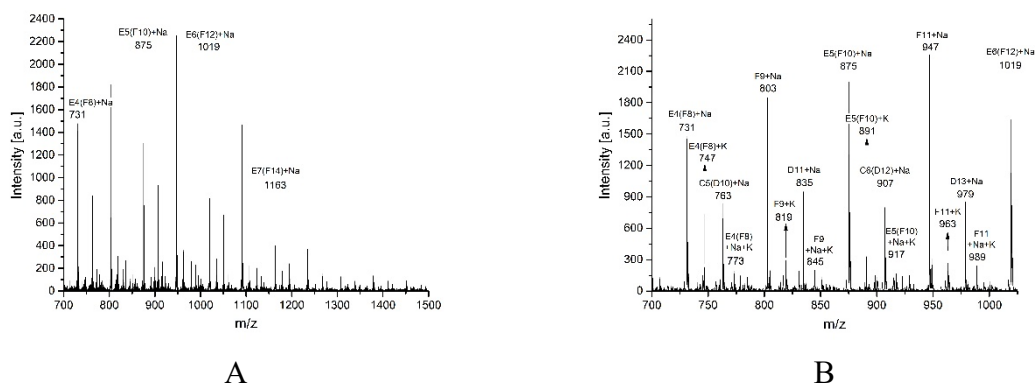


Figure S3. MALDI-TOF spectrum of oligomers derived from bulk ROP of L-LA catalyzed by $\text{In}(\text{OAc})_3$ in presence of 1-octanol as initiators [Table 4, Exp. 5]. A: Full spectrum; B: Magnification (700-1025 m/z). The chemical structures are illustrated in Scheme S1.

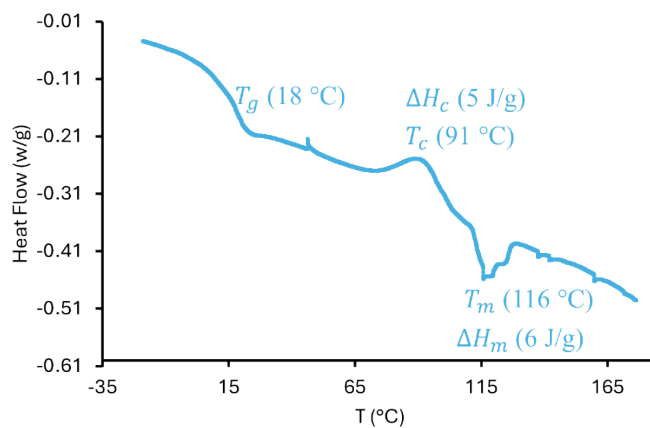


Figure S4. Thermogram (DSC) of oligomers obtained from ROP of L-LA using $\text{In}(\text{OAc})_3$ and 1-octanol as catalyst and initiator (Table 4, Exp. 5), respectively.

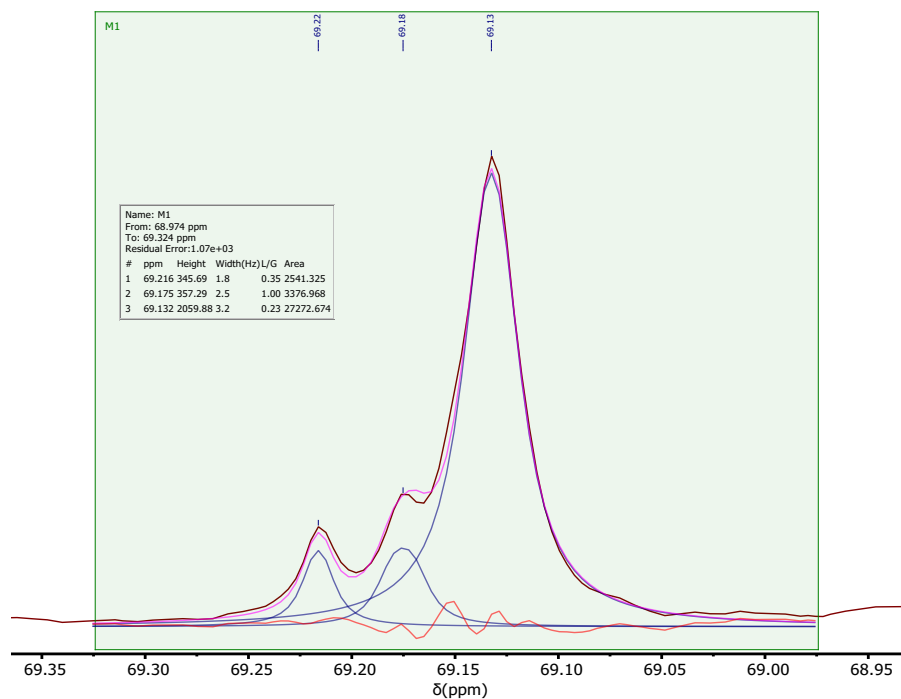


Figure S5. Deconvoluted methine region of the inverse-gated $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of L-LA oligomers obtained after 5 h.

