A DFT Case Study on the Comparison of Ruthenium-Catalyzed C–H Allylation, C–H Alkenylation, and Hydroarylation

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Table S1. Cartesian coordinates of the stationary points involved in the main C-H allylation reaction, optimized at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.

| Names | Cartesian Coordinates |
|-------|-----------------------|
| 6     | 2.462380000 0.725427000 0.403532000 |
| 6     | 2.396763000 -0.209700000 -0.642803000 |
| 6     | 2.428020000 -1.592912000 -0.317845000 |
| 6     | 2.109893000 -2.008803000 0.983210000 |
| 6     | 1.930864000 -1.050368000 2.025597000 |
| 6     | 2.125957000 0.315414000 1.721003000 |
| 1     | 2.489470000 1.782728000 0.192350000 |
| 1     | 2.445951000 -2.325788000 -1.114309000 |
| 1     | 1.900476000 -3.052624000 1.173571000 |
| 1     | 1.918863000 1.067062000 2.468045000 |
| 6     | 1.483490000 -1.484127000 3.385269000 |
| 1     | 0.983772000 -0.672085000 3.911717000 |
| 1     | 0.806477000 -2.335672000 3.321850000 |
| 1     | 2.354170000 -1.788327000 3.972986000 |
| 6     | 2.868355000 0.199336000 -2.071154000 |
| 1     | 2.511740000 -0.621383000 -2.700454000 |
| 6     | 4.384244000 0.337221000 -2.278549000 |
| 1     | 4.910670000 -0.579861000 -2.007880000 |
| 1     | 4.600405000 0.556910000 -3.325254000 |
| 6     | 2.123116000 1.467332000 -2.491374000 |
| 1     | 2.284234000 1.651976000 -3.554276000 |
| 1     | 1.050211000 1.369276000 -2.319554000 |
| 1     | 2.478527000 2.346488000 -1.950273000 |
| 44    | 0.645549000 -0.500084000 0.324783000 |
| 6     | -1.500555000 -1.669986000 -0.318521000 |
| 8     | -1.216335000 -1.553000000 0.897108000 |
| 8     | -0.704009000 -1.319312000 -1.221544000 |
| 6     | -2.890195000 -2.200423000 -0.715528000 |
| 6     | -0.604462000 2.248914000 0.547880000 |
| 8     | 0.307814000 2.785260000 1.149886000 |
| 8     | -0.730067000 1.048762000 0.128413000 |
| 6     | -1.867589000 3.085887000 0.186216000 |
| 9     | -1.768709000 4.354430000 0.607108000 |
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| 9     | -2.977129000 2.559103000 0.744856000 |
| 9     | -3.751253000 -1.171289000 -0.830944000 |
| 9     | -2.851758000 -2.840217000 -1.891681000 |
| 9     | -3.374555000 -3.042967000 0.205825000 |
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**INT-1**

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| 9 | -2.201286000 | -4.637645000 | -2.197353000 |
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| 6 | 5.292708000 | 3.652300000 | -1.025645000 |
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TS-3

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| 6 | 1.322449000 | 1.360394000 | 2.421033000 |
| 1 | 3.412423000 | 0.946331000 | 2.035819000 |
| 1 | 0.792837000 | -2.484056000 | 2.251887000 |
| 1 | -1.136800000 | -0.998760000 | 2.576546000 |
| 1 | 1.467155000 | 2.431563000 | 2.383132000 |
| 6 | -1.170812000 | 1.747313000 | 2.711442000 |
| 1 | -0.949525000 | 2.751193000 | 2.350391000 |
| 1 | -2.027600000 | 1.352414000 | 2.165608000 |
| 1 | -1.446971000 | 1.819480000 | 3.767124000 |
| 6 | 3.405691000 | -1.848030000 | 1.868365000 |
| 1 | 2.978886000 | -2.661772000 | 1.274764000 |
| 6 | 3.901895000 | -2.438631000 | 3.198008000 |
| 1 | 3.092060000 | -2.915590000 | 3.752749000 |
|     |     |     |     |
|-----|-----|-----|-----|
| 1   | 4.671599000 | -3.188902000 | 3.010024000 |
| 1   | 4.333338000 | -1.658497000 | 3.829523000 |
| 6   | 4.556930000 | -1.238077000 | 1.070784000 |
| 1   | 5.275773000 | -2.016714000 | 0.812779000 |
| 1   | 4.207005000 | -0.780725000 | 0.144081000 |
| 1   | 5.092107000 | -0.479917000 | 1.646616000 |
| 44  | 0.894444000 | 0.086609000 | 0.676108000 |
| 6   | 1.659381000 | -1.110637000 | -1.925826000 |
| 6   | 1.756381000 | -0.711145000 | -2.355452000 |
| 6   | 1.356166000 | -1.549120000 | -0.774549000 |
| 6   | 1.966502000 | -2.214203000 | -2.963360000 |
| 6   | -0.285595000 | 3.768107000 | -1.135263000 |
| 6   | 0.832069000 | 4.603355000 | -1.043763000 |
| 6   | 2.095176000 | 4.111350000 | -0.737226000 |
| 6   | 2.275366000 | 2.756849000 | -0.490877000 |
| 6   | 1.183843000 | 1.887431000 | -0.540560000 |
| 6   | -0.087852000 | 2.402585000 | -0.881522000 |
| 1   | 0.705580000 | 5.664749000 | -1.224018000 |
| 1   | 2.939415000 | 4.789845000 | -0.693287000 |
| 1   | 3.265207000 | 2.373515000 | -0.272461000 |
| 6   | -1.164167000 | 1.375562000 | -0.929718000 |
| 6   | 1.506246000 | 0.801504000 | -1.384015000 |
| 6   | -4.288488000 | -0.413538000 | 0.142220000 |
| 8   | -3.953332000 | -0.223367000 | -1.098690000 |
| 8   | -3.942601000 | 0.200232000 | 1.124687000 |
| 6   | -5.253038000 | -1.624251000 | 0.270529000 |
| 8   | -0.868821000 | 0.226621000 | -0.433490000 |
| 8   | -2.283306000 | 1.597641000 | -1.443506000 |
| 1   | -3.235237000 | 0.545195000 | -1.211276000 |
| 6   | -1.621240000 | 4.370898000 | -1.475829000 |
| 6   | -1.984876000 | 4.006598000 | -2.437275000 |
| 6   | -2.381077000 | 4.104540000 | -0.740912000 |
| 1   | -1.540381000 | 5.456987000 | -1.520778000 |
| 9   | 3.218456000 | -2.073627000 | -3.429697000 |
| 9   | 1.850339000 | -3.435793000 | -2.438493000 |
| 9   | 1.121305000 | -2.119396000 | -4.002185000 |
| 9   | -5.676957000 | -1.779440000 | 1.529552000 |
| 9   | -6.336246000 | -1.474667000 | -0.514350000 |
| 9   | -4.634326000 | -2.763666000 | -0.099290000 |

INT-3

|     |     |     |
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| 6   | -2.209457000 | -1.932223000 | -1.729255000 |
| 6   | -2.236377000 | -2.416390000 | -0.407046000 |
| 6   | -1.016601000 | -2.913930000 | 0.168483000 |
| 6   | 0.188399000 | -2.801395000 | -0.508867000 |
| 6   | 0.243732000 | -2.194425000 | -1.810466000 |
|   | -0.972563000 | -1.815753000 | -2.422564000 |
|---|-------------|-------------|-------------|
| 1 | -3.112859000 | -1.573657000 | -2.198882000 |
| 1 | -1.025400000 | -3.282182000 | 1.186437000  |
| 1 | 1.109695000  | -3.087104000 | -0.018080000 |
| 1 | -0.953416000 | -1.359978000 | -3.403145000 |
| 6 | 1.558590000  | -2.004534000 | -2.500235000 |
| 1 | 1.469019000  | -1.291281000 | -3.318946000 |
| 1 | 2.316842000  | -1.639440000 | -1.807673000 |
| 1 | 1.903449000  | -2.956795000 | -2.912734000 |
| 6 | -3.505197000 | -2.494870000 | 0.412282000  |
| 1 | -3.215626000 | -2.285140000 | 1.447499000  |
| 1 | -0.953416000 | -1.359978000 | -3.403145000 |
| 6 | -4.059373000 | -3.927377000 | 0.354031000  |
| 1 | -3.317475000 | -4.658041000 | 0.680383000  |
| 1 | -4.933431000 | -4.019683000 | 1.000946000  |
| 1 | -4.360976000 | -4.181583000 | -0.664827000 |
| 6 | -4.573544000 | -1.478804000 | 0.011540000  |
| 1 | -5.404690000 | -1.521800000 | 0.716566000  |
| 1 | -4.184455000 | -0.459274000 | 0.011942000  |
| 1 | -4.978593000 | -1.686583000 | -0.981036000 |
| 44| -0.777064000 | -0.725855000 | -0.544520000 |
| 6 | -2.035698000 | 1.126537000  | 1.710577000  |
| 8 | -2.480422000 | 2.076979000  | 0.940831000  |
| 8 | -1.443805000 | 0.115532000  | 1.390168000  |
| 6 | -2.348531000 | 1.402732000  | 3.200054000  |
| 6 | -0.004826000 | 3.266429000  | -1.961048000 |
| 6 | -1.161521000 | 3.633733000  | -2.653925000 |
| 6 | -2.246596000 | 2.775974000  | -2.749716000 |
| 6 | -2.204972000 | 1.512423000  | -2.161223000 |
| 6 | -1.068547000 | 1.095997000  | -1.463839000 |
| 6 | 0.021022000  | 1.992031000  | -1.367663000 |
| 1 | -1.207805000 | 4.611188000  | -3.119153000 |
| 1 | -3.133805000 | 3.089577000  | -3.288786000 |
| 1 | -3.064926000 | 0.860586000  | -2.254742000 |
| 6 | 1.154181000  | 1.460655000  | -0.571520000 |
| 1 | -2.235754000 | 1.896302000  | -0.006338000 |
| 6 | 4.584337000  | -0.039605000 | 0.203141000  |
| 8 | 3.987838000  | 0.901052000  | 0.865515000  |
| 8 | 4.427162000  | -0.381877000 | -0.946513000 |
| 6 | 5.618929000  | -0.770097000 | 1.103307000  |
| 8 | 0.986206000  | 0.290671000  | -0.072412000 |
| 8 | 2.214184000  | 2.105854000  | -0.378589000 |
| 1 | 3.210310000  | 1.382762000  | 0.298914000  |
| 6 | 1.133858000  | 4.246188000  | -1.885304000 |
| 1 | 1.367066000  | 4.506011000  | -0.852270000 |
|   | 1    | 2.048162000 | 3.827393000 | -2.306443000 |
|---|------|-------------|-------------|--------------|
|   | 1    | 0.879484000 | 5.156502000 | -2.428299000 |
|   | 9    | -3.667408000 | 1.566573000 | 3.374773000  |
|   | 9    | -1.938737000 | 0.392225000 | 3.962060000  |
|   | 9    | -1.727264000 | 2.522091000 | 3.597061000  |
|   | 9    | 6.285326000  | -1.709510000| 0.422482000  |
|   | 9    | 6.522985000  | 0.091463000 | 1.607987000  |
|   | 9    | 5.006346000  | -1.373084000| 2.142424000  |
|   | 6    | 3.233285000  | -1.093345000| 0.857333000  |
|   | 6    | 2.922810000  | -1.850358000| -0.292934000 |
|   | 6    | 1.712417000  | -2.624775000| -0.306147000 |
|   | 6    | 0.783339000  | -2.512173000| 0.717648000  |
|   | 6    | 1.001613000  | -1.590171000| 1.793186000  |
|   | 6    | 2.268907000  | -0.939245000| 1.880091000  |
|   | 1    | 4.150548000  | -0.526243000| 0.905783000  |
|   | 1    | 1.476959000  | -3.217374000| -1.181278000 |
|   | 1    | -0.170823000 | -3.016626000| 0.638632000  |
|   | 1    | 2.460168000  | -0.260343000| 2.700326000  |
|   | 6    | -0.046155000 | -1.386164000| 2.842382000  |
|   | 1    | 0.090040000  | -0.433009000| 3.351965000  |
|   | 1    | -1.044161000 | -1.407626000| 2.405222000  |
|   | 1    | 0.015440000  | -2.184190000| 3.588020000  |
|   | 6    | 3.854889000  | -1.943432000| -1.480300000 |
|   | 1    | 3.218555000  | -2.091866000| -2.358686000 |
|   | 6    | 4.748638000  | -3.184452000| -1.326465000 |
|   | 1    | 4.156539000  | -4.092370000| -1.199154000 |
|   | 1    | 5.374827000  | -3.308951000| -2.211564000 |
|   | 1    | 5.403460000  | -3.081463000| -0.457988000 |
|   | 6    | 4.690118000  | -0.684740000| -1.715909000 |
|   | 1    | 5.246858000  | -0.783218000| -2.648855000 |
|   | 1    | 4.061691000  | 0.204539000 | -1.786797000 |
|   | 1    | 5.418812000  | -0.526111000| -0.918170000 |
| 44 | 1.300376000 | -0.380690000 | 0.041996000 |
|   | 6    | 0.361864000  | 3.788494000 | -0.127692000 |
|   | 6    | 1.559250000  | 4.437188000 | 0.180496000  |
|   | 6    | 2.709981000  | 3.724423000 | 0.493606000  |
|   | 6    | 2.696677000  | 2.334352000 | 0.513847000  |
|   | 6    | 1.525669000  | 1.642734000 | 0.210428000  |
|   | 6    | 0.365326000  | 2.382566000 | -0.099948000 |
|   | 1    | 1.585722000  | 5.520601000 | 0.175226000  |
|   | 1    | 3.623768000  | 4.260036000 | 0.727434000  |
|   | 1    | 3.607776000  | 1.802468000 | 0.758011000  |
|   | 6    | -0.814843000 | 1.536693000 | -0.406422000 |
|   | 6    | -4.266169000 | -0.145050000| 0.012479000  |
|   |      |            |            |            |
|---|------|------------|------------|------------|
| 8 | -3.788068000 | 0.382808000 | -1.072835000 |   |
| 8 | -3.937803000 | 0.045982000 | 1.159975000 |   |
| 6 | -5.405663000 | -1.145747000 | 0.324825000 |   |
| 8 | -0.630916000 | 0.259856000 | -0.325580000 |   |
| 8 | -1.927628000 | 2.007206000 | -0.727771000 |   |
| 1 | -2.975883000 | 1.042579000 | 0.882979000 |   |
| 6 | -0.847475000 | 4.617335000 | -0.466005000 |   |
| 1 | -1.216037000 | 4.394892000 | 0.783712000 |   |
| 1 | -1.675117000 | 4.413249000 | 0.214143000 |   |
| 1 | -0.600233000 | 5.677725000 | -0.411730000 |   |
| 9 | -5.941484000 | 0.294446000 | -1.285484000 |   |
| 9 | -6.392594000 | -0.544924000 | -1.016584000 |   |
| 9 | -4.941144000 | -2.163513000 | -1.076824000 |   |

**INT-3-2**

|   |      |            |            |            |
|---|------|------------|------------|------------|
| 6 | 4.256573000 | -0.234874000 | -0.012413000 |   |
| 6 | 3.922336000 | 0.450321000 | 1.170011000 |   |
| 6 | 3.224974000 | 1.691139000 | 1.039349000 |   |
| 6 | 2.808846000 | 2.167614000 | -0.203080000 |   |
| 6 | 3.150438000 | 1.468564000 | -1.406341000 |   |
| 6 | 3.906074000 | 0.294446000 | -1.285484000 |   |
| 1 | 4.789248000 | -1.172461000 | 0.034780000 |   |
| 1 | 2.936833000 | 2.228036000 | 1.934943000 |   |
| 1 | 2.207222000 | 3.064737000 | -0.265310000 |   |
| 1 | 4.144516000 | -0.274370000 | -2.174311000 |   |
| 6 | 2.692583000 | 1.984055000 | -2.733727000 |   |
| 1 | 2.783380000 | 1.217219000 | -3.501884000 |   |
| 1 | 1.653184000 | 2.310200000 | -2.684320000 |   |
| 1 | 3.303503000 | 2.840943000 | -3.030210000 |   |
| 6 | 4.352798000 | -0.020046000 | 2.540823000 |   |
| 1 | 3.568470000 | 0.283185000 | 3.241710000 |   |
| 6 | 5.641502000 | 0.716991000 | 2.947890000 |   |
| 1 | 5.519730000 | 1.800018000 | 2.907029000 |   |
| 1 | 5.930970000 | 0.442008000 | 0.957358000 |   |
| 1 | 6.460512000 | 0.450997000 | 2.269527000 |   |
| 6 | 4.530867000 | -1.533455000 | 2.653404000 |   |
| 1 | 4.730437000 | -1.803104000 | 3.691115000 |   |
| 1 | 3.640042000 | -2.072629000 | 2.329497000 |   |
| 1 | 5.376834000 | -1.884707000 | 2.058823000 |   |
| 44 | 2.023597000 | 0.019543000 | -0.044160000 |   |
| 6 | 0.326195000 | -2.792148000 | -2.849901000 |   |
| 6 | 1.162333000 | -3.903884000 | -2.791930000 |   |
| 6 | 2.233277000 | -3.950730000 | -1.906037000 |   |
| 6 | 2.508433000 | -2.881060000 | -1.062617000 |   |
| 6 | 1.713612000 | -1.740827000 | -1.109438000 |   |
| 6 | 0.618089000 | -1.712555000 | -1.991498000 |   |
|   | 1     | 2     | 3       |
|---|-------|-------|---------|
|   | x     | y     | z       |
| 1 | 0.965161000 | -4.747950000 | -3.442039000 |
| 1 | 2.860979000 | -4.834805000 | -1.876260000 |
| 1 | 3.341549000 | -2.951664000 | -0.375665000 |
| 6 | -0.192874000 | -0.490412000 | -1.876260000 |
| 6 | -1.765247000 | 2.893519000 | -2.129348000 |
| 8 | -0.829673000 | 3.050074000 | -2.880893000 |
| 6 | -2.395340000 | 4.116957000 | -1.408416000 |
| 8 | 0.240956000 | 0.384980000 | -1.038584000 |
| 8 | -1.255716000 | -0.284180000 | -2.515858000 |
| 1 | -1.848998000 | 0.909898000 | -2.140807000 |
| 6 | -0.834946000 | -2.796228000 | -3.805925000 |
| 1 | -1.784865000 | -2.729794000 | -3.273805000 |
| 1 | -0.802255000 | -1.940652000 | -4.481141000 |
| 1 | -0.827613000 | -3.712157000 | -4.397188000 |
| 9 | -2.100245000 | 4.077578000 | -0.083100000 |
| 9 | -1.925826000 | 5.271805000 | -1.892585000 |
| 9 | -3.734674000 | 4.135149000 | -1.522437000 |
| 6 | 0.792050000 | -1.263971000 | 1.304972000 |
| 6 | 0.773163000 | 0.026551000 | 1.824245000 |
| 1 | -0.062872000 | -1.641056000 | 0.765842000 |
| 1 | 1.426557000 | -2.010922000 | 1.760053000 |
| 1 | 1.446222000 | 0.244888000 | 2.643840000 |
| 6 | -0.395317000 | 0.968855000 | 1.706565000 |
| 1 | -0.726022000 | 1.059347000 | 0.676897000 |
| 1 | -0.113461000 | 1.953733000 | 2.074887000 |
| 7 | -1.609490000 | 0.515917000 | 2.480511000 |
| 6 | -1.309479000 | 0.251655000 | 3.924182000 |
| 1 | -0.924678000 | 1.173717000 | 4.360925000 |
| 1 | -0.503695000 | -0.479923000 | 3.931845000 |
| 6 | -2.771475000 | 1.446347000 | 2.244346000 |
| 1 | -3.659621000 | 0.906074000 | 2.564099000 |
| 1 | -2.837526000 | 1.558951000 | 1.162713000 |
| 6 | -2.505306000 | -0.282740000 | 4.691891000 |
| 1 | -3.284669000 | 0.467511000 | 4.822490000 |
| 1 | -2.172388000 | -0.592323000 | 5.683145000 |
| 1 | -2.942226000 | -1.146204000 | 4.189943000 |
| 6 | -2.655148000 | 2.797649000 | 2.924011000 |
| 1 | -3.521852000 | 3.395919000 | 2.641145000 |
| 1 | -1.767007000 | 3.347276000 | 2.613017000 |
| 1 | -2.652456000 | 2.716764000 | 4.011237000 |
| 1 | -1.917235000 | -0.407836000 | 2.042408000 |
| 6 | -3.621191000 | -1.946804000 | 1.207334000 |
| 8 | -4.542146000 | -1.393807000 | 1.808892000 |
|   |     |          |          |          |
|---|-----|----------|----------|----------|
| 8 | -2.381398000 | -1.725156000 | 1.240113000 |
| 6 | -3.992938000 | -3.110666000 | 0.233371000 |
| 9 | -3.364231000 | -4.259415000 | 0.575699000 |
| 9 | -5.310676000 | -3.378368000 | 0.205405000 |
| 9 | -3.621667000 | -2.820991000 | -1.035678000 |
| 9 | 3.034197000 | 3.067277000 | 0.271061000 |
| 6 | 2.111307000 | 2.234232000 | -0.189752000 |
| 1 | 4.089153000 | 2.815496000 | 0.250507000 |
| 1 | 2.766847000 | 4.034740000 | -0.160746000 |
| 6 | 2.436120000 | 0.914264000 | -0.814678000 |
| 1 | 2.107623000 | 0.897945000 | -1.856021000 |
| 1 | 3.507380000 | 0.718049000 | -0.785380000 |
| 7 | 1.721818000 | -0.227247000 | -0.140139000 |
| 6 | 2.186578000 | -0.402586000 | 1.276240000 |
| 1 | 1.032501000 | -2.159406000 | -0.521880000 |
| 1 | 1.367713000 | -1.198617000 | -1.944939000 |
| 6 | 1.433451000 | -1.487817000 | 2.023889000 |
| 1 | 1.672078000 | -2.486770000 | 1.658954000 |
| 1 | 1.717610000 | -1.443326000 | 3.075862000 |
| 1 | 0.355379000 | -1.345160000 | 1.951604000 |
| 6 | 3.127637000 | -2.122525000 | -1.093496000 |
| 1 | 3.063703000 | -3.003343000 | -1.730159000 |
| 1 | 3.856951000 | -1.457282000 | -1.556701000 |
| 1 | 3.520786000 | -2.453150000 | -0.131732000 |
| 1 | 0.687234000 | 0.053070000 | -0.098818000 |
| 6 | -1.669538000 | -0.341600000 | -0.069805000 |
| 8 | -1.515212000 | -1.562479000 | -0.037916000 |
| 8 | -0.811288000 | 0.581828000 | -0.098869000 |
| 6 | -3.134306000 | 0.201173000 | -0.071863000 |
| 9 | -4.059889000 | -0.773588000 | -0.053647000 |
| 9 | -3.376323000 | 0.955663000 | -1.688960000 |
| 9 | -3.365498000 | 0.986215000 | 1.006273000 |
| 6 | 4.180546000 | -0.315801000 | -0.370978000 |
| 6 | 3.993747000 | -0.277256000 | 1.030054000 |
| 6 | 3.383271000 | 0.891126000 | 1.574259000 |
| 6 | 2.948237000 | 1.927435000 | 0.735785000 |
| 6 | 3.203603000 | 1.903082000 | -0.678365000 |
| 6 | 3.852080000 | 0.790510000 | -1.207356000 |
| 1 | 4.597752000 | -1.200523000 | -0.829736000 |
| 1 | 3.172705000 | 0.939961000 | 2.634757000 |

**R2+HOTFA**

**TS-4**
|   |       |       |       |
|---|-------|-------|-------|
| 1 | 2.392561000 | 2.753832000 | 1.157649000 |
| 1 | 4.003463000 | 0.709969000 | -2.275886000 |
| 6 | 2.717197000 | 3.030753000 | -1.538885000 |
| 1 | 2.736681000 | 2.753978000 | -2.592369000 |
| 1 | 1.698380000 | 3.312489000 | -1.269195000 |
| 1 | 3.354074000 | 3.909187000 | -1.402657000 |
| 6 | 4.443249000 | -1.385087000 | 1.954928000 |
| 1 | 3.756067000 | -1.378411000 | 2.806908000 |
| 6 | 5.849462000 | -1.062825000 | 2.484432000 |
| 1 | 5.877893000 | -0.087317000 | 2.972939000 |
| 1 | 6.162834000 | -1.815785000 | 3.209782000 |
| 1 | 6.575182000 | -1.054115000 | 1.667678000 |
| 6 | 4.400687000 | -2.777893000 | 1.327234000 |
| 1 | 4.644285000 | -3.529164000 | 2.079620000 |
| 1 | 3.412854000 | -3.010573000 | 0.927104000 |
| 1 | 5.127833000 | -2.880241000 | 0.519035000 |
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**INT-4-1**

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|   | 1   | 4.934310000 | -4.301688000| -1.362753000 |
|   | 1   | 4.092015000 | -3.167484000| -0.307666000 |
|   | 1   | 5.782263000 | -2.888750000| -0.747102000 |
|   | 1   | 3.719347000 | -0.652289000| -2.953826000 |
|   | 6   | -0.481939000| -2.799802000| 0.292916000  |
|   | 8   | -0.506985000| -3.206577000| 1.444265000  |
|   | 8   | -0.124254000| -1.682381000| -0.193138000 |
|    |     |          |          |          |
|----|-----|----------|----------|----------|
| 6  | -0.940745000 | -3.76113000 | -0.846187000 |
| 9  | 0.076109000  | -4.016332000 | -1.702162000 |
| 9  | -1.368702000 | -4.942461000 | -0.375754000 |
| 9  | -1.946833000 | -3.228623000 | -1.570230000 |
| 6  | 2.693625000  | -1.434802000 | 1.021150000 |
| 6  | 1.741699000  | -2.476375000 | 1.176335000 |
| 6  | 0.503870000  | -2.110395000 | 1.739466000 |
| 6  | 0.244314000  | -0.791931000 | 2.207490000 |
| 6  | 1.230261000  | 0.205942000  | 2.128680000 |
| 6  | 2.445617000  | -0.118878000 | 1.467885000 |
| 1  | 3.631526000  | -1.634574000 | 0.523593000 |
| 1  | -0.289980000 | -2.843883000 | 1.771142000 |
| 1  | -0.735820000 | -0.546393000 | 2.592509000 |
| 1  | 3.190715000  | 0.646763000  | 1.305946000 |
| 6  | 0.968818000  | 1.576860000  | 2.654957000 |
| 1  | 1.731081000  | 2.277039000  | 2.326146000 |
| 1  | -0.015826000 | 1.927717000  | 2.346131000 |
| 1  | 0.985236000  | 1.543010000  | 3.747883000 |
| 6  | 1.995533000  | -3.915573000 | 0.792637000 |
| 1  | 1.057868000  | -4.284360000 | 0.371757000 |
| 6  | 2.306871000  | -4.719591000 | 2.066342000 |
| 1  | 1.501840000  | -4.637835000 | 2.798312000 |
| 1  | 2.435876000  | -5.774615000 | 1.819373000 |
| 1  | 3.228831000  | -4.365360000 | 2.534056000 |
| 6  | 3.095573000  | -4.104883000 | -0.246049000 |
| 1  | 3.160828000  | -5.157599000 | -0.523854000 |
| 1  | 2.912938000  | -3.534361000 | -1.156263000 |
| 1  | 4.078218000  | -3.815812000 | 0.144332000 |
| 44 | 0.818698000  | -0.726859000 | 0.041406000 |
| 6  | 2.512442000  | 3.567895000  | 0.030239000 |
| 6  | 3.896622000  | 3.710679000  | 0.138613000 |
| 6  | 4.764266000  | 2.893358000  | -0.571236000 |
| 6  | 4.258096000  | 1.919311000  | -1.421129000 |
| 6  | 2.885639000  | 1.723240000  | -1.525300000 |
| 6  | 2.015246000  | 2.526967000  | -0.773546000 |
| 1  | 4.295267000  | 4.487388000  | 0.780820000 |
| 1  | 5.835054000  | 3.029672000  | -0.478023000 |
| 1  | 4.931433000  | 1.310882000  | -2.014830000 |
| 6  | 0.545390000  | 2.261913000  | -0.859023000 |
| 6  | -2.931911000 | 2.197435000  | 0.473184000 |
| 8  | -2.652889000 | 2.673238000  | -0.701669000 |
| 8  | -2.200383000 | 2.031289000  | 1.421353000 |
| 6  | -4.443213000 | 1.856569000  | 0.582823000 |
| 8  | 0.102613000  | 1.070266000  | -0.763362000 |
|     |      |                   |                   |                   |
|-----|------|-------------------|-------------------|-------------------|
| 8   | -0.236010000 | 3.222915000 | -1.053273000 |
| 1   | -1.621221000 | 2.877330000 | -0.823733000 |
| 6   | 1.625321000  | 4.545008000 | 0.757566000  |
| 1   | 1.275963000  | 5.318999000 | 0.070845000  |
| 1   | 0.734397000  | 4.081311000 | 1.174761000  |
| 1   | 2.179176000  | 5.030792000 | 1.561281000  |
| 9   | -4.876871000 | 1.145161000 | -0.470586000 |
| 9   | -4.703696000 | 1.153400000 | 1.690924000  |
| 9   | -5.170562000 | 2.992972000 | 0.636194000  |
| 6   | 2.351964000  | 0.682002000 | -2.480397000 |
| 6   | 2.190186000  | -0.691937000 | -1.892732000 |
| 1   | 1.409849000  | 1.001958000 | -2.922851000 |
| 1   | 3.067763000  | 0.576560000 | -3.303070000 |
| 1   | 3.111158000  | -1.157520000 | -1.564985000 |
| 6   | 1.079044000  | -1.469651000 | -2.094283000 |
| 1   | 0.237190000  | -1.058887000 | -2.634200000 |
| 1   | 1.107389000  | -2.542474000 | -1.980977000 |
| 6   | -1.624042000 | -2.360316000 | -0.721199000 |
| 8   | -1.056966000 | -3.440713000 | -0.684376000 |
| 8   | -1.178766000 | -1.182244000 | -0.532069000 |
| 6   | -3.151131000 | -2.324202000 | -1.029208000 |
| 9   | -3.431312000 | -1.505202000 | -2.062370000 |
| 9   | -3.630592000 | -3.537942000 | -1.337937000 |
| 9   | -3.843059000 | -1.877685000 | 0.041489000  |