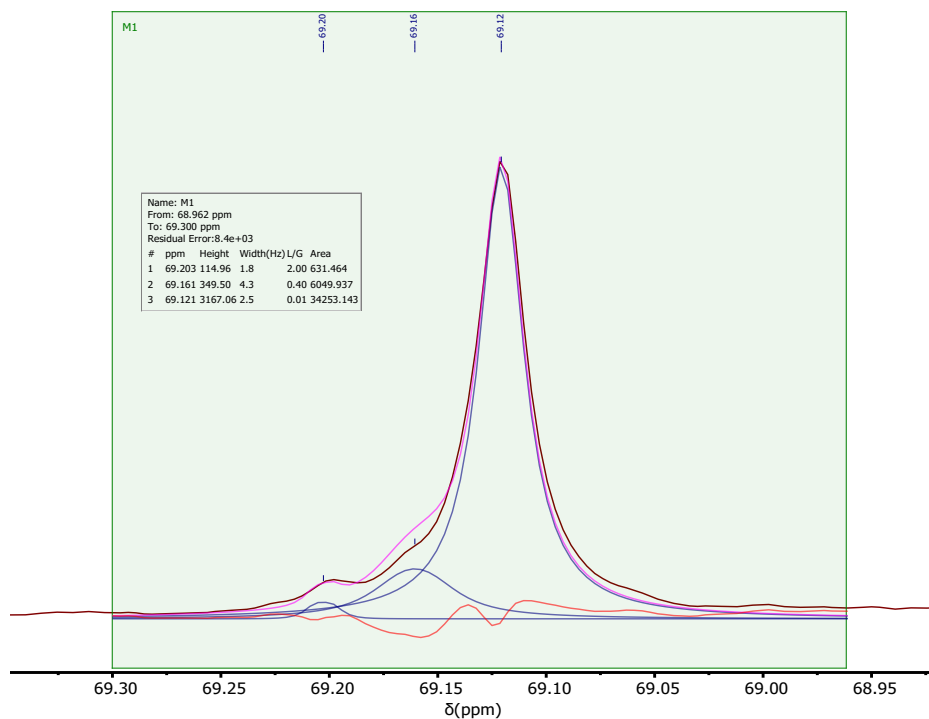


Figure S6. Deconvoluted methine region of the inverse-gated $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of L-LA oligomers obtained after 72 h.

Table S1. Optimized cartesian coordinates (xyz) for all species in the energy profile of Figure 7. Coordinates are given in Å.

ADD E(scf)= -990.613266611				TS₁ E(scf)= -990.596887123 v_{min}= -727.4434			
49	-0.141672000	-0.012585000	0.069311000	49	0.281950000	0.084471000	0.244135000
8	1.636155000	-0.963652000	0.502065000	8	-1.621945000	-1.089278000	-0.011943000
8	0.209428000	2.112538000	0.656303000	8	1.895483000	-1.399198000	0.583666000
8	-2.375666000	0.036357000	0.080508000	8	1.280919000	2.050755000	0.474003000
6	2.586265000	-1.485868000	-0.264486000	6	-2.753844000	-0.952415000	-0.734423000
6	-2.412140000	-0.960159000	-0.694432000	6	0.418947000	2.597200000	-0.273865000
6	0.397875000	2.434711000	-0.551588000	6	2.066259000	-1.535589000	-0.663745000
6	0.755099000	3.847607000	-0.908611000	6	3.121421000	-2.468034000	-1.180015000
8	0.309123000	1.548460000	-1.450832000	8	1.353225000	-0.861382000	-1.460190000
8	-1.324262000	-1.485763000	-1.075639000	8	-0.507885000	1.889297000	-0.765464000
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6	-4.304756000	0.286481000	0.080453000	6	-3.784862000	0.315107000 -0.519833000
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1	-3.707977000	3.696382000	-1.354051000	1	3.391254000	-3.471406000 -1.708711000
1	-3.052627000	4.260001000	0.207799000	1	2.785367000	-4.187302000 -0.194939000

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1	1.958070000	-1.290341000	-2.138421000	1	-3.311933000	0.479742000	2.991445000
1	0.253150000	-1.849540000	-2.107951000	1	-2.568300000	2.106187000	3.078531000
1	1.955071000	-0.339531000	3.196579000	1	-1.175175000	-2.932391000	0.955154000
1	3.279101000	0.565728000	2.408469000	1	-1.361528000	-2.337239000	-0.717209000
6	2.806311000	-0.425372000	2.505499000	6	-1.894564000	-2.522806000	0.230080000
1	3.541660000	-1.138792000	2.910659000	1	-2.692004000	-3.262296000	0.053450000
1	4.440252000	2.349607000	0.348769000	1	-1.333985000	-0.511415000	-2.906176000
6	4.014022000	2.261948000	-0.664181000	6	-1.498202000	0.556480000	-2.686890000
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8	0.343261000	0.395410000	1.323649000	8	-0.358487000	-0.510135000	1.587203000
6	2.324140000	-0.914251000	1.151529000	6	-2.498681000	-1.241097000	0.773839000
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6	3.111961000	1.042068000	-0.758271000	6	-2.020606000	0.736693000	-1.273052000
6	3.914751000	-0.247252000	-0.553441000	6	-3.387304000	0.070770000	-1.076823000
8	4.907160000	-0.465123000	-1.188051000	8	-4.297191000	0.354082000	-1.802352000
1	2.715491000	0.971418000	-1.790751000	1	-2.180976000	1.806603000	-1.056773000
TS₃ E(scf)= -1295.56857403 v_{min}= -116.4967				INT₆ E(scf)= -1295.56648597			
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8	2.154547000	-1.108451000	1.391921000	8	1.921856000	2.015988000	-0.754779000
8	1.120660000	2.067720000	0.755649000	8	2.117919000	-1.554337000	-1.254120000
6	2.050866000	2.356917000	-0.052053000	6	2.930649000	-1.627647000	-0.284191000
6	2.391578000	-2.016637000	0.546514000	6	1.420889000	2.556606000	0.269087000
6	3.238096000	-3.198415000	0.918670000	6	1.626258000	4.018683000	0.539154000
8	1.930327000	-1.906514000	-0.628242000	8	0.714621000	1.861243000	1.058878000
8	2.436432000	1.488781000	-0.886247000	8	2.773010000	-0.865064000	0.708515000
6	2.668514000	3.723675000	-0.026018000	6	4.046558000	-2.629409000	-0.320422000
1	4.292004000	-2.949245000	0.704017000	1	1.861283000	4.174259000	1.603088000
1	2.961746000	-4.075687000	0.316603000	1	0.681430000	4.546741000	0.324956000
1	3.145990000	-3.411733000	1.993006000	1	2.421644000	4.425601000	-0.099545000
1	2.900767000	4.003385000	1.013031000	1	4.541792000	-2.596296000	-1.302791000
1	1.930829000	4.449328000	-0.407974000	1	3.615142000	-3.637337000	-0.199809000
1	3.572112000	3.757530000	-0.649397000	1	4.768614000	-2.441429000	0.485429000
8	-2.115423000	-1.266711000	-1.833545000	8	-2.179936000	-0.411509000	2.215498000
6	-1.249187000	-2.296355000	-2.292012000	6	-1.487984000	0.424859000	3.150196000
1	-0.552102000	-2.590008000	-1.490817000	1	-0.867458000	1.159704000	2.613185000
1	-0.676821000	-1.959699000	-3.169916000	1	-0.849648000	-0.192062000	3.801043000
1	-1.901768000	-3.138519000	-2.556954000	1	-2.274153000	0.919641000	3.733865000
1	-1.398328000	2.645287000	-1.331819000	1	-0.857281000	-3.438580000	0.028609000
1	-1.369349000	2.075708000	0.355642000	1	-0.968596000	-2.204360000	-1.275679000
6	-2.008974000	2.199415000	-0.531232000	6	-1.541600000	-2.796505000	-0.549656000
1	-2.829180000	2.891393000	-0.282932000	1	-2.253085000	-3.439885000	-1.091040000
1	-1.112742000	1.184022000	2.459173000	1	-2.048957000	1.761087000	-2.826111000
6	-1.263938000	0.115153000	2.686848000	6	-1.911302000	2.072556000	-1.778678000
1	-0.289189000	-0.321388000	2.963604000	1	-0.954444000	2.616102000	-1.699001000
8	-0.408845000	0.195555000	-1.826623000	8	-0.240582000	-1.088099000	1.380837000
6	-2.598609000	0.881460000	-0.997302000	6	-2.325244000	-1.890387000	0.382534000
1	-1.950678000	0.027242000	3.543292000	1	-2.737876000	2.744862000	-1.499974000
6	-1.557278000	-0.145395000	-1.427600000	6	-1.463811000	-1.082481000	1.352667000
1	-3.213518000	1.066665000	-1.894308000	1	-2.934967000	-2.522847000	1.052166000
8	-0.985449000	-0.569169000	0.376205000	8	-0.797130000	0.007923000	-1.220327000
8	-3.531328000	0.352508000	-0.067776000	8	-3.303024000	-1.115044000	-0.281493000