**TS-6**

|     |      |                   |                   |                   |
|-----|------|-------------------|-------------------|-------------------|
| 6   | 1.720055000  | -0.225904000 | 2.162996000  |
| 6   | 1.886878000  | -1.580970000 | 1.784443000  |
| 6   | 0.761309000  | -2.451293000 | 1.893466000  |
| 6   | -0.467049000 | -1.997683000 | 2.397589000  |
| 6   | -0.649815000 | -0.634343000 | 2.736887000  |
| 6   | 0.468296000  | 0.244568000  | 2.605911000  |
| 1   | 2.523988000  | 0.477311000  | 2.012668000  |
| 1   | 0.837883000  | -3.464361000 | 1.520342000  |
| 1   | -1.324620000 | -2.656049000 | 2.379919000  |
| 1   | 0.321542000  | 1.302350000  | 2.778776000  |
| 6   | -1.978272000 | -0.129016000 | 3.196605000  |
| 1   | -2.110590000 | 0.918508000  | 2.937129000  |
| 1   | -2.791323000 | -0.714225000 | 2.769256000  |
| 1   | -2.030195000 | -0.224183000 | 4.285745000  |
| 6   | 3.193824000  | -2.146796000 | 1.286267000  |
| 1   | 2.953464000  | -2.782554000 | 0.429829000  |
| 6   | 3.780123000  | -3.042455000 | 2.393710000  |
| 1   | 3.092606000  | -3.838960000 | 2.681749000  |
| 1   | 4.703473000  | -3.502881000 | 2.039536000  |
| 1   | 4.013023000  | -2.453032000 | 3.283331000  |
| 6  | 4.203977000  | -1.094019000  | 0.845684000  |
| 1  | 5.066829000  | -1.581845000  | 0.391635000  |
| 1  | 3.784876000  | -0.410170000  | 0.111957000  |
| 1  | 4.568183000  | -0.510510000  | 1.694078000  |
| 44 | 0.139928000  | -0.739466000  | 0.696133000  |
| 6  | 3.147033000  | 2.562040000   | -0.241168000 |
| 6  | 4.535657000  | 2.577940000   | -0.335775000 |
| 6  | 5.193172000  | 1.817119000   | -1.294457000 |
| 6  | 4.467828000  | 1.000894000   | -1.107504000 |
| 1  | 5.105057000  | 3.201989000   | 0.343325000  |
| 1  | 6.273372000  | 1.856809000   | -1.369891000 |
| 1  | 4.982373000  | 0.402775000   | -2.891271000 |
| 6  | 0.930797000  | 1.752486000   | -1.045085000 |
| 6  | -2.401153000 | 2.506884000   | 0.332324000  |
| 8  | -2.138984000 | 2.662544000   | -0.929658000 |
| 8  | -1.643385000 | 2.562278000   | 1.272942000  |
| 6  | -3.896847000 | 2.160303000   | 0.555031000  |
| 8  | 0.288519000  | 0.692497000   | -0.725841000 |
| 8  | 0.341690000  | 2.807049000   | -1.348692000 |
| 1  | -1.105825000 | 2.735066000   | -1.092472000 |
| 6  | 2.452071000  | 3.431397000   | 0.774119000  |
| 1  | 2.069983000  | 4.343312000   | 0.310190000  |
| 1  | 1.593724000  | 2.931468000   | 1.226029000  |
| 1  | 3.141057000  | 3.717976000   | 1.568459000  |
| 9  | -4.095421000 | 0.851388000   | 0.289036000  |
| 9  | -4.260524000 | 2.378087000   | 1.824813000  |
| 9  | -4.713418000 | 2.869344000   | -0.237975000 |
| 6  | 2.341234000  | -0.060796000  | -2.940440000 |
| 6  | 2.510314000  | -1.472804000  | -2.443939000 |
| 1  | 1.280566000  | 0.174074000   | -3.013757000 |
| 1  | 2.761554000  | 0.099491000   | -3.949422000 |
| 1  | 3.536859000  | -1.797854000  | -2.293759000 |
| 6  | 1.512428000  | -2.310368000  | -2.187769000 |
| 1  | 0.483126000  | -2.018967000  | -2.346050000 |
| 1  | 1.702783000  | -3.320748000  | -1.845546000 |
| 6  | -1.938965000 | -1.374464000  | -1.555888000 |
| 8  | -1.430257000 | -1.578911000  | -0.398201000 |
| 8  | -1.542997000 | -0.725230000  | -2.502767000 |
| 6  | -3.260842000 | -2.187750000  | -1.717236000 |
| 9  | -2.975681000 | -3.503376000  | -1.866918000 |
| 9  | -4.071899000 | -2.074393000  | -0.648520000 |
| 9  | -3.959657000 | -1.804479000  | -2.795139000 |
|   |       |       |       |
|---|-------|-------|-------|
| 6 | -2.523358000 | 0.214452000 | -1.577280000 |
| 6 | -2.539031000 | -1.199721000 | -1.702353000 |
| 6 | -1.567229000 | -1.812483000 | -2.539681000 |
| 6 | -0.589605000 | 0.381844000 | -3.070228000 |
| 6 | -1.555599000 | 0.980622000 | -2.267976000 |
| 1 | 3.198734000 | 0.713149000 | -0.899392000 |
| 1 | -1.515294000 | -2.891101000 | -3.738708000 |
| 6 | -3.532143000 | -2.077908000 | -0.981821000 |
| 6 | -3.017355000 | -3.020140000 | -2.195029000 |
| 1 | 3.143673000 | 2.043043000 | -2.874652000 |
| 6 | -4.695023000 | -2.826159000 | -2.874652000 |
| 1 | -4.344251000 | -1.020800000 | -3.832422000 |
| 6 | -5.397704000 | -3.621790000 | -4.742864000 |
| 6 | -4.041560000 | -1.507933000 | -0.981821000 |
| 1 | -3.224524000 | -2.405570000 | -0.981821000 |
| 1 | -4.630451000 | -0.600973000 | -0.981821000 |
| 44 | -0.525005000 | -0.551251000 | -1.069606000 |
| 6 | -1.743941000 | 3.252002000 | 0.282264000 |
| 6 | -3.098432000 | 3.583473000 | 0.316880000 |
| 6 | -3.978783000 | 2.877573000 | 1.124620000 |
| 6 | -3.514941000 | 1.840998000 | 1.926163000 |
| 6 | -2.171815000 | 1.474418000 | 1.907422000 |
| 6 | -1.304663000 | 2.173088000 | 1.056155000 |
| 1 | -3.460181000 | 4.408222000 | -0.295434000 |
| 1 | -5.029396000 | 3.141957000 | 1.139256000 |
| 1 | -4.203451000 | 1.307350000 | 2.568685000 |
| 6 | 0.130943000 | 1.749037000 | 0.967580000 |
| 6 | 3.774180000 | 1.491554000 | 0.046683000 |
| 8 | 3.320105000 | 1.446408000 | 1.265442000 |
| 8 | 3.300995000 | 2.038099000 | -0.919871000 |
| 6 | 5.103469000 | 0.696758000 | -0.919871000 |
| 8 | 0.434523000 | 0.721960000 | 0.275182000 |
| 8 | 1.001685000 | 2.401254000 | 1.581151000 |
| 1 | 2.364579000 | 1.865911000 | 1.347791000 |
| 6 | -0.782809000 | 4.062501000 | -0.549171000 |
| 1 | -0.295434000 | 4.825224000 | 0.063302000 |
|    | X       | Y       | Z       |
|----|---------|---------|---------|
| 1  | 0.01507 | 3.45183 | -0.97539|
| 1  | -1.30110| 4.57198 | -1.36217|
| 9  | 4.89930 | -0.60916| 0.19784 |
| 9  | 5.62666 | 0.79188 | -1.29075|
| 9  | 6.01950 | 1.15088 | 0.81215 |
| 6  | -1.63881| 0.35611 | 2.78498 |
| 6  | -2.50515| 0.00687 | 3.95686 |
| 1  | -1.45631| -0.53675| 2.18304 |
| 1  | -0.65572| 0.66016 | 3.16221 |
| 1  | -2.73122| 0.81891 | 4.64068 |
| 6  | -2.98044| -1.20657| 4.20671 |
| 1  | -2.77891| -2.04124| 3.54386 |
| 1  | -3.58123| -1.41064| 5.08474 |
| 6  | 0.90452 | -2.08607| 0.33965 |
| 8  | 1.38677 | -1.60141| -0.70962|
| 8  | -0.30472| -1.93361| 0.64182 |
| 6  | 1.82312 | -2.83698| 1.31978 |
| 9  | 2.89124 | -3.34927| 0.69788 |
| 9  | 2.25940 | -1.98919| 2.26980 |
| 9  | 1.16907 | -3.83691| 1.92734 |

**TS-7**

|    | X       | Y       | Z       |
|----|---------|---------|---------|
| 6  | 1.71608 | -1.86729| -2.22242|
| 6  | 2.84154 | -1.46234| -1.44600|
| 6  | 3.17442 | -0.08640| -1.45027|
| 6  | 2.45173 | 0.84808 | -2.23989|
| 6  | 1.35384 | 0.44877 | -3.02951|
| 6  | 0.99288 | -0.92936| -2.99704|
| 1  | 1.35033 | -2.88119| -2.16386|
| 1  | 3.93495 | 0.27824 | -0.77384|
| 1  | 2.65316 | 1.90093 | -2.10356|
| 1  | 0.08165 | -1.24806| -3.48522|
| 6  | 0.53247 | 1.44806 | -3.77929|
| 1  | -0.49094| 1.09587 | -3.90597|
| 1  | 0.51668 | 2.40025 | -3.25232|
| 1  | 0.96035 | 1.60505 | -4.77295|
| 6  | 3.62717 | -2.41546| -0.57839|
| 1  | 3.85795 | -1.87518| 0.34520 |
| 6  | 4.95578 | -2.73121| -1.28795|
| 1  | 5.52586 | -1.82546| -1.49952|
| 1  | 5.56588 | -3.37883| -0.65635|
| 1  | 4.77543 | -3.25020| -2.23221|
| 6  | 2.88253 | -3.69845| -0.21342|
| 1  | 3.48410 | -4.27693| 0.48900 |
| 1  | 1.92288 | -3.48508| 0.25556 |
| 1  | 2.71558 | -4.32804| -1.09073 |
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| 44| 1.072318000 | -0.250552000 | -0.951897000 |
| 6 | -4.429461000  | 0.281800000  | -1.483257000  |
| 6 | -5.683953000  | -0.313080000  | -1.594603000  |
| 6 | -5.981178000  | -1.487055000  | -0.916543000  |
| 6 | -5.019832000  | -2.092520000  | -0.121196000  |
| 6 | -3.743744000  | -1.547443000  | -0.001369000  |
| 6 | -3.462028000  | -0.352148000  | -0.683118000  |
| 6 | -5.019832000  | 0.152038000   | -1.011235000  |
| 1 | -6.964619000  | -1.932108000  | -0.537472000  |
| 1 | -5.254949000  | -3.003939000  | 0.415644000   |
| 6 | -2.102157000  | 0.249589000   | -0.586848000  |
| 6 | 1.064827000   | 3.030450000   | 0.057358000   |
| 8 | 0.285589000   | 2.220678000   | -0.537472000  |
| 8 | 2.186691000   | 3.385599000   | -0.275148000  |
| 6 | 0.492348000   | 3.693057000   | 1.347993000   |
| 8 | -1.107433000  | -0.410588000  | -0.926811000  |
| 8 | -2.051077000  | 1.468335000   | -0.150614000  |
| 1 | -1.080715000  | 1.845904000   | -0.207811000  |
| 6 | -4.145910000  | 1.556068000   | -2.236930000  |
| 1 | -4.100446000  | 2.412823000   | -1.562539000  |
| 1 | -3.191882000  | 1.515500000   | -2.766160000  |
| 1 | -4.928734000  | 1.741244000   | -2.971215000  |
| 9 | -0.525887000  | 3.003673000   | 1.895362000   |
| 9 | 1.432527000   | 3.840955000   | 2.295767000   |
| 9 | 0.020761000   | 4.929387000   | 1.054012000   |
| 6 | -2.744769000  | -2.217029000  | 0.920729000   |
| 6 | -2.641935000  | -1.507577000  | 2.243665000   |
| 1 | -3.057686000  | -3.248538000  | 1.088491000   |
| 1 | -1.759441000  | -2.242410000  | 0.453971000   |
| 1 | -2.304883000  | -0.474355000  | 2.209434000   |
| 6 | -2.937391000  | -2.051988000  | 3.416260000   |
| 1 | -3.281347000  | -3.077965000  | 3.494020000   |
| 1 | -2.837749000  | -1.494809000  | 4.339562000   |
| 6 | 1.105182000   | -0.571853000  | 1.694506000   |
| 8 | 1.540263000   | 0.534525000   | 1.341226000   |
| 8 | 0.703905000   | -1.449543000  | 0.887816000   |
| 6 | 1.055185000   | -0.880446000  | 3.206699000   |
| 9 | 2.248870000   | -0.625465000  | 3.775448000   |
| 9 | 0.141762000   | -0.098388000  | 3.812780000   |
| 9 | 0.745793000   | -2.156442000  | 3.462392000   |

INT-7

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| 6 | 0.901355000  | -2.334533000  | -1.884373000  |
| 6 | 1.998485000  | -2.323496000  | -0.983685000  |
| 6 | 2.958915000  | -1.284998000  | -1.119850000  |
| 6 | 2.837398000  | -0.310834000  | -2.132523000  |
| row | x   | y   | z   |
|-----|-----|-----|-----|
| 6   | 1.748205000 | -0.307889000 | -3.035976000 |
| 6   | 0.784227000  | -1.337896000 | -2.880041000 |
| 1   | 0.103422000  | -3.051423000 | -1.768717000 |
| 1   | 3.750172000  | -1.190984000 | -0.383240000 |
| 1   | 3.531166000  | 0.516606000  | -2.139205000 |
| 1   | -0.122382000 | -1.299444000 | -3.470770000 |
| 6   | 1.589073000  | 0.762952000  | -4.070532000 |
| 6   | 2.056596000  | 0.762952000  | -4.275654000 |
| 1   | 2.064501000  | 1.691233000  | -3.743736000 |
| 6   | 3.531166000  | 0.516606000  | -2.139205000 |
| 6   | 0.840983000  | -3.988312000 | 0.567257000  |
| 1   | 2.584675000  | -2.810438000 | 0.970326000  |
| 6   | 3.162389000  | -4.055890000 | -0.344812000 |
| 1   | 4.121833000  | -3.960063000 | -0.612005000 |
| 6   | 2.064501000  | -0.328570000 | -1.205534000 |
| 1   | 2.064501000  | 2.002607000  | 0.273572000  |
| 6   | 1.425022000  | -4.633555000 | -0.209892000 |
| 44  | 0.991792000  | -0.343200000 | -0.950601000 |
| 6   | 4.012573000  | 2.123721000  | -0.735668000 |
| 6   | -5.395917000 | 1.969335000  | -0.787326000 |
| 6   | -5.981312000 | 0.723078000  | -0.621626000 |
| 6   | -5.192190000 | -0.398576000 | -0.409327000 |
| 6   | -3.804335000 | -0.299844000 | -0.370570000 |
| 6   | -3.225093000 | 0.975160000  | -0.532556000 |
| 1   | -6.017028000 | 2.839726000  | -0.962629000 |
| 1   | -7.059831000 | 0.624070000  | -0.659868000 |
| 1   | -5.656056000 | -1.366790000 | -0.273801000 |
| 6   | -1.748363000 | 1.084456000  | -0.511023000 |
| 6   | 2.405305000  | 2.153124000  | 0.180843000  |
| 8   | 1.286975000  | 1.602721000  | -0.132977000 |
| 8   | 3.537425000  | 1.763220000  | -0.006861000 |
| 6   | 2.188018000  | 3.534620000  | 0.863936000  |
| 8   | -1.052325000 | 0.328570000  | -1.205534000 |
| 8   | -1.249120000 | 2.002607000  | 0.273572000  |
| 1   | -0.248750000 | 1.993418000  | -0.204198000 |
| 6   | -3.422302000 | 3.497235000  | -0.928936000 |
| 1   | -3.062945000 | 3.909845000  | 0.015118000  |
| 1   | -2.574820000 | 3.487845000  | -1.616054000 |
| 1   | -4.176038000 | 4.173699000  | -1.330276000 |
| 9   | 1.193010000  | 3.498052000  | 1.772382000  |
| 9   | 3.291636000  | 3.962579000  | 1.485015000  |
|   | 1.852304000  | 4.459500000  | -0.062754000  |
|---|-------------|-------------|--------------|
| 6 | -2.964216000 | -1.545625000 | -0.138430000 |
| 6 | -3.661525000 | -2.627097000 | 0.630795000  |
| 1 | -2.632235000 | -1.938607000 | -1.104078000 |
| 1 | -2.055252000 | -1.274375000 | 0.401350000  |
| 1 | -4.006442000 | -2.356121000 | 1.626114000  |
| 6 | -3.849903000 | -3.865319000 | 0.192459000  |
| 1 | -3.523592000 | -4.170811000 | -0.796306000 |
| 1 | -4.330963000 | -4.617777000 | 0.805342000  |
| 6 | 0.915717000  | -0.625773000 | 2.057122000  |
| 8 | 2.121661000  | -0.534814000 | 2.205693000  |
| 8 | 0.213467000  | -0.648127000 | 0.993066000  |
| 6 | 0.005348000  | -0.737575000 | 3.316450000  |
| 9 | 0.713962000  | -0.746693000 | 4.454333000  |
| 9 | -0.857241000 | 0.298374000  | 3.386162000  |
| 9 | -0.729562000 | -1.870641000 | 3.290086000  |

|   | 1.415048000  | -2.165330000 | -1.760275000 |
|---|-------------|-------------|--------------|
| 6 | 2.677444000  | -1.840985000 | -1.225759000 |
| 6 | 3.218320000  | -0.556720000 | -1.546187000 |
| 6 | 2.526193000  | 0.336552000  | -2.397367000 |
| 6 | 1.257198000  | -0.002272000 | -2.953262000 |
| 6 | 0.721769000  | -1.257584000 | -2.610668000 |
| 1 | 0.908638000  | -3.066388000 | -1.449321000 |
| 1 | 4.130697000  | -0.228297000 | -1.068133000 |
| 1 | 2.919357000  | 1.332951000  | -2.535614000 |
| 1 | -0.295697000 | -1.488950000 | -2.892744000 |
| 6 | 0.484639000  | 0.981644000  | -3.773176000 |
| 1 | -0.586224000 | 0.825044000  | -3.653974000 |
| 1 | 0.725016000  | 2.003762000  | -3.481884000 |
| 1 | 0.736415000  | 0.863346000  | -4.830369000 |
| 6 | 3.425484000  | -2.734152000 | -0.267328000 |
| 1 | 3.890280000  | -2.072095000 | 0.468888000  |
| 6 | 4.545279000  | -3.456007000 | -1.035177000 |
| 1 | 5.212383000  | -2.750261000 | -1.532883000 |
| 1 | 5.140311000  | -4.056439000 | -0.345417000 |
| 1 | 4.126858000  | -4.122428000 | -1.792913000 |
| 6 | 2.539144000  | -3.728960000 | 0.480312000  |
| 1 | 3.129574000  | -4.243504000 | 1.239164000  |
| 1 | 1.703172000  | -3.235840000 | 0.977372000  |
| 1 | 2.135829000  | -4.491379000 | -0.190113000 |
| 44 | 1.259778000 | -0.224008000 | -0.748391000 |
| 6 | -4.556904000 | 1.276423000  | -0.364246000 |
| 6 | -5.903779000 | 0.921227000  | -0.397757000 |
| 6 | -6.294558000 | -0.406828000 | -0.320157000 |
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | -5.340270000 | -1.408684000 | -0.222483000 |
| 6 | -3.980796000 | -1.105693000 | -0.207119000 |
| 6 | -3.597566000 | 0.249450000 | -0.268029000 |
| 1 | -6.651505000 | 1.700203000 | -0.489749000 |
| 1 | -7.347347000 | -0.663248000 | -0.174240000 |
| 1 | -5.649692000 | -2.443979000 | -0.163117000 |
| 6 | -2.147864000 | 0.583931000 | -0.280337000 |
| 6 | 1.685334000 | 2.697684000 | -0.056132000 |
| 8 | 0.795188000 | 1.780793000 | -0.174240000 |
| 6 | 1.062011000 | 4.033397000 | 0.443042000 |
| 8 | -1.339418000 | 0.004628000 | -0.992399000 |
| 8 | -1.792450000 | 1.558994000 | 0.546154000 |
| 1 | -0.831059000 | 1.749244000 | 0.392969000 |
| 6 | -4.192809000 | 2.736312000 | -0.469785000 |
| 1 | -3.862595000 | 3.134401000 | 0.490599000 |
| 1 | -3.381878000 | 2.907253000 | -1.179094000 |
| 1 | -5.057958000 | 3.311589000 | -0.798299000 |
| 9 | 0.301101000 | 3.846208000 | 1.540938000 |
| 9 | 1.995759000 | 4.940998000 | 0.745394000 |
| 9 | 0.266582000 | 4.564798000 | -0.511113000 |
| 6 | -2.966711000 | -2.235286000 | -0.126040000 |
| 6 | -3.465309000 | -3.459793000 | 0.581430000 |
| 1 | -2.650312000 | -2.501625000 | -1.139195000 |
| 1 | -2.068404000 | -1.884560000 | 0.381951000 |
| 1 | -3.776430000 | -3.318214000 | 1.614246000 |
| 6 | -3.524715000 | -4.673370000 | 0.047427000 |
| 1 | -3.230044000 | -4.853178000 | -0.981389000 |
| 1 | -3.864651000 | -5.529354000 | 0.617650000 |
| 6 | 0.993133000 | 0.629427000 | 1.902234000 |
| 8 | -0.067180000 | -1.058160000 | 1.319271000 |
| 8 | 1.954699000 | -0.170994000 | 1.320930000 |
| 6 | 0.990659000 | -0.620724000 | 3.446349000 |
| 9 | -0.103632000 | -1.161672000 | 3.995416000 |
| 9 | 2.058088000 | -1.315541000 | 3.886441000 |
| 9 | 1.104820000 | 0.638980000 | 3.909392000 |

|   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 1.720452000 | 0.845928000 | -0.033564000 |
| 6 | 1.377119000 | 2.196494000 | -0.041653000 |
| 6 | 0.047747000 | 2.593113000 | -0.046212000 |
| 6 | -0.963848000 | 1.643108000 | -0.051618000 |
| 6 | -0.664588000 | 0.282481000 | -0.060604000 |
| 6 | 0.685394000 | -0.102577000 | -0.047408000 |
| 1 | 2.164561000 | 2.941185000 | -0.046239000 |
| 1 | -0.201887000 | 3.647637000 | -0.047980000 |

P
| Cart. Pos | $x$  | $y$  | $z$  |
|----------|------|------|------|
| 1        | -1.999716000 | 1.956684000 | -0.052818000 |
| 6        | 1.022904000 | -1.558019000 | -0.106582000 |
| 8        | 0.713171000 | -2.295600000 | 0.843112000 |
| 8        | 1.712461000 | -1.979061000 | 0.965696000 |
| 1        | 1.924077000 | -2.932669000 | 0.843112000 |
| 6        | 3.173898000 | 0.446458000 | -0.033148000 |
| 1        | 3.474152000 | 0.045213000 | 0.936455000 |
| 1        | 3.383895000 | -0.324305000 | -0.777704000 |
| 1        | 3.803438000 | 1.307696000 | -0.033148000 |
| 6        | -1.782770000 | -0.745960000 | -0.089479000 |
| 6        | -3.063940000 | -0.283139000 | 0.538175000 |
| 1        | -1.968747000 | -1.046735000 | -1.124812000 |
| 1        | -1.451243000 | -1.650413000 | 0.428860000 |
| 1        | -3.004731000 | 0.001450000 | 1.586659000 |
| 6        | -4.230900000 | -0.213686000 | -0.089439000 |
| 6        | -4.326728000 | -0.480579000 | -1.136768000 |
| 1        | -4.218624000 | -0.003301000 | 1.178776000 |
| 1        | -0.931667000 | 2.730515000 | 1.779776000 |
| 1        | 0.442195000 | 0.886819000 | 2.658219000 |
| 1        | -0.726590000 | -2.697517000 | 2.840122000 |
| 1        | 0.724571000 | -1.701337000 | 2.626095000 |
| 1        | -0.185426000 | -1.626595000 | 4.138585000 |
| 6        | -3.498188000 | 2.674453000 | 0.857222000 |
| 1        | -2.805873000 | 3.313645000 | 0.300235000 |
| 6        | -4.037790000 | 3.496679000 | 2.039541000 |
| 1        | -3.233360000 | 3.833619000 | 2.695363000 |
| 1        | -4.568143000 | 4.377224000 | 1.673257000 |
| 1        | -4.734539000 | 2.901618000 | 2.634451000 |
| 6        | -4.630200000 | 2.268142000 | -0.085097000 |