6	-1.825691000	-0.633232000	1.479890000	6	-1.850991000	0.845462000	-0.878254000
6	-3.244908000	-0.148997000	1.148850000	6	-3.178024000	0.067891000	-0.941002000
8	-4.127663000	-0.270590000	1.949208000	8	-4.146313000	0.478052000	-1.510244000
1	-1.976915000	-1.691290000	1.771404000	1	-1.773561000	1.212181000	0.172091000
P				L-LA			
E(scf)= -1295.59106521				E(scf)= -533.788651882			
49	1.377190000	-0.201156000	0.144102000	8	0.258302000	-1.338278000	-0.106845000
8	3.564383000	0.131774000	0.254106000	6	-1.028068000	-0.965598000	-0.060152000
8	0.607336000	0.802932000	1.988690000	6	-1.254298000	0.465284000	0.428453000
6	0.295739000	1.839840000	1.339061000	8	-1.905151000	-1.713347000	-0.372300000
6	3.659224000	0.086625000	-1.007307000	8	-0.258305000	1.338279000	-0.106856000
6	5.000245000	0.226238000	-1.667414000	6	1.254323000	-0.465268000	0.428373000
8	2.621377000	-0.104200000	-1.700973000	6	1.028091000	0.965592000	-0.060207000
8	0.573573000	1.905666000	0.106266000	8	1.905135000	1.713412000	-0.372273000
6	-0.452199000	2.951699000	2.012420000	6	2.613460000	-1.003950000	0.042296000
1	4.888900000	0.660975000	-2.671011000	1	1.154371000	-0.456939000	1.532253000
1	5.441060000	-0.780045000	-1.772087000	1	2.719301000	-1.021999000	-1.053667000
1	5.671674000	0.835455000	-1.045826000	1	2.732488000	-2.026330000	0.433260000
1	-0.178645000	3.012910000	3.075623000	1	3.400734000	-0.358060000	0.458153000
1	-1.525072000	2.701133000	1.941076000	6	-2.613470000	1.003883000	0.042265000
1	-0.270568000	3.909997000	1.504765000	1	-1.154445000	0.457093000	1.532317000
8	-3.048400000	1.508596000	-1.432371000	1	-2.719328000	1.021764000	-1.053694000
6	-2.697573000	2.837752000	-1.059237000	1	-2.732545000	2.026299000	0.433122000
1	-1.639641000	2.862619000	-0.750266000	1	-3.400651000	0.357975000	0.458270000
1	-3.340606000	3.194196000	-0.238728000				
1	-2.849149000	3.450158000	-1.957706000				
1	-5.349409000	-0.470661000	-1.467565000				
1	-5.007973000	-1.167170000	0.152398000				
6	-4.719987000	-1.183437000	-0.911212000				
1	-4.889813000	-2.194536000	-1.314171000				
1	-0.902917000	-1.316511000	2.437876000				
6	-0.971649000	-2.356731000	2.077512000				
1	-0.362586000	-2.993428000	2.738015000				
8	-2.759335000	0.801153000	0.677557000				
6	-3.259538000	-0.801985000	-1.062474000				
1	-2.022508000	-2.687303000	2.119687000				
6	-2.978957000	0.588755000	-0.485420000				
1	-2.949559000	-0.806680000	-2.118210000				
8	0.939127000	-2.150304000	0.591570000				
8	-2.488126000	-1.773916000	-0.347672000				
6	-0.394811000	-2.462789000	0.656159000				
6	-1.197254000	-1.549196000	-0.263117000				
8	-0.676081000	-0.611779000	-0.855738000				
1	-0.565761000	-3.494489000	0.279807000				
CH₃COOH							
E(scf)= -228.829458179							
8	0.637418000	1.194311000	-0.000008000				
6	0.093135000	0.123847000	0.000056000				
6	-1.392391000	-0.113987000	0.000008000				
8	0.780575000	-1.032413000	0.000011000				
1	-1.678268000	-0.701772000	0.887969000				
1	-1.678305000	-0.699821000	-0.889248000				
1	-1.918252000	0.850159000	0.001008000				
1	1.726409000	-0.802909000	-0.000135000				

Table S2. Optimized cartesian coordinates (xyz) for all species in the energy profile of Figure 8. Coordinates are given in Å.