**Table S2.** Cartesian coordinates of the stationary points involved in the formation of the ruthenium-(η³-allyl) complex and in the reaction pathway without the promotion of HOTFA, optimized at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.
|   |       |          |          |          |
|---|-------|----------|----------|----------|
| 1 | -5.084328000 | 3.159944000 | -0.518487000 |          |
| 1 | -4.274383000 | 1.639763000 | -0.902200000 |          |
| 1 | -5.418069000 | 1.726788000 | 0.443066000  |          |
| 44| -1.337968000 | 0.014860000 | 0.329183000  |          |
| 6 | -1.343510000 | -3.735156000 | -1.812129000 |          |
| 6 | -2.679907000 | -3.964862000 | -2.120866000 |          |
| 6 | -3.664124000 | -3.039534000 | -1.786238000 |          |
| 6 | -3.343817000 | -1.862513000 | -1.122587000 |          |
| 6 | -2.023387000 | -1.598047000 | -0.772302000 |          |
| 6 | -1.031869000 | -2.534479000 | -1.136536000 |          |
| 1 | -2.953747000 | -4.877232000 | -2.636726000 |          |
| 1 | -4.696855000 | -3.242334000 | -2.049195000 |          |
| 1 | -4.131295000 | -1.159266000 | -0.885633000 |          |
| 6 | 0.310757000  | -2.094718000 | -0.771671000 |          |
| 6 | 3.621427000  | -1.595553000 | 0.947847000  |          |
| 8 | 3.482342000  | -1.756715000 | -0.299290000 |          |
| 8 | 2.988028000  | -2.076658000 | 1.882549000  |          |
| 6 | 4.756874000  | -0.585969000 | 1.304660000  |          |
| 8 | 0.431513000  | -0.978703000 | -0.193116000 |          |
| 8 | 1.355650000  | -2.803976000 | -1.039945000 |          |
| 1 | 2.255051000  | -2.347414000 | -0.678798000 |          |
| 6 | -0.315551000 | -4.759858000 | -2.208243000 |          |
| 1 | 0.421807000  | -4.342623000 | -2.895369000 |          |
| 1 | 0.241078000  | -5.124744000 | -1.344285000 |          |
| 1 | -0.802516000 | -5.609555000 | -2.692657000 |          |
| 9 | 4.307243000  | 0.685835000  | 1.154191000  |          |
| 9 | 5.177707000  | -0.705080000 | 2.576386000  |          |
| 9 | 5.841631000  | -0.716650000 | 0.514675000  |          |
| 6 | -1.389854000 | 0.779686000  | -1.789419000 |          |
| 6 | -0.593416000 | 1.654926000  | -1.071859000 |          |
| 1 | -0.926397000 | 0.048964000  | -2.437707000 |          |
| 1 | -2.414543000 | 1.029923000  | -2.024701000 |          |
| 1 | -1.049424000 | 2.567009000  | -0.708331000 |          |
| 6 | 0.909502000  | 1.709424000  | -1.192041000 |          |
| 1 | 1.257917000  | 0.802096000  | -1.679602000 |          |
| 1 | 1.383817000  | 1.733090000  | -0.200985000 |          |
| 7 | 1.287535000  | 2.872158000  | -2.002259000 |          |
| 6 | 1.395337000  | 4.081662000  | -1.184777000 |          |
| 1 | 2.237385000  | 4.016304000  | -0.475869000 |          |
| 1 | 0.492913000  | 4.139228000  | -0.571722000 |          |
| 6 | 2.445034000  | 2.607726000  | -2.863620000 |          |
| 1 | 2.553693000  | 3.448570000  | -3.551036000 |          |
| 1 | 2.189491000  | 1.742846000  | -3.480669000 |          |
| 6 | 1.508898000  | 5.362218000  | -2.000401000 |          |
| 1  | 2.451945000 | 5.421161000 | 2.545831000 |
| 1  | 1.459282000 | 6.229385000 | 1.339020000 |
| 1  | 0.692876000 | 5.432228000 | 2.722436000 |
| 1  | 3.779160000 | 2.349632000 | 2.155828000 |
| 1  | 4.553882000 | 2.133753000 | 2.895008000 |
| 1  | 3.718790000 | 1.496871000 | 1.477391000 |
| 1  | 4.107805000 | 3.215925000 | 1.578747000 |
| 6  | 3.027771000 | -1.250657000 | -1.393553000 |
| 6  | 2.855286000 | 0.032084000 | -1.966036000 |
| 6  | 1.605636000 | 0.300988000 | 2.597491000 |
| 6  | 0.584958000 | -0.660819000 | -2.595866000 |
| 6  | 0.800254000 | -1.986099000 | 2.080984000 |
| 6  | 2.042240000 | -2.273294000 | -1.517583000 |
| 1  | 3.942031000 | -1.479830000 | -0.865407000 |
| 1  | 1.409544000 | 1.285929000 | -3.000487000 |
| 1  | -0.391043000 | -0.398700000 | 2.981121000 |
| 1  | 2.219950000 | -3.239388000 | 1.063356000 |
| 6  | -0.316402000 | -2.983548000 | 2.105734000 |
| 1  | -0.098127000 | -3.831571000 | 1.457497000 |
| 1  | -1.251799000 | -2.526501000 | -1.779147000 |
| 1  | -0.465106000 | -3.357535000 | -3.122557000 |
| 6  | 3.936789000 | 1.088216000 | -1.969589000 |
| 1  | 3.427061000 | 2.056622000 | 1.951607000 |
| 6  | 4.728907000 | 0.999936000 | -3.283378000 |
| 1  | 4.072478000 | 1.085987000 | 4.151023000 |
| 1  | 5.468426000 | 1.801159000 | -3.335550000 |
| 1  | 5.256266000 | 0.045309000 | -3.351191000 |
| 6  | 4.871826000 | 1.028241000 | -0.762970000 |
| 1  | 5.560454000 | 1.874014000 | -0.786154000 |
| 6  | 4.319837000 | 1.070181000 | 0.177643000 |
| 1  | 5.475502000 | 0.118213000 | -0.762518000 |
| 44  | 1.216348000 | -0.355604000 | -0.501232000 |
| 6  | 0.389610000 | -2.912908000 | 2.719391000 |
| 6  | 1.639662000 | -3.406056000 | 3.100852000 |
| 6  | 2.814701000 | -2.758824000 | 2.736369000 |
| 6  | 2.770319000 | -1.596999000 | 1.983531000 |
| 6  | 1.544522000 | -1.089666000 | 1.551165000 |
| 6  | 0.354664000 | -1.749533000 | 1.936647000 |
| 1  | 1.688796000 | -4.311734000 | 3.693599000 |
| 1  | 3.770855000 | -3.160761000 | 3.051097000 |
| 1  | 3.688194000 | -1.077659000 | 1.737361000 |
| 6  | -0.887554000 | -1.180412000 | 1.359432000 |
| 6  | -4.183692000 | -0.883419000 | -0.480645000 |
| 8  | -3.908234000 | -0.356100000 | 0.666862000 |
|    |     |        |        |        |
|----|-----|--------|--------|--------|
| 8  | -3.695108000 | -1.856222000 | -1.009473000 |
| 6  | -5.301490000 | -0.080502000 | -1.202223000 |
| 8  | -0.742650000 | -0.480030000 | 0.302655000  |
| 8  | -2.014872000 | -1.363246000 | 1.889278000  |
| 1  | -3.064645000 | -0.818653000 | 1.158626000  |
| 6  | -0.847179000 | -3.667371000 | 3.129353000  |
| 1  | -1.461499000 | -3.079206000 | 3.811781000  |
| 1  | -1.479013000 | -3.900915000 | 2.271948000  |
| 9  | -0.742650000 | -0.480030000 | 0.302655000  |
| 8  | -2.014872000 | -1.363246000 | 1.889278000  |
| 1  | -3.064645000 | -0.818653000 | 1.158626000  |
| 6  | -0.847179000 | -3.667371000 | 3.129353000  |
| 1  | -1.461499000 | -3.079206000 | 3.811781000  |
| 1  | -1.479013000 | -3.900915000 | 2.271948000  |
| 9  | -6.400435000 | 0.035213000  | -0.432309000 |
| 6  | 1.551019000  | 0.770001000  | 1.554810000  |
| 6  | 1.235046000  | 1.564029000  | 0.377491000  |
| 1  | 0.810078000  | 0.843497000  | 2.343264000  |
| 1  | 2.558109000  | 0.887060000  | 1.933151000  |
| 1  | 2.087702000  | 2.093649000  | -0.032775000 |
| 6  | -0.037094000 | 2.381251000  | 0.358203000  |
| 1  | -0.892059000 | 1.734163000  | 0.537740000  |
| 1  | -0.160056000 | 2.798932000  | -0.654237000 |
| 7  | -0.056876000 | 3.426835000  | 1.390329000  |
| 6  | 0.880232000  | 4.509344000  | 1.094692000  |
| 1  | 0.602091000  | 5.049813000  | 0.173383000  |
| 1  | 1.848534000  | 4.048172000  | 0.892633000  |
| 6  | -1.419953000 | 3.869849000  | 1.698851000  |
| 1  | -1.379887000 | 4.500765000  | 2.588856000  |
| 1  | -1.985114000 | 2.978268000  | 1.982282000  |
| 6  | 1.049139000  | 5.503658000  | 2.236255000  |
| 1  | 0.149629000  | 6.097263000  | 2.406520000  |
| 1  | 1.859944000  | 6.197957000  | 2.006729000  |
| 1  | 1.294630000  | 4.984366000  | 3.165067000  |
| 6  | -2.175881000 | 4.610228000  | 0.589054000  |
| 1  | -3.179318000 | 4.869395000  | 0.934144000  |
| 1  | -2.281445000 | 3.995110000  | -0.306439000 |
| 1  | -1.675625000 | 5.537815000  | 0.304080000  |

**INT-4-NA**

|    |     |        |        |        |
|----|-----|--------|--------|--------|
| 6  | 2.451865000 | -2.072659000 | -1.153776000 |
| 6  | 2.902831000 | -0.801480000 | -1.585981000 |
| 6  | 1.971577000 | -0.011953000 | -2.316130000 |
| 6  | 0.670365000 | -0.486345000 | -2.576939000 |
| 6  | 0.286950000 | -1.836873000 | -2.261761000 |
| 6  | 1.203306000 | -2.625637000 | -1.573945000 |
| 1  | 3.083073000 | -2.669898000 | -0.510512000 |
| 1  | 2.234216000 | 0.999352000  | -2.597091000  |
| 1  | -0.047406000 | 0.169288000  | -3.051529000  |
|    |   x     |    y     |    z     |
|----|---------|---------|---------|
| 1  | 0.930824| -3.62278| -1.25464|
| 6  | -1.08990| -2.31536| -2.60360|
| 1  | -1.28581| -3.29764| -2.17453|
| 1  | -1.84298| -1.61985| -2.22839|
| 1  | -1.20982| -2.38272| -3.68768|
| 6  | 4.29244| -0.26748| -1.32817|
| 1  | 4.18944| 0.81256| -1.18078|
| 6  | 5.15949| -0.48889| -2.57769|
| 1  | 4.71009| -0.03431| -3.46236|
| 1  | 6.14914| -0.05048| -2.43558|
| 1  | 5.28576| -1.55687| -2.77344|
| 6  | 4.96448| -0.84812| -0.08641|
| 1  | 5.91688| -0.34479| 0.08694|
| 1  | 4.34408| -0.72091| 0.79966|
| 1  | 5.17668| -1.91336| -0.20370|
| 44 | 1.00768| -0.58793| -0.43315|
| 6  | 0.38737| -2.73694| 1.95338|
| 6  | 1.56335| -3.23189| 2.48194|
| 6  | 2.59778| -2.37314| 2.87382|
| 6  | 2.47649| -1.01153| 2.70719|
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**TS-allyl**

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| 1 | -2.612000000 | -5.614039000 | 1.857036000   |
| 1 | -0.697687000 | -4.275879000 | 1.119519000   |
| 6 | -3.210020000 | -0.516330000 | 0.483190000   |
| 6 | -3.677606000 | 3.013814000  | -1.101932000  |
| 8 | -3.416715000 | 4.542470000  | -1.179737000  |
| 8 | -2.070784000 | 0.005289000  | 0.150680000   |
| 8 | -4.237563000 | 0.184461000  | 0.528627000   |
| 1 | -4.027580000 | 1.621183000  | 0.226030000   |
| 6 | -5.662752000 | -2.148498000 | 1.343951000   |
| 1 | -5.712467000 | -1.319573000 | 2.050989000   |
| 1 | -5.997223000 | -1.752136000 | 0.384350000   |
| 1 | -6.355052000 | -2.926538000 | 1.664816000   |
| 9 | -2.289699000 | 4.862044000  | -0.512668000  |
| 9 | -3.272812000 | 4.946451000  | -2.445160000  |
| 9 | -4.427894000 | 5.241685000  | -0.633587000  |
| 6 | -0.182468000 | -1.217897000 | 2.125227000   |
| 6 | 0.833505000  | -0.466184000 | 1.532058000   |
| 1 | -1.088685000 | -0.728760000 | 2.452209000   |
| 1 | 0.061527000  | -2.149104000 | 2.614019000   |
| 1 | 1.849160000  | -0.836477000 | 1.478355000   |
| 6 | 0.492873000  | 0.680304000  | 0.801595000   |
| 1 | -0.411853000 | 1.227390000  | 1.013877000   |
| 1 | 1.243618000  | 1.160178000  | 0.199383000   |
| 7 | 2.264582000  | 2.274524000  | 2.266253000   |
| 6 | 2.445635000  | 3.703038000  | 2.019106000   |
| 1 | 1.683915000  | 4.253425000  | 2.576416000   |
| 1 | 2.232835000  | 3.877178000  | 0.960614000   |
| 6 | 2.312206000  | 1.834191000  | 3.657819000   |
| 1 | 3.200283000  | 2.207175000  | 4.188835000   |
| 1 | 2.405106000  | 0.745319000  | 3.645027000   |
| 6 | 3.833421000  | 4.260601000  | 2.349812000   |
| 1 | 4.067753000  | 4.163229000  | 3.411399000   |
| 1 | 3.889551000  | 5.321634000  | 2.094307000   |
| 1 | 4.606044000  | 3.734220000  | 1.784110000   |
| 6 | 1.060522000  | 2.221867000  | 4.436939000   |
| 1 | 1.107824000  | 1.827942000  | 5.454358000   |
| 1 | 0.166804000  | 1.823980000  | 3.952095000   |
| 1 | 0.948789000  | 3.305305000  | 4.509668000   |
| 1 | 2.922666000  | 1.738453000  | 1.705882000   |
|   |       |        |        |
|---|-------|--------|--------|
| 6 | 4.836578000 | 0.487801000 | 0.108707000 |
| 8 | 5.737630000 | 0.506873000 | 0.952249000 |
| 8 | 3.598945000 | 0.343327000 | 0.242222000 |
| 6 | 5.268851000 | 0.699541000 | -1.381739000 |
| 9 | 4.756290000 | -0.258203000 | -2.196491000 |
| 9 | 4.813475000 | 1.888623000 | -1.849790000 |
| 9 | 6.601113000 | 0.691310000 | -1.568337000 |