INT₃ E(scf)= -1295.56773628				EM-TS₁ E(scf)= -1295.53472203 v_{min}= -977.6394			
49	1.263131000	0.104655000	0.128425000	49	1.215933000	0.183571000	-0.020262000
8	2.889176000	-1.147704000	1.035042000	8	3.035377000	-0.850767000	0.842540000
8	1.994319000	2.194632000	0.533117000	8	1.187117000	2.146913000	0.965278000
6	2.547825000	2.218813000	-0.599648000	6	1.912477000	2.650817000	0.054770000
6	2.622485000	-2.094755000	0.244472000	6	3.044170000	-1.644414000	-0.135326000
6	3.434229000	-3.357984000	0.269240000	6	4.110959000	-2.690543000	-0.273217000
8	1.685749000	-1.961751000	-0.597128000	8	2.148901000	-1.539833000	-1.029932000
8	2.457439000	1.206379000	-1.356146000	8	2.308932000	1.917697000	-0.892538000
6	3.281069000	3.440620000	-1.071070000	6	2.258322000	4.109634000	0.088301000
1	4.225434000	-3.272222000	-0.495329000	1	4.855442000	-2.328693000	-1.002773000
1	2.805346000	-4.222450000	0.010688000	1	3.679681000	-3.621542000	-0.670267000
1	3.908366000	-3.494803000	1.251175000	1	4.610467000	-2.865997000	0.689376000
1	3.577301000	4.067564000	-0.218722000	1	2.290719000	4.474416000	1.124734000
1	2.604554000	4.020772000	-1.721698000	1	1.467128000	4.660007000	-0.449435000
1	4.157320000	3.149823000	-1.669033000	1	3.214170000	4.289060000	-0.423681000
8	-0.302131000	-0.104277000	1.422148000	8	-0.104260000	-0.862515000	1.322552000
6	-0.118085000	0.064160000	2.795120000	6	0.288128000	-1.969034000	2.105188000
1	0.668393000	-0.601487000	3.207512000	1	0.624038000	-2.814534000	1.475523000
1	-1.060983000	-0.178937000	3.325206000	1	-0.566177000	-2.301990000	2.720175000
1	0.151367000	1.107003000	3.063308000	1	1.113527000	-1.673606000	2.771693000
1	-0.560180000	-2.423131000	-1.407178000	1	-0.264150000	-2.285105000	-1.269875000
1	-1.848706000	-2.027131000	-2.592293000	1	-1.812223000	-2.668096000	-2.076862000
6	-1.647262000	-2.322134000	-1.550368000	6	-1.340649000	-2.443198000	-1.103691000
1	-2.128859000	-3.292549000	-1.354368000	1	-1.465770000	-3.325234000	-0.453962000
1	-4.653400000	2.466569000	-0.185661000	1	-5.015839000	1.995557000	-0.716480000
6	-4.204313000	2.091290000	0.747217000	6	-4.518604000	1.973370000	0.266121000
1	-3.523768000	2.853474000	1.157118000	1	-3.995484000	2.928591000	0.428446000
8	-0.530861000	0.289595000	-1.308369000	8	-0.509919000	0.402750000	-1.296180000
6	-2.200264000	-1.296727000	-0.584838000	6	-1.984128000	-1.238884000	-0.459012000
1	-5.012118000	1.897496000	1.468226000	1	-5.287388000	1.840177000	1.041328000
6	-1.618920000	0.092137000	-0.792353000	6	-1.653750000	0.070919000	-0.874391000
1	-1.929556000	-1.566102000	0.451966000	1	-1.079939000	-1.065440000	0.702272000
8	-2.363238000	1.099685000	-0.412167000	8	-2.513443000	1.060298000	-0.649112000
8	-3.623455000	-1.264882000	-0.712206000	8	-3.361181000	-1.503714000	-0.232639000
6	-3.442077000	0.813151000	0.494388000	6	-3.531757000	0.831180000	0.329879000
6	-4.311167000	-0.301652000	-0.085225000	6	-4.189920000	-0.533739000	0.140220000
8	-5.501992000	-0.329092000	-0.005857000	8	-5.353063000	-0.738048000	0.339022000
1	-2.975083000	0.445830000	1.427191000	1	-3.028094000	0.808531000	1.317650000
EM-INT₁ E(scf)= -1295.54668803				EM-INT₂ E(scf)= -1295.55128053			
49	1.202492000	0.013109000	-0.305808000	8	-3.854882000	0.233002000	1.022273000
8	3.069664000	-0.086761000	0.968702000	6	-4.024705000	-0.527270000	-0.063820000
8	0.259820000	1.720928000	0.830691000	6	-2.724963000	-0.889807000	-0.780382000
6	0.658579000	2.522053000	-0.059498000	8	-5.113566000	-0.863322000	-0.430886000
6	3.641665000	-0.742751000	0.057894000	8	-1.735472000	-1.193669000	0.200755000
6	5.070910000	-1.177839000	0.191019000	6	-2.572696000	0.604306000	1.442028000
8	2.999809000	-1.017380000	-1.002685000	6	-1.517141000	-0.155925000	1.100134000
8	1.346466000	2.082970000	-1.029138000	8	-0.282608000	-0.035066000	1.502150000
6	0.302131000	3.977910000	-0.005556000	6	-2.551150000	1.799034000	2.328284000
1	5.694443000	-0.514179000	-0.431915000	1	-3.113952000	1.616971000	3.261765000
1	5.189165000	-2.201793000	-0.194007000	1	-3.009499000	2.671494000	1.828464000
1	5.404408000	-1.109517000	1.235349000	1	-1.511175000	2.044431000	2.590909000
1	-0.061684000	4.256022000	0.992996000	6	-2.870880000	-2.069937000	-1.712000000
1	-0.491970000	4.163446000	-0.748786000	1	-2.383491000	0.005884000	-1.335999000

1	1.171874000	4.589836000	-0.289259000	1	-3.185660000	-2.967363000	-1.155053000
8	0.328799000	-1.320030000	1.335282000	1	-1.911803000	-2.266482000	-2.219031000
6	0.382679000	-0.945083000	2.707555000	1	-3.636399000	-1.851038000	-2.471011000
1	0.072233000	-1.794541000	3.338055000	49	1.218441000	0.174184000	0.074449000
1	-0.252626000	-0.065523000	2.903891000	8	-0.052820000	0.988298000	-1.568817000
1	1.429902000	-0.690358000	2.920220000	8	3.241770000	-0.184526000	-0.849728000
1	-0.911252000	-3.403678000	-0.806773000	6	3.744310000	-0.311117000	0.298999000
1	-2.592031000	-3.767632000	-1.287280000	6	0.257437000	2.174180000	-1.246245000
6	-1.966836000	-3.258094000	-0.531500000	6	-0.393795000	3.334418000	-1.938466000
1	-2.158934000	-3.750667000	0.438858000	8	1.086156000	2.364891000	-0.312699000
1	-3.794345000	2.375158000	-0.685080000	8	2.991523000	-0.221328000	1.316796000
6	-3.282314000	2.144249000	0.262575000	6	5.209472000	-0.576093000	0.483062000
1	-2.409653000	2.85013000	0.379641000	1	0.203419000	4.247988000	-1.813378000
8	-0.292185000	-0.916850000	-1.408501000	1	-1.383860000	3.492464000	-1.476630000
6	-2.280866000	-1.800999000	-0.475957000	1	-0.547762000	3.106916000	-3.003385000
1	-3.986175000	2.318298000	1.089882000	1	5.338689000	-1.541306000	0.999417000
6	-1.496919000	-0.789786000	-0.926761000	1	5.637136000	0.202277000	1.134938000
1	-0.582964000	-1.556563000	1.059229000	1	5.730238000	-0.591996000	-0.483483000
8	-1.945765000	0.491891000	-0.818629000	8	0.680483000	-1.916739000	-0.569794000
8	-3.612170000	-1.530698000	-0.139367000	1	-0.270276000	-1.946967000	-0.292430000
6	-2.824069000	0.705564000	0.271961000	6	1.413149000	-3.060393000	-0.159523000
6	-3.981294000	-0.291682000	0.208475000	1	0.963797000	-3.968048000	-0.594432000
8	-5.119183000	-0.030137000	0.470972000	1	2.433758000	-2.944805000	-0.551947000
1	-2.266518000	0.491619000	1.209739000	1	1.444358000	-3.146118000	0.940463000
EM-INT₃ E(scf)= -1295.54393421				EM-TS₂ E(scf)= -1295.53703923 v_{min}= -883.3651			
8	3.456369000	-0.892336000	0.947551000	8	-3.327365000	0.477035000	1.148185000
6	4.356870000	-0.094865000	0.358372000	6	-4.318811000	-0.044343000	0.430393000
6	3.929307000	0.423136000	-1.015561000	6	-4.006925000	-0.252219000	-1.052725000
8	5.403223000	0.152737000	0.883916000	8	-5.382439000	-0.299140000	0.916708000
8	2.547173000	0.742005000	-1.005670000	8	-2.635149000	-0.606815000	-1.247458000
6	2.208478000	-1.130036000	0.353187000	6	-2.056457000	0.773493000	0.591274000
6	1.745515000	-0.270040000	-0.594388000	6	-1.738269000	0.164067000	-0.644962000
8	0.569812000	-0.297970000	-1.151379000	8	-0.585915000	0.183268000	-1.165918000
6	1.579206000	-2.408571000	0.800254000	6	-1.617194000	2.181444000	0.921504000
1	0.833639000	-0.029501000	1.502991000	1	-1.001140000	0.014574000	1.284160000
1	1.507657000	-2.464021000	1.902210000	1	-1.601207000	2.331143000	2.013740000
1	2.178672000	-3.278522000	0.473643000	1	-2.306919000	2.929230000	0.488282000
1	0.566548000	-2.511925000	0.381810000	1	-0.602209000	2.375347000	0.541346000
6	4.708530000	1.647656000	-1.439074000	6	-4.865997000	-1.325684000	-1.681091000
1	4.091656000	-0.405762000	-1.735705000	1	-4.178235000	0.718215000	-1.557569000
1	4.557460000	2.465105000	-0.716111000	1	-4.687143000	-2.294740000	-1.188552000
1	4.366964000	1.978928000	-2.432323000	1	-4.628222000	-1.417513000	-2.752357000
1	5.782744000	1.413798000	-1.479680000	1	-5.927564000	-1.065304000	-1.560391000
49	-1.238239000	0.125268000	-0.245545000	49	1.270211000	-0.099913000	-0.121407000
8	-2.808062000	1.303354000	0.898393000	8	2.985519000	-1.244113000	0.818373000
8	-1.936612000	-1.899409000	0.421512000	8	1.832369000	1.985939000	0.457468000
6	-2.612918000	-2.020162000	-0.640312000	6	2.448562000	2.140756000	-0.638463000
6	-2.550408000	2.306416000	0.182600000	6	2.745860000	-2.204044000	0.039908000
6	-3.247848000	3.616785000	0.399694000	6	3.592984000	-3.442376000	0.055085000
8	-1.662131000	2.212745000	-0.720961000	8	1.790530000	-2.107907000	-0.792736000
8	-2.612420000	-1.079588000	-1.486636000	8	2.476401000	1.192433000	-1.471323000
6	-3.379423000	-3.279356000	-0.918672000	6	3.107878000	3.451681000	-0.951220000
1	-3.399187000	4.128936000	-0.561631000	1	4.373892000	-3.333947000	-0.717151000
1	-2.599506000	4.254277000	1.025071000	1	2.985929000	-4.323976000	-0.196998000
1	-4.203950000	3.465010000	0.919373000	1	4.080165000	-3.564807000	1.032453000
1	-2.754145000	-3.928625000	-1.555413000	1	3.869908000	3.326155000	-1.732698000
1	-4.301775000	-3.049106000	-1.471368000	1	3.546772000	3.881631000	-0.038986000
1	-3.602842000	-3.811224000	0.016519000	1	2.335567000	4.149515000	-1.317733000
8	-0.072035000	0.321194000	1.675104000	8	0.028685000	-0.430424000	1.592522000