**INT-allyl**

|   |       |        |        |
|---|-------|--------|--------|
| 6 | -0.757721000 | -2.581354000 | 1.538351000 |
| 6 | -1.824464000 | -1.698822000 | 1.301532000 |
| 6 | -1.586753000 | -0.317258000 | 1.539483000 |
| 6 | -0.341792000 | 0.152732000 | 1.994502000 |
| 6 | 0.707761000 | -0.751293000 | 2.313015000 |
| 6 | 0.477049000 | -2.115195000 | 2.062812000 |
| 1 | -0.869060000 | -3.636939000 | 1.339535000 |
| 1 | -2.357937000 | 0.402012000 | 1.272220000 |
| 1 | -0.179587000 | 1.217346000 | 2.102660000 |
| 1 | 1.276265000 | -2.825439000 | 2.293820000 |
| 6 | 2.020361000 | -0.258912000 | 2.822346000 |
| 1 | 2.800080000 | -1.006507000 | 2.683902000 |
| 1 | 2.312654000 | 0.665360000 | 2.325022000 |
| 1 | 1.932729000 | -0.054570000 | 3.893439000 |
| 6 | -3.189110000 | -2.150566000 | 0.848134000 |
| 1 | -3.580743000 | -1.363687000 | 0.199207000 |
| 6 | -4.105306000 | -2.235944000 | 2.082417000 |
| 1 | -4.151169000 | -1.283530000 | 2.613108000 |
| 1 | -5.116961000 | -2.496518000 | 1.768474000 |
| 1 | -3.755274000 | -3.001054000 | 2.779459000 |
| 6 | -3.183699000 | -3.464643000 | 0.070182000 |
| 1 | -4.186043000 | -3.664390000 | -0.309271000 |
| 1 | -2.506270000 | -3.429384000 | -0.785606000 |
| 1 | -2.898765000 | -4.312879000 | 0.696965000 |
| 44 | 0.085567000 | -1.011940000 | 0.076492000 |
| 6 | 3.858010000 | -2.858951000 | -1.004736000 |
| 6 | 3.582854000 | -4.220953000 | -1.097025000 |
| 6 | 2.291927000 | -4.708907000 | -0.940034000 |
| 6 | 1.232739000 | -3.849611000 | -0.668224000 |
| 6 | 1.486309000 | -2.494290000 | -0.543388000 |
| 6 | 2.778741000 | -1.994174000 | -0.730106000 |
| 1 | 4.392657000 | -4.909186000 | -1.306958000 |
| 1 | 2.103233000 | -5.772330000 | -1.033082000 |
| 1 | 0.235122000 | -4.254978000 | -0.566705000 |
| 6 | 2.875738000 | -0.526556000 | -0.664902000 |
| 6 | 3.356170000 | 3.181338000 | 0.328530000 |
| 8 | 3.698375000 | 2.638870000 | -0.803980000 |
Table S3. Cartesian coordinates of the stationary points involved in the β-H elimination processes, optimized at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.

| Names       | Cartesian Coordinates |
|-------------|-----------------------|
| TS-BHE-1    |                       |
| 6           | 0.172472000 1.645123000 2.472197000 |
| 6           | 1.586324000 1.599630000 2.476979000 |
| 6           | 2.200298000 0.375193000 2.874292000 |
| 6           | 1.437772000 -0.737567000 3.232983000 |
| 6           | 0.006367000 -0.665051000 3.255723000 |
| 6           | -0.611037000 0.542466000 2.909567000 |
| 1           | -0.338161000 2.531631000 2.129503000 |
| 1           | 3.278726000 0.286070000 2.839044000 |
| 1           | 1.920791000 -1.677543000 3.452786000 |
| 1           | -1.690086000 0.611611000 2.886200000 |
| 6           | -0.800442000 -1.866507000 3.638395000 |
|   | x         | y         | z         |
|---|-----------|-----------|-----------|
| 1 | -1.798216000 | -1.822865000 | 3.203782000 |
| 1 | -0.307619000  | -2.781146000  | 3.315253000  |
| 1 | -0.903511000  | -1.905718000  | 4.726542000  |
| 6 | 2.454573000  | 2.801159000  | 2.159941000  |
| 1 | 3.182774000  | 2.489988000  | 1.405261000  |
| 6 | 3.238549000  | 3.207872000  | 3.419609000  |
| 1 | 3.854863000  | 2.392557000  | 3.800515000  |
| 1 | 3.895703000  | 4.049387000  | 3.194093000  |
| 1 | 2.554211000  | 3.515535000  | 4.213828000  |
| 1 | 1.683932000  | 3.999915000  | 1.612016000  |
| 1 | 2.384736000  | 4.785950000  | 1.329121000  |
| 1 | 1.096545000  | 3.748125000  | 0.732068000  |
| 1 | 1.013379000  | 4.413796000  | 2.369121000  |
| 44 | 0.742971000  | -0.051205000 | 1.164585000  |
| 6  | -0.482251000 | 4.080871000  | -1.729688000 |
| 6  | 0.681156000  | 4.729503000  | -2.142724000 |
| 6  | 1.899004000  | 4.069272000  | -2.151634000 |
| 6  | 1.969988000  | 2.743431000  | -1.751386000 |
| 6  | 0.828267000  | 2.053701000  | -1.342050000 |
| 6  | -0.400078000 | 2.737117000  | -1.338023000 |
| 1  | 0.624416000  | 5.764212000  | -2.459907000 |
| 1  | 2.796170000  | 4.584564000  | -2.472525000 |
| 1  | 2.925820000  | 2.238525000  | -1.767030000 |
| 6  | -1.657833000 | 2.060054000  | -0.869300000 |
| 6  | -5.165695000 | 0.190609000  | -1.073834000 |
| 8  | -4.024105000 | -0.271744000 | -0.801612000 |
| 8  | -5.486905000 | 1.190651000  | -1.713323000 |
| 6  | -6.316461000 | -0.685458000 | -0.481296000 |
| 8  | -2.280781000 | 2.455733000  | 0.099978000  |
| 8  | -2.003646000 | 1.028159000  | -1.613256000 |
| 1  | -2.863306000 | 0.560976000  | -1.256196000 |
| 6  | -1.788625000 | 4.831176000  | -1.719797000 |
| 1  | -2.592325000 | 4.252599000  | -2.178925000 |
| 1  | -2.102706000 | 5.053994000  | -0.698754000 |
| 1  | -1.691154000 | 5.770816000  | -2.262628000 |
| 9  | -6.224234000 | -0.772085000 | 0.866450000  |
| 9  | -7.542504000 | -0.207145000 | -0.759745000 |
| 9  | -6.269049000 | -1.950457000 | -0.961375000 |
| 6  | 0.949983000  | 0.606652000  | -0.970285000 |
| 6  | 2.170008000  | 0.069019000  | -0.445332000 |
| 1  | -0.301070000 | 0.448684000  | 0.060676000  |
| 1  | 0.397034000  | -0.059815000 | -1.627534000 |
| 1  | 2.937210000  | 0.772805000  | -0.145483000 |
| 6  | 2.675667000  | -1.254294000 | -0.925127000 |
|     | 1.850904000 | -1.888390000 | -1.227833000 |
|-----|-------------|--------------|--------------|
| 1   | 3.268441000 | -1.767650000 | -0.172363000 |
| 7   | 3.570784000 | -1.141863000 | -2.162847000 |
| 6   | 4.926390000 | -0.583467000 | -1.808291000 |
| 1   | 5.382333000 | -1.287115000 | -1.114116000 |
| 1   | 4.734874000 | 0.340197000  | -1.265544000 |
| 6   | 3.620167000 | -2.449115000 | -2.928855000 |
| 1   | 4.161335000 | -2.250224000 | -3.851688000 |
| 1   | 2.585227000 | -2.668610000 | -3.191314000 |
| 6   | 5.806781000 | -0.320976000 | -3.014408000 |
| 1   | 6.123339000 | -1.237986000 | -3.510262000 |
| 1   | 6.703896000 | 0.199430000  | -2.678098000 |
| 1   | 5.305234000 | 0.319083000  | -3.743645000 |
| 6   | 4.241943000 | -3.594726000 | -2.156148000 |
| 1   | 4.211167000 | -4.480778000 | -2.790906000 |
| 1   | 3.693060000 | -3.824309000 | -1.243599000 |
| 1   | 5.286295000 | -3.409525000 | -1.904451000 |
| 1   | 3.116618000 | -0.464388000 | -2.791589000 |
| 6   | 0.529420000 | -3.049404000 | 0.628099000  |
| 8   | 0.106225000 | -1.897686000 | 0.295262000  |
| 8   | 1.365508000 | -3.841200000 | 1.454273000  |
| 6   | -0.110702000 | -4.162198000 | -0.253696000 |
| 9   | 0.039885000 | -5.383194000 | 0.278340000  |
| 9   | -1.422628000 | -3.972855000 | -0.470553000 |
| 9   | 0.499733000 | -4.177276000 | -1.469035000 |
|     |             |             |              |
| 6   | 0.936723000 | 1.617642000 | 2.659790000  |
| 6   | 2.274190000 | 1.451705000 | 2.243487000  |
| 6   | 2.856401000 | 0.160977000 | 2.414578000  |
| 6   | 2.138934000 | -0.904338000 | 2.959889000  |
| 6   | 0.798874000 | -0.712667000 | 3.420075000  |
| 6   | 0.223413000 | 0.556403000 | 3.283739000  |
| 1   | 0.440681000 | 2.565785000 | 2.524534000  |
| 1   | 3.864664000 | -0.012431000 | 2.058226000  |
| 1   | 2.583304000 | -1.886683000 | 3.020390000  |
| 1   | -0.800783000 | 0.714747000 | 3.593883000  |
| 6   | 0.039958000 | -1.840007000 | 4.046181000  |
| 1   | -1.034024000 | -1.703366000 | 3.925634000  |
| 1   | 0.332903000 | -2.792476000 | 3.611440000  |
| 1   | 0.258719000 | -1.871204000 | 5.117426000  |
| 6   | 3.118834000 | 2.593232000 | 1.717633000  |
| 1   | 3.571042000 | 2.256676000 | 0.779058000  |
| 6   | 4.259493000 | 2.880319000 | 2.709310000  |
| 1   | 4.884179000 | 2.002848000 | 2.881838000  |
| 1   | 4.897294000 | 3.676271000 | 2.321554000  |
|   |          |          |          |
|---|----------|----------|----------|
| 1 | 3.857930000 | 3.205966000 | 3.671726000 |
| 6 | 2.328284000 | 3.868972000 | 1.438402000 |
| 1 | 2.978989000 | 4.606364000 | 0.968495000 |
| 1 | 1.488166000 | 3.695195000 | 0.769033000 |
| 1 | 1.950134000 | 4.306780000 | 2.365868000 |
| 44 | 0.889944000 | -0.053453000 | 1.185819000 |
| 6 | -0.146027000 | 4.141063000 | -2.168919000 |
| 6 | 1.060105000 | 4.665130000 | -2.102192000 |
| 6 | 2.197125000 | 3.879775000 | -2.168919000 |
| 6 | 2.146743000 | 2.550815000 | -1.778613000 |
| 6 | 0.958493000 | 1.981971000 | -1.312872000 |
| 6 | -0.189502000 | 2.794104000 | -1.253164000 |
| 1 | 1.098743000 | 5.702787000 | -2.416895000 |
| 1 | 3.129074000 | 4.298389000 | -2.534555000 |
| 1 | 3.035220000 | 1.943966000 | -1.856738000 |
| 6 | -1.488280000 | 2.248253000 | -0.731727000 |
| 6 | -5.192256000 | 0.666810000 | -0.858458000 |
| 8 | -4.080979000 | 0.152775000 | -0.559078000 |
| 8 | -5.453988000 | 1.665459000 | -1.527621000 |
| 6 | -6.395428000 | -0.133666000 | -0.262389000 |
| 8 | -2.028662000 | 2.701845000 | -0.261788000 |
| 8 | -1.976158000 | 1.264684000 | -1.462015000 |
| 1 | -2.855019000 | 0.886519000 | -1.063495000 |
| 6 | -1.364913000 | 5.024636000 | -1.574497000 |
| 1 | -2.240535000 | 4.540005000 | -2.010624000 |
| 1 | -1.618983000 | 5.265199000 | -0.540980000 |
| 1 | -1.187929000 | 5.956176000 | -2.111290000 |
| 9 | -6.320164000 | -0.205627000 | 1.087192000 |
| 9 | -7.590908000 | 0.407699000 | -0.558839000 |
| 9 | -6.414996000 | -1.406688000 | -0.723840000 |
| 6 | 0.920244000 | 0.540127000 | -0.958654000 |
| 6 | 2.072848000 | -0.209171000 | -0.640168000 |
| 1 | -0.474235000 | 0.570075000 | 0.745081000 |
| 1 | 0.098132000 | -0.009658000 | -1.400675000 |
| 1 | 3.000339000 | 0.322358000 | -0.464029000 |
| 6 | 2.234154000 | -1.607870000 | -1.146725000 |
| 1 | 1.265798000 | -2.073971000 | -1.281380000 |
| 1 | 2.848528000 | -2.225000000 | -0.496718000 |
| 7 | 2.887866000 | -1.643802000 | -2.528415000 |
| 6 | 4.366905000 | -1.357393000 | -2.445146000 |
| 1 | 4.804109000 | -2.146506000 | -1.836031000 |
| 1 | 4.458620000 | -0.423253000 | -1.894183000 |
| 6 | 2.543754000 | -2.923045000 | -3.265169000 |
| 1 | 2.936535000 | -2.817980000 | -4.274376000 |
|   |        |                |                |                |
|---|--------|----------------|----------------|----------------|
| 1 | 1.456085000 | -2.931943000  | -3.331322000  |
| 6 | 5.038764000 | -1.244358000  | -3.799586000  |
| 1 | 5.079920000 | -2.195843000  | -4.328757000  |
| 1 | 6.064467000 | -0.907839000  | -3.646550000  |
| 1 | 4.538948000 | -0.508735000  | -4.433581000  |
| 6 | 3.062180000 | -4.179026000  | -2.594161000  |
| 1 | 2.745997000 | -5.032862000  | -3.194128000  |
| 1 | 2.654267000 | -4.311219000  | -1.592627000  |
| 1 | 4.150671000 | -4.203430000  | -2.539613000  |
| 1 | 2.458483000 | -0.880707000  | -3.070857000  |
| 6 | 0.113694000 | -2.961835000  | 0.743777000   |
| 8 | -0.197449000 | -1.752929000  | 0.501844000   |
| 8 | 1.073408000 | -3.435429000  | 1.334533000   |
| 6 | -0.886922000 | -3.952031000  | 0.077925000   |
| 9 | -0.860641000 | -5.162228000  | 0.654993000   |
| 9 | -2.157127000 | -3.519774000  | 0.099021000   |
| 9 | -0.540429000 | -4.122393000  | -1.225930000  |