6	-0.602119000	-0.144499000	2.913169000	6	0.439271000	-0.102113000	2.903782000
1	-1.582242000	0.336211000	3.037136000	1	1.377921000	-0.634425000	3.127325000
1	-0.728262000	-1.239517000	2.899529000	1	0.610226000	0.984002000	3.015780000
1	0.066617000	0.157131000	3.735409000	1	-0.334604000	-0.425541000	3.620833000
EM-INT₄ E(scf)= -1295.56544642							
8	-3.390700000	-0.983722000	1.016302000				
6	-4.419357000	-0.686156000	0.221350000				
6	-4.111475000	0.265437000	-0.935717000				
8	-5.510430000	-1.133340000	0.410573000				
8	-2.760413000	0.114628000	-1.405419000				
6	-2.144911000	-0.298937000	0.902322000				
6	-1.784702000	-0.037563000	-0.541988000				
8	-0.636164000	0.047136000	-0.939595000				
6	-2.116701000	0.983821000	1.728702000				
1	-1.368290000	-0.985019000	1.287309000				
1	-2.352315000	0.730500000	2.774114000				
1	-2.850463000	1.728794000	1.374377000				
1	-1.107452000	1.427466000	1.695022000				
6	-5.035736000	0.061670000	-2.115279000				
1	-4.211788000	1.297456000	-0.552586000				
1	-4.930046000	-0.959400000	-2.514358000				
1	-4.793174000	0.786229000	-2.907911000				
1	-6.076845000	0.205253000	-1.791986000				
49	1.416744000	-0.099445000	0.080571000				
8	3.598104000	-0.661240000	0.156079000				
8	1.149037000	1.885492000	1.143566000				
6	1.513932000	2.507663000	0.102761000				
6	3.467823000	-1.284813000	-0.933251000				
6	4.650621000	-1.949333000	-1.577738000				
8	2.337607000	-1.324991000	-1.504552000				
8	1.813624000	1.858645000	-0.934036000				
6	1.574547000	4.008999000	0.113886000				
1	5.076517000	-1.249702000	-2.317380000				
1	4.334447000	-2.857762000	-2.110843000				
1	5.420274000	-2.180298000	-0.828041000				
1	1.990221000	4.392730000	-0.827498000				
1	2.186889000	4.341946000	0.966860000				
1	0.558160000	4.409573000	0.263063000				
8	0.570963000	-1.337445000	1.446526000				
6	1.245581000	-1.670783000	2.621739000				
1	2.272207000	-2.048916000	2.436270000				
1	1.329730000	-0.813675000	3.323939000				
1	0.690714000	-2.473700000	3.145382000				

Table S3. Optimized cartesian coordinates (xyz) for all species in the energy profile of Figure 9. Coordinates are given in Å.

ADD E(scf)= -1411.18787182				EL-TS₁ E(scf)= -1411.14833580 v_{min}= -663.3968			
8	-0.683824000	-3.259692000	-0.311907000	8	0.556979000	3.132781000	1.167067000
6	0.719485000	-3.478376000	-0.516208000	6	1.571081000	2.803679000	2.114662000
1	1.249663000	-3.050216000	0.348690000	1	2.224451000	2.005479000	1.728871000
1	1.054785000	-2.992550000	-1.443952000	1	1.115417000	2.469837000	3.059699000
1	0.841780000	-4.567663000	-0.569373000	1	2.133524000	3.733865000	2.272315000
1	-3.143767000	-4.013227000	-0.280871000	1	-0.377645000	4.428620000	-0.846742000
1	-3.563229000	-2.943388000	-1.658376000	1	-1.997256000	4.403889000	-0.092751000