TS-BHE-2

|   |        |                |                |                |
|---|--------|----------------|----------------|----------------|
| 6 | 0.897813000 | 3.073069000   | -0.870343000  |
| 6 | -0.184203000 | 2.819822000  | -1.756807000  |
| 6 | 0.021406000 | 1.889776000   | -2.802246000  |
| 6 | 1.256760000 | 1.215743000   | -2.960171000  |
| 6 | 2.314828000 | 1.422527000   | -2.060317000  |
| 6 | 2.092805000 | 2.359746000   | -1.008151000  |
| 1 | 0.785573000 | 3.755807000   | -0.042000000  |
| 1 | -0.776971000 | 1.703748000   | -3.507670000  |
| 1 | 1.365962000 | 0.489654000   | -3.755592000  |
| 1 | 2.870100000 | 2.499546000   | -0.270164000  |
| 6 | 3.618119000 | 0.694915000   | -2.173836000  |
| 1 | 3.967668000 | 0.359602000   | -1.197401000  |
| 1 | 3.519573000 | -0.176301000  | -2.820260000  |
| 1 | 4.383207000 | 1.350391000   | -2.598901000  |
| 6 | -1.481273000 | 3.596306000  | -1.700697000  |
| 1 | -2.282449000 | 2.902790000  | -1.974415000  |
| 6 | -1.442721000 | 4.703602000  | -2.768624000  |
| 1 | -1.279762000 | 4.294944000  | -3.766814000  |
| 1 | -2.387177000 | 5.250053000  | -2.773314000  |
| 1 | -0.640269000 | 5.413801000  | -2.556094000  |
| 6 | -1.803363000 | 4.183572000  | -0.328214000  |
| 1 | -2.800780000 | 4.624486000  | -0.343755000  |
| 1 | -1.776042000 | 3.429297000  | 0.455749000   |
| 1 | -1.101528000 | 4.974615000  | -0.056034000  |
| 44 | 0.452997000 | 0.793699000   | -0.869017000  |
| 6 | 2.240164000 | 2.481162000  | 2.663390000   |
| 6 | 1.708803000 | 3.685640000  | 3.125731000   |
|   |       |       |       |
|---|-------|-------|-------|
|   |       |       |       |
| 1 | -1.180306000 | -2.346129000 | -3.572341000 |
| 1 | -3.032027000 | -1.245210000 | -0.446181000 |
| 6 | -4.992479000 | -2.114539000 | 0.471809000  |
| 8 | -5.061984000 | -3.007480000 | -0.369981000 |
| 8 | -4.138277000 | -1.192146000 | 0.602055000  |
| 6 | -6.103995000 | -2.058013000 | 1.566155000  |
| 9 | -6.785416000 | -3.043600000 | 1.506715000  |
| 9 | -7.006058000 | -3.047140000 | 1.451072000  |
| 9 | -5.574935000 | -2.145163000 | 2.807610000  |

**INT-BHE-2**

|   |       |       |       |
|---|-------|-------|-------|
| 6 | -1.980017000 | 1.904271000 | 1.547809000 |
| 6 | -0.774567000 | 2.172630000 | 2.198226000 |
| 6 | -0.157998000 | 1.079820000 | 2.871970000 |
| 6 | -0.828322000 | -0.145855000 | 3.067899000 |
| 6 | -2.139210000 | -0.347925000 | 2.547064000 |
| 6 | -2.646607000 | 0.651055000 | 1.711092000 |
| 1  | -2.444610000 | 2.653943000 | 0.926320000 |
| 1  | 0.811500000 | 1.223395000 | 3.327087000 |
| 1  | -0.362368000 | -0.921686000 | 3.660563000 |
| 1  | -3.569465000 | 0.472454000 | 1.177317000 |
| 6  | -2.908080000 | -1.602722000 | 2.821177000 |
| 1  | -3.601890000 | -1.815436000 | 2.010830000 |
| 1  | -2.243125000 | -2.452410000 | 2.960573000 |
| 1  | -3.485808000 | -1.475712000 | 3.741011000 |
| 6  | -0.092628000 | 3.521168000 | 2.206288000 |
| 1  | 0.939533000 | 3.358172000 | 1.875486000 |
| 6  | -0.041841000 | 4.051178000 | 3.651224000 |
| 1  | 0.472813000 | 3.364300000 | 4.324186000 |
| 1  | 0.486730000 | 5.005216000 | 3.674647000 |
| 1  | -1.051506000 | 4.212050000 | 4.035927000 |
| 6  | -0.741782000 | 4.546315000 | 1.284058000 |
| 1  | -0.152600000 | 5.464077000 | 1.281855000 |
| 1  | -0.804608000 | 4.191162000 | 0.258736000 |
| 1  | -1.747936000 | 4.802326000 | 1.625514000 |
| 44 | -0.579461000 | 0.117920000 | 0.870645000 |
| 6  | -2.231735000 | 3.093727000 | -2.192785000 |
| 6  | -1.731971000 | 4.384937000 | -2.356205000 |
| 6  | -0.368469000 | 4.639256000 | -2.316822000 |
| 6  | 0.520548000 | 3.603701000 | -2.069761000 |
| 6  | 0.058980000 | 2.305196000 | -1.872234000 |
| 6  | -1.320497000 | 2.048438000 | -1.955522000 |
| 1  | -2.426472000 | 5.199870000 | -2.524040000 |
| 1  | -0.000658000 | 5.647766000 | -2.463579000 |
| 1  | 1.586100000 | 3.798528000 | -2.033532000 |
| 6  | -1.794052000 | 0.627809000 | -1.912869000 |
|   |                  |                  |                  |
|---|------------------|------------------|------------------|
| 6 | -4.197773000     | -2.073999000     | -1.199387000     |
| 8 | -3.580730000     | -1.984216000     | -2.334327000     |
| 8 | -4.448800000     | -1.205266000     | -0.394709000     |
| 6 | -4.627362000     | -3.541294000     | -0.923213000     |
| 8 | -1.341886000     | -0.200272000     | -1.060065000     |
| 8 | -2.613990000     | 0.256236000      | -2.791711000     |
| 1 | -3.167281000     | -1.007000000     | -2.504814000     |
| 6 | -3.720889000     | 2.876474000      | -2.267359000     |
| 1 | -0.798424000     | 0.327710000      | -2.232379000     |
| 1 | 2.037506000      | 1.532296000      | -1.960063000     |
| 1 | 1.745922000      | 1.461552000      | 0.444933000      |
| 6 | 1.296705000      | -0.621658000     | 0.088783000      |
| 1 | 1.110793000      | -1.277875000     | -0.751714000     |
| 1 | -0.610056000     | -1.436369000     | 0.770035000      |
| 7 | 2.400055000      | -1.215221000     | 0.888520000      |
| 6 | 2.676335000      | -0.568709000     | 2.205652000      |
| 1 | 1.849845000      | -0.797542000     | 2.871177000      |
| 1 | 2.681420000      | 0.503741000      | 2.026401000      |
| 6 | 2.336239000      | -2.720617000     | 0.948825000      |
| 1 | 3.359190000      | -3.051354000     | 1.115616000      |
| 1 | 2.061194000      | -3.040334000     | -0.055619000     |
| 6 | 4.001888000      | -0.998717000     | 2.809234000      |
| 1 | 4.006100000      | -2.050414000     | 3.093853000      |
| 1 | 4.174939000      | -0.410080000     | 3.710880000      |
| 1 | 4.828729000      | -0.825980000     | 2.122068000      |
| 6 | 1.384647000      | -3.298146000     | 1.978682000      |
| 1 | 1.402248000      | -4.384798000     | 1.884195000      |
| 1 | 0.360690000      | -2.964890000     | 1.821792000      |
| 1 | 1.680796000      | -3.056779000     | 2.999971000      |
| 1 | 3.267767000      | -1.002823000     | 0.274039000      |
| 6 | 5.394106000      | -1.386325000     | -0.683856000     |
| 8 | 5.546736000      | -2.447047000     | -0.080640000     |
| 8 | 4.428049000      | -0.574060000     | -0.662172000     |
| 6 | 6.544244000      | -0.921289000     | -1.632009000     |
| 9 | 7.037657000      | 0.279036000      | -1.247664000     |
| 9 | 7.578586000      | -1.778812000     | -1.666681000     |
|   | x        | y        | z        |
|---|----------|----------|----------|
| 9 | 6.104466000 | -0.779147000 | -2.903410000 |
| 6 | 2.128396000 | -1.568732000 | 0.582819000  |
| 6 | 1.768544000 | -1.914073000 | -0.753280000 |
| 6 | 0.555011000 | -2.598480000 | -0.919550000 |
| 6 | -0.258283000 | -2.895095000 | 0.212358000  |
| 6 | 1.768544000 | -1.914073000 | -0.753280000 |
| 9 | 1.374897000 | -1.971359000 | 1.721283000  |
| 1 | 1.736539000 | -1.732794000 | 0.748170000  |
| 1 | 0.213589000 | -2.873774000 | -1.909166000 |
| 6 | -0.258283000 | -2.895095000 | 0.212358000  |
| 6 | 0.149208000 | -2.637737000 | 1.554842000  |
| 6 | 0.555011000 | -2.598480000 | -0.919550000 |
| 6 | -0.258283000 | -2.895095000 | 0.212358000  |
| 6 | 0.149208000 | -2.637737000 | 1.554842000  |
| 6 | 0.555011000 | -2.598480000 | -0.919550000 |
| 6 | -0.258283000 | -2.895095000 | 0.212358000  |
| 1 | -1.361531000 | -0.841304000 | 0.942939000  |
| 6 | -0.500815000 | -2.480651000 | 3.595904000  |
| 6 | -1.737150000 | -3.083729000 | 0.212358000  |
| 6 | -4.136846000 | -3.984990000 | 0.212358000  |
| 6 | 2.663804000 | -1.596438000 | -1.930670000 |
| 6 | 3.861504000 | -2.557449000 | -1.961853000 |
| 6 | 4.475141000 | -2.378112000 | -2.847309000 |
| 6 | 4.493626000 | -2.419108000 | -1.081040000 |
| 6 | 3.125905000 | -0.136789000 | -1.957907000 |
| 6 | 3.725873000 | 0.051738000 | -2.850373000 |
| 1 | 2.270692000 | 0.540489000 | -1.968161000 |
| 1 | 3.743410000 | 0.107759000 | -1.990965000 |
| 44 | 0.127359000 | -0.707890000 | 0.293722000  |
| 6 | 2.663804000 | -1.596438000 | -1.930670000 |
| 8 | -3.124890000 | -1.529955000 | -0.434487000 |
| 8 | -1.720188000 | 0.216584000 | -0.093412000 |
| 6 | -4.021276000 | 0.661514000 | -0.618000000 |
| 6 | 1.461417000 | 2.105280000 | 0.626326000  |
| 8 | 2.573923000 | 1.803355000 | 1.291094000  |
| 8 | 0.557854000 | 1.343794000 | 0.312530000  |
| 6 | 1.393715000 | 3.585239000 | 0.281498000  |
| 9 | 1.350836000 | 4.347820000 | 1.395592000  |
| 9 | 2.483262000 | 3.971358000 | -0.416555000 |
| 9 | 0.312011000 | 3.860239000 | -0.450322000 |
| 9 | -5.016108000 | 0.426216000 | 0.264922000  |
| 9 | -3.681347000 | 1.949041000 | -0.527908000 |
| 9 | -4.532959000 | 0.446573000 | -1.849331000 |
| 1 | -2.296730000 | -2.024449000 | -0.263382000 |
| 1 | 2.478503000 | 0.933680000 | 1.734814000  |
| P' | 6 | -3.713969000 | 0.204459000 | 0.276802000  |
| 6 | -3.968591000 | 1.564699000 | 0.432206000  |
|   |   |   |   |
|---|---|---|---|
| 6 | -2.973463000 | 2.507893000 | 0.203945000 |
| 6 | -1.703938000 | 2.105837000 | -0.091321000 |
| 6 | -1.393510000 | 0.747940000 | -0.310850000 |
| 6 | -2.418676000 | -0.191364000 | -0.091321000 |
| 1 | -4.956840000 | 1.885981000 | 0.730442000 |
| 1 | -3.195374000 | 3.563051000 | 0.311572000 |
| 1 | -0.944076000 | 2.847671000 | -0.381136000 |
| 6 | -2.098430000 | -1.649405000 | -0.184746000 |
| 8 | -1.306049000 | -2.223842000 | 0.528918000 |
| 8 | -2.788271000 | -2.273361000 | -1.152843000 |
| 1 | -2.554262000 | -3.229478000 | -1.133217000 |
| 6 | -4.812893000 | -0.795372000 | 0.530792000 |
| 1 | -5.156872000 | -1.250365000 | -0.399743000 |
| 1 | -4.480182000 | -1.607363000 | 1.181052000 |
| 1 | -5.663940000 | -0.310627000 | 1.007837000 |
| 6 | -0.047060000 | 0.314673000 | -0.709982000 |
| 6 | 1.078996000 | 1.061440000 | -0.530761000 |
| 1 | 0.029663000 | -0.662464000 | -1.774050000 |
| 1 | 1.064396000 | 1.962723000 | -0.015882000 |
| 6 | 2.428929000 | 0.545292000 | -0.987169000 |
| 1 | 2.800768000 | 1.247893000 | -1.740981000 |
| 1 | 2.332335000 | -0.432745000 | -1.486093000 |
| 7 | 3.400943000 | 0.531408000 | 0.106927000 |
| 6 | 3.130303000 | -0.552796000 | 1.052858000 |
| 1 | 3.288962000 | -1.543025000 | 0.593417000 |
| 1 | 2.067881000 | -0.501399000 | 1.297179000 |
| 6 | 4.786700000 | 0.598238000 | -0.366507000 |
| 1 | 5.430814000 | 0.770582000 | 0.497690000 |
| 1 | 4.867205000 | 1.493502000 | -0.988609000 |
| 6 | 3.937385000 | -0.452337000 | 2.340273000 |
| 1 | 5.003412000 | -0.618437000 | 2.176383000 |
| 1 | 3.595178000 | -1.206470000 | 3.051792000 |
| 1 | 3.812670000 | 0.531935000 | 2.796421000 |
| 6 | 5.309518000 | -0.610137000 | -1.152071000 |
| 1 | 6.339562000 | -0.428302000 | -1.466694000 |
| 1 | 4.716906000 | -0.797082000 | -2.049720000 |
| 1 | 5.304789000 | -1.520405000 | -0.549758000 |

|   |   |   |   |
|---|---|---|---|
| 6 | -3.141434000 | -0.564467000 | 0.606679000 |
| 6 | -4.055324000 | 0.446573000 | 0.900574000 |
| 6 | -3.825654000 | 1.754064000 | 0.499519000 |
| 6 | -2.677411000 | 2.067686000 | -0.214160000 |
| 6 | -1.746317000 | 1.086317000 | -0.547304000 |
| 6 | -1.987562000 | -0.232260000 | -0.123794000 |
| 1 | -4.956090000 | 0.199068000 | 1.450049000 |
### Table S4.
Cartesian coordinates of the stationary points involved in the protonation-demetalation processes, optimized at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.