6	-3.515104000	-3.016204000	-0.559812000	6	-1.326419000	3.872624000	-0.794812000
1	-4.529870000	-2.884954000	-0.152827000	1	-1.788228000	3.898712000	-1.796079000
1	-1.767446000	1.801518000	-1.893445000	1	-3.556293000	-0.268241000	1.812209000
6	-2.859726000	1.851976000	-1.753081000	6	-4.274019000	0.109763000	1.065144000
1	-3.220913000	2.832337000	-2.103753000	1	-5.232713000	-0.415050000	1.202104000
8	-0.537070000	-1.108632000	-0.915384000	8	-0.149187000	1.010313000	1.253531000
6	-2.600731000	-1.944493000	0.007047000	6	-1.055566000	2.452284000	-0.382574000
1	-3.338402000	1.061819000	-2.353080000	1	-4.427399000	1.188852000	1.221875000
6	-1.154440000	-2.055488000	-0.460262000	6	-0.242413000	2.156695000	0.762848000
1	-2.555150000	-2.004416000	1.108714000	1	-0.014930000	1.668543000	-1.270706000
8	-2.697660000	2.754070000	0.482902000	8	-3.659604000	-1.546661000	-0.549102000
8	-3.116610000	-0.679951000	-0.374681000	8	-2.315863000	1.735506000	-0.310706000
6	-3.211412000	1.697763000	-0.275115000	6	-3.755326000	-0.168366000	-0.341623000
6	-2.682797000	0.390593000	0.286862000	6	-2.389844000	0.467146000	-0.550192000
8	-1.953120000	0.343083000	1.245663000	8	-1.463955000	-0.239875000	-0.929567000
1	-4.314597000	1.662542000	-0.166699000	1	-4.440607000	0.295578000	-1.082114000
1	-2.143668000	2.380608000	1.193027000	1	-2.845129000	-1.725464000	-1.051211000
49	1.091735000	0.143164000	0.230180000	49	0.653032000	-0.630276000	-0.138496000
8	3.303572000	0.594278000	0.306526000	8	2.642933000	-1.452144000	-0.865671000
8	0.569477000	2.199176000	1.089379000	8	-0.223966000	-2.653274000	-0.779447000
6	0.418519000	2.628634000	-0.081759000	6	-0.512844000	-2.879299000	0.420355000
6	3.513599000	-0.196594000	-0.651775000	6	3.263637000	-0.803614000	0.014083000
6	4.902414000	-0.370576000	-1.200479000	6	4.760443000	-0.886396000	0.126047000
8	2.544190000	-0.818939000	-1.175747000	8	2.617434000	-0.058754000	0.809319000
8	0.508479000	1.811618000	-1.055615000	8	-0.163324000	-2.046101000	1.315869000
6	0.104467000	4.068840000	-0.350667000	6	-1.336052000	-4.073601000	0.805276000
1	5.063072000	0.395109000	-1.978947000	1	5.034602000	-1.150976000	1.159697000
1	5.015391000	-1.361748000	-1.662646000	1	5.191845000	0.106402000	-0.084267000
1	5.650349000	-0.218058000	-0.409027000	1	5.165885000	-1.625567000	-0.577957000
1	0.541323000	4.706740000	0.431091000	1	-1.198429000	-4.889409000	0.081576000
1	-0.994054000	4.169931000	-0.317619000	1	-2.393487000	-3.754796000	0.781828000
1	0.465106000	4.362395000	-1.346781000	1	-1.094503000	-4.402920000	1.825985000
8	0.731209000	-1.268857000	1.626444000	8	0.815237000	0.978775000	-1.609725000
6	0.575761000	-0.950445000	2.976000000	6	2.007386000	1.686112000	-1.862859000
1	1.487801000	-0.498525000	3.419057000	1	2.381354000	2.202715000	-0.959270000
1	0.365685000	-1.881545000	3.539081000	1	1.833392000	2.431674000	-2.658794000
1	-0.268220000	-0.254740000	3.153792000	1	2.773707000	0.975074000	-2.210639000
EL-INT₁ E(scf)= -1411.16479932				EL-INT₂ E(scf)= -1411.14911595			
8	0.119104000	2.982280000	0.708965000	8	-0.063722000	3.625384000	-0.373029000
6	0.933573000	3.084805000	1.862397000	6	1.301863000	3.812501000	-0.657824000
1	1.654123000	2.254201000	1.931081000	1	1.555118000	3.478348000	-1.677693000
1	0.313832000	3.114804000	2.777076000	1	1.946313000	3.276289000	0.063603000
1	1.482365000	4.033073000	1.764650000	1	1.481685000	4.893918000	-0.568828000
1	-1.896482000	4.367692000	0.109772000	1	-2.065231000	4.098982000	1.002251000
1	-3.553503000	3.771153000	0.437237000	1	-2.786780000	2.817908000	2.017688000
6	-2.616568000	3.566839000	-0.112362000	6	-2.576001000	3.125182000	0.974644000
1	-2.852260000	3.601504000	-1.193302000	1	-3.543178000	3.256909000	0.457047000
1	-2.266209000	-1.472592000	1.513154000	1	-1.993202000	-1.772031000	1.113874000
6	-3.330986000	-1.401566000	1.234549000	6	-3.091414000	-1.734899000	1.031907000
1	-3.824870000	-2.363495000	1.446588000	1	-3.468504000	-2.769626000	1.077897000
8	-0.397612000	0.781506000	1.095267000	8	0.228808000	1.446683000	-0.908483000
6	-2.044488000	2.249491000	0.280224000	6	-1.708373000	2.131547000	0.282413000
1	-3.784138000	-0.616397000	1.858918000	1	-3.490461000	-1.179479000	1.898553000
6	-0.794497000	1.971784000	0.708984000	6	-0.520964000	2.353915000	-0.328568000
1	-0.450360000	0.775421000	-1.869206000	1	-1.051411000	0.130928000	1.536328000
8	-3.124092000	-2.136134000	-1.089340000	8	-3.004740000	-1.795086000	-1.400050000
8	-2.944530000	1.171371000	0.233360000	8	-2.129359000	0.778754000	0.336190000
6	-3.495185000	-1.084637000	-0.256775000	6	-3.514169000	-1.105920000	-0.291899000
6	-2.725063000	0.183272000	-0.614531000	6	-3.200874000	0.393242000	-0.415631000
8	-1.965356000	0.240062000	-1.558671000	8	-3.808582000	1.146439000	-1.112082000
1	-4.563297000	-0.878589000	-0.453212000	1	-4.609580000	-1.163891000	-0.385484000

1	-2.151430000	-2.126824000	-1.186151000	1	-2.030835000	-1.707319000	-1.426457000
49	0.961280000	-0.385391000	0.046372000	49	1.038749000	-0.261703000	-0.127591000
8	2.931101000	-1.061594000	-0.823752000	8	1.085435000	-2.508971000	0.454135000
8	-0.326538000	-2.085458000	-0.601536000	8	2.917549000	0.279623000	0.914450000
6	-0.063817000	-2.735513000	0.461561000	6	3.594800000	0.010034000	-0.123102000
6	3.544571000	-0.232968000	-0.102890000	6	0.183288000	-2.726689000	-0.382552000
6	5.043529000	-0.157530000	-0.115343000	6	-0.412246000	-4.085004000	-0.597803000
8	2.882152000	0.531732000	0.664539000	8	-0.255642000	-1.748619000	-1.084037000
8	0.724363000	-2.233537000	1.302476000	8	3.000181000	-0.386782000	-1.163771000
6	-0.702643000	-4.074362000	0.674018000	6	5.087914000	0.153114000	-0.096847000
1	5.422772000	-0.707148000	0.763074000	1	0.011185000	-4.508069000	-1.524771000
1	5.372094000	0.888284000	-0.023008000	1	-1.499447000	-3.986878000	-0.744711000
1	5.449565000	-0.619240000	-1.025795000	1	-0.178862000	-4.752889000	-0.242507000
1	-0.212541000	-4.805622000	0.009049000	1	5.501144000	-0.596302000	0.598539000
1	-1.763230000	-4.015564000	0.381995000	1	5.354426000	1.147464000	0.294135000
1	-0.595217000	-4.399151000	1.717659000	1	5.514608000	0.004940000	-1.097778000
8	0.543688000	0.738552000	-1.817066000	8	-0.115892000	-0.082657000	1.761227000
6	1.173598000	1.949291000	-2.215293000	6	0.063318000	-0.810937000	2.965074000
1	0.953599000	2.759511000	-1.501405000	1	-0.412002000	-1.804055000	2.902022000
1	0.835320000	2.218968000	-3.228847000	1	-0.353995000	-0.239356000	3.809729000
1	2.256779000	1.760469000	-2.242734000	1	1.145169000	-0.937014000	3.108255000
EL-TS₂ E(scf)= -1411.14745395 v_{min}= -368.2259				EL-INT₃ E(scf)= -1411.18453648			
8	-0.186342000	3.533209000	-0.206689000	8	-1.353696000	3.330517000	-0.331876000
6	1.072996000	3.911939000	-0.738807000	6	-0.459462000	4.011264000	-1.210888000
1	1.123541000	3.693801000	-1.816931000	1	-0.390059000	3.466146000	-2.164331000
1	1.892786000	3.384573000	-0.222899000	1	0.538635000	4.089243000	-0.752949000
1	1.153694000	4.994039000	-0.568196000	1	-0.897022000	5.005899000	-1.362636000
1	-2.016546000	3.709365000	1.585367000	1	-3.086181000	3.211213000	1.661521000
1	-3.066622000	2.350958000	2.069767000	1	-3.947991000	1.665456000	1.909632000
6	-2.537882000	2.812034000	1.217627000	6	-3.315971000	2.234131000	1.209252000
1	-3.290025000	3.131789000	0.472830000	1	-3.868047000	2.402205000	0.271958000
1	-2.669917000	-1.879421000	0.824507000	1	-2.104816000	-2.520083000	0.600111000
6	-3.649329000	-1.678004000	0.360577000	6	-3.109368000	-2.436250000	0.156104000
1	-4.153831000	-2.638818000	0.165817000	1	-3.436788000	-3.435165000	-0.175387000
8	0.286566000	1.433805000	-0.806855000	8	-0.008610000	1.580455000	-0.358647000
6	-1.549724000	1.841955000	0.636208000	6	-2.038131000	1.453109000	0.964205000
1	-4.253527000	-1.099298000	1.080048000	1	-3.801259000	-2.076143000	0.935239000
6	-0.488829000	2.244039000	-0.190543000	6	-1.056060000	2.106380000	0.001583000
1	-0.518511000	1.162287000	1.628128000	1	-1.454662000	1.311677000	1.889250000
8	-2.764546000	-1.673066000	-1.909092000	8	-2.293042000	-1.993292000	-2.096806000
8	-2.083134000	0.563579000	0.316530000	8	-2.310255000	0.117710000	0.549666000
6	-3.475918000	-0.931193000	-0.957537000	6	-3.085609000	-1.508961000	-1.053720000
6	-2.854395000	0.464877000	-0.795964000	6	-2.679389000	-0.065041000	-0.729256000
8	-3.009640000	1.366975000	-1.566576000	8	-2.665248000	0.831841000	-1.531491000
1	-4.464629000	-0.744045000	-1.405554000	1	-4.106327000	-1.421311000	-1.465628000
1	-1.841193000	-1.771163000	-1.606190000	1	-1.361827000	-1.931766000	-1.802244000
49	1.055758000	-0.310602000	0.116321000	49	1.198333000	-0.155679000	0.450350000
8	0.981326000	-2.452271000	0.915650000	8	1.748055000	-2.367149000	0.453202000
8	3.101531000	0.373074000	0.586718000	8	3.097738000	0.982871000	0.607128000
6	3.544730000	-0.092694000	-0.506475000	6	3.338013000	0.831681000	-0.627870000
6	0.100902000	-2.736792000	0.068782000	6	0.804770000	-2.627350000	-0.330461000
6	-0.488793000	-4.110501000	-0.037710000	6	0.573846000	-4.022466000	-0.835100000
8	-0.288921000	-1.828428000	-0.736403000	8	0.042645000	-1.684382000	-0.721621000
8	2.749100000	-0.670915000	-1.295504000	8	2.518206000	0.201052000	-1.344930000
6	5.005311000	0.013700000	-0.832311000	6	4.610706000	1.372772000	-1.214726000
1	-0.537438000	-4.585546000	0.952587000	1	0.738370000	-4.749193000	-0.025655000
1	0.169542000	-4.719814000	-0.680652000	1	1.312000000	-4.229056000	-1.628801000
1	-1.482874000	-4.060641000	-0.505478000	1	-0.437397000	-4.123453000	-1.254922000
1	5.525543000	-0.834939000	-0.355769000	1	5.398943000	0.610761000	-1.088170000

1	5.423159000	0.943419000	-0.419923000	1	4.925168000	2.281243000	-0.681053000
1	5.163708000	-0.043731000	-1.918191000	1	4.486557000	1.568320000	-2.289241000
8	0.194987000	0.398153000	1.974729000	8	0.320066000	0.075038000	2.255532000
6	-0.375482000	-0.434943000	2.966439000	6	-0.120677000	-1.028213000	2.984032000
1	-1.271697000	-0.954681000	2.584089000	1	-0.989247000	-1.535548000	2.510073000
1	-0.658076000	0.181174000	3.836844000	1	-0.447958000	-0.692617000	3.988166000
1	0.371848000	-1.179269000	3.278285000	1	0.668715000	-1.793193000	3.137723000