| Names | Cartesian Coordinates |
|-------|-----------------------|
|       | X         | Y         | Z         |
| pre-1 |           |           |           |
| 6     | -0.011185000 | -1.697994000 | 2.107941000 |
| 6     | -1.251313000 | -1.093507000 | 2.412631000 |
| 6     | -1.227930000 | 0.293932000 | 2.736506000 |
| 6     | -0.040750000 | 0.987469000 | 2.791762000 |
| 6     | 1.262373000 | 0.320410000 | 2.649265000 |
| 6     | 1.237664000 | -1.022056000 | 2.298488000 |
|   | 0.007690000  | -2.715643000  | 1.749263000  |
|---|--------------|---------------|--------------|
| 1 | -2.153380000 | 0.827022000   | 2.900116000  |
| 1 | -0.013024000 | 2.049713000   | 2.996030000  |
| 1 | 2.156913000  | -1.531545000  | 2.044018000  |
| 6 | 2.541870000  | 1.084482000   | 2.789150000  |
| 1 | 3.374846000  | 0.536137000   | 2.353857000  |
| 1 | 2.475691000  | 2.060998000   | 2.307998000  |
| 1 | 2.759092000  | 1.259311000   | 3.846309000  |
| 6 | -2.561392000 | -1.842718000  | 2.434201000  |
| 1 | -3.317660000 | -1.177500000  | 2.007714000  |
| 6 | -2.949649000 | -2.105900000  | 3.899146000  |
| 1 | -3.012517000 | -1.179396000  | 4.471943000  |
| 1 | -3.921112000 | -2.601055000  | 3.944179000  |
| 1 | -2.213797000 | -2.754169000  | 4.380564000  |
| 6 | -2.557295000 | -3.138524000  | 1.629258000  |
| 1 | -3.562748000 | -3.560773000  | 1.610420000  |
| 1 | -2.242211000 | -2.974158000  | 0.601078000  |
| 1 | -1.897983000 | -3.884638000  | 2.078140000  |
| 44 | 0.191851000  | 0.049799000   | 0.813742000  |
| 6 | -0.777270000 | -3.981391000  | -1.693317000 |
| 6 | -2.023839000 | -4.573929000  | -1.871857000 |
| 6 | -3.162992000 | -3.803808000  | -2.068359000 |
| 6 | -3.076172000 | -2.421430000  | -2.057064000 |
| 6 | -1.854298000 | -1.779420000  | -1.854981000 |
| 6 | -0.704390000 | -2.572971000  | -1.690480000 |
| 1 | -2.100039000 | -5.654050000  | -1.854168000 |
| 1 | -4.121309000 | -4.285757000  | -2.217946000 |
| 1 | -3.965442000 | -1.820361000  | -2.201871000 |
| 6 | 0.598563000  | -1.885014000  | -1.545378000 |
| 6 | 4.150034000  | -1.383075000  | -0.494122000 |
| 8 | 3.763588000  | -1.266887000  | -1.691405000 |
| 8 | 3.758381000  | -2.132395000  | 0.397214000  |
| 6 | 5.296025000  | -0.382098000  | -0.145511000 |
| 8 | 0.755820000  | -0.865338000  | -0.852977000 |
| 8 | 1.590580000  | -2.373621000  | -2.225768000 |
| 1 | 2.507820000  | -1.898921000  | -1.973535000 |
| 6 | 0.420540000  | -4.867869000  | -1.467357000 |
| 1 | 1.038949000  | -4.934900000  | -2.363520000 |
| 1 | 1.060588000  | -4.494221000  | -0.667824000 |
| 1 | 0.092882000  | -5.873085000  | -1.203563000 |
| 9 | 4.861769000  | 0.897822000   | -0.237579000 |
| 9 | 5.773151000  | -0.544195000  | 1.101894000  |
| 9 | 6.343726000  | -0.505638000  | -0.989570000 |
| 6 | -1.842816000 | -0.276453000  | -1.792160000 |
|   | x   | y   | z   |
|---|-----|-----|-----|
| 6 | -1.975071000 | 0.255059000 | -0.356889000 |
| 1 | -0.955160000 | 0.142652000 | -2.269723000 |
| 1 | -2.706569000 | 0.084839000 | -2.357132000 |
| 1 | -2.723195000 | -0.356889000 | 0.151719000 |
| 6 | -2.477433000 | 1.700453000 | -0.384335000 |
| 1 | -1.825533000 | -0.352265000 | 0.151719000 |
| 1 | -2.420149000 | 2.134248000 | 0.630613000 |
| 7 | -3.838031000 | 1.509753000 | -0.912131000 |
| 6 | -4.847821000 | 1.700453000 | -0.384335000 |
| 1 | -4.873133000 | 2.265427000 | 0.898775000 |
| 1 | -4.544053000 | 0.575659000 | 0.570082000 |
| 6 | -4.066539000 | 3.087788000 | -1.628571000 |
| 1 | -5.022010000 | 3.012619000 | -2.150665000 |
| 1 | -3.300521000 | 3.154231000 | -2.404952000 |
| 6 | -6.246997000 | 1.326595000 | -0.477120000 |
| 1 | -6.658067000 | 2.257588000 | -0.870380000 |
| 1 | -6.923471000 | 0.974174000 | 0.303989000 |
| 1 | -6.239879000 | 0.590180000 | -1.283351000 |
| 6 | -4.051173000 | 4.376140000 | -0.038195000 |
| 1 | -4.211064000 | 5.236370000 | -1.441679000 |
| 1 | -3.095882000 | 4.514679000 | -0.283390000 |
| 1 | -4.839812000 | 4.376140000 | -0.038195000 |
| 6 | 0.707545000 | 2.950894000 | -0.233035000 |
| 8 | -0.057277000 | 3.723328000 | 0.501665000 |
| 8 | 0.672519000 | 1.745011000 | -0.324138000 |
| 6 | 1.735238000 | 3.777010000 | -1.038083000 |
| 9 | 1.103544000 | 4.646987000 | -1.838447000 |
| 9 | 2.523307000 | 4.468549000 | -0.201909000 |
| 9 | 2.493949000 | 2.980412000 | -1.783043000 |
| 1 | -0.752003000 | 3.190503000 | 0.936014000 |

| TS-prot-1 |
|-----------|
| 6 | -0.679125000 | -1.839097000 | 1.983458000 |
| 6 | -1.649920000 | -0.895407000 | 2.364697000 |
| 6 | -1.196993000 | 0.358530000 | 2.873899000 |
| 6 | 0.170372000 | 0.585152000 | 3.092708000 |
| 6 | 1.156351000 | -0.410575000 | 2.807231000 |
| 6 | 0.709450000 | -1.599198000 | 2.214540000 |
| 1 | -0.976626000 | -2.757558000 | 1.502988000 |
| 1 | -1.906335000 | 1.142517000 | 3.093940000 |
| 1 | 0.493405000 | 1.561591000 | 3.425445000 |
| 1 | 1.437018000 | -2.317368000 | 1.864180000 |
| 6 | 2.608636000 | -0.134990000 | 3.034412000 |
| 1 | 3.227573000 | -0.810893000 | 2.448142000 |
| 1 | 2.852026000 | 0.892446000 | 2.764809000 |
| 1 | 2.848966000 | -0.270518000 | 4.092175000 |
|   |    x   |    y   |    z   |
|---|--------|--------|--------|
| 6 | -3.134396000 | -1.149140000 | 2.266906000 |
| 1 | -3.586124000 | -0.247344000 | 1.845975000 |
| 6 | -3.692221000 | -1.316696000 | 3.692174000 |
| 1 | -3.484771000 | -0.444749000 | 4.313445000 |
| 1 | -4.773596000 | -1.454473000 | 3.648881000 |
| 1 | -3.255139000 | -2.193060000 | 4.175415000 |
| 6 | -3.515512000 | -2.341644000 | 1.395244000 |
| 1 | -4.600373000 | -2.387219000 | 1.292646000 |
| 1 | -3.088548000 | -2.276895000 | 0.396052000 |
| 1 | -3.188620000 | -3.281349000 | 1.845606000 |
| 44 | -0.084042000 | 0.063926000 | 0.979961000 |
| 6 | -0.749396000 | -3.602064000 | -1.642030000 |
| 6 | -1.991644000 | -4.190092000 | -1.869484000 |
| 6 | -3.098743000 | -3.417739000 | -2.196732000 |
| 6 | -2.986904000 | -2.037044000 | -2.252950000 |
| 6 | -1.770207000 | -1.405458000 | -1.992194000 |
| 6 | -0.648856000 | -2.201763000 | -1.712975000 |
| 1 | -2.086030000 | -5.266986000 | -1.799443000 |
| 1 | -4.051962000 | -3.893320000 | -2.392081000 |
| 1 | -3.852416000 | -1.431889000 | -2.492967000 |
| 6 | 0.691369000 | -1.549106000 | -1.576612000 |
| 6 | 4.194125000 | -1.198849000 | -0.545963000 |
| 8 | 3.795782000 | -0.913057000 | -1.745503000 |
| 8 | 3.736234000 | -1.995779000 | 0.240916000 |
| 6 | 5.422261000 | -0.331779000 | -0.155759000 |
| 8 | 0.887330000 | -0.613212000 | -0.743088000 |
| 8 | 1.613483000 | -1.933630000 | -2.342690000 |
| 1 | 2.853829000 | -1.374973000 | -1.983882000 |
| 6 | 0.435326000 | -4.474733000 | -1.317777000 |
| 1 | 1.088314000 | -4.587968000 | -2.184830000 |
| 1 | 1.043911000 | -4.053921000 | -0.516387000 |
| 1 | 0.101889000 | -5.465712000 | -1.010248000 |
| 9 | 5.072595000 | 0.968519000 | -0.073257000 |
| 9 | 5.923099000 | -0.694532000 | 1.031331000 |
| 9 | 6.408723000 | -0.431180000 | -1.066215000 |
| 6 | -1.715966000 | 0.098767000 | -1.975582000 |
| 6 | -1.817729000 | 0.647174000 | -0.527481000 |
| 1 | -0.817441000 | 0.454833000 | -2.482288000 |
| 1 | -2.569352000 | 0.485986000 | -2.535055000 |
| 1 | -2.340733000 | -0.113773000 | 0.033896000 |
| 6 | -2.642538000 | 1.941606000 | -0.381194000 |
| 1 | -2.106454000 | 2.792216000 | -0.804070000 |
| 1 | -2.740648000 | 2.143946000 | 0.697345000 |
| 7 | -3.943011000 | 1.901369000 | -1.052973000 |
|   | 6     | -4.887361000 | 0.989982000 | -0.412680000 |
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|   | 1     | -4.389965000 | 0.024715000 | -0.318648000 |
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|   | 1     | -6.799015000 | 1.676922000 | -1.222973000 |
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**INT-prot-1**

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| 8 | 1.566532000 | 3.525689000 | 0.322537000 |
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| 6   | 2.742895000  | -2.039244000 | 0.541488000   |
| 6   | 2.311108000  | -1.628511000 | 1.825095000   |
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| 6   | 4.389546000  | -0.193852000 | 0.432799000   |
| 6   | 3.768635000  | -1.330191000 | -0.132130000  |
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| 8 | 2.353987000 | 2.286703000 | 0.330316000 |
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| INT-prot-2 |
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| 1  | -2.431756000 | -1.089203000 |
| 1  | -1.724332000 | 1.289107000  |
| 6  | -1.615363000 | 0.398223000  |
| 1  | -1.400045000 | -0.592095000 |
| 1  | -1.076251000 | 1.119371000  |
| 7  | -3.089449000 | 0.656335000  |
| 6  | -3.338283000 | 2.130881000  |
| 1  | -2.791854000 | 2.454474000  |
| 1  | -2.879411000 | 2.606404000  |
| 6  | -3.679230000 | -0.195780000 |
| 1  | -4.757676000 | -0.074427000 |
| 1  | -3.456681000 | -1.223416000 |
| 6  | -4.807947000 | 2.496480000  |
| 1  | -5.273436000 | 2.123868000  |
| 1  | -4.890386000 | 3.583798000  |
| 1  | -5.362724000 | 2.116240000  |
| 6  | -3.149956000 | 0.112575000  |
| 1  | -3.593263000 | -0.594957000 |
| 1  | -2.066680000 | 0.004459000  |
| 1  | -3.419159000 | 1.115609000  |
| 6  | 2.313974000  | -0.643924000 |
| 8  | 1.631869000  | 0.234504000  |
| 8  | 3.366863000  | -1.106367000 |
| 6  | 1.787716000  | -1.199788000 |
| 9  | 0.791824000  | -2.078229000 |
| 9  | 1.293203000  | -0.218644000 |
| 9  | 2.742885000  | -1.832789000 |
| 1  | -0.134550000 | 0.752105000  |

| i  | x   | y   | z   |
|----|-----|-----|-----|
| 6  | -1.078031000 | 0.414720000 |
| 6  | -0.668067000 | 0.933552000 |
| 6  | -1.479088000 | 1.932431000 |
| 6  | -2.723109000 | 1.617143000 |
| 6  | -3.170190000 | 0.300033000 |
| 6  | -2.281051000 | -0.709015000 |
| 1  | -0.465153000 | -1.229247000 |
| 1  | -1.184317000 | 2.968972000 |
| 1  | -3.311196000 | 2.415535000 |
| 1  | -2.529136000 | -1.745932000 |

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| 6  | -4.458931000 | 1.493748000 | -0.051120000 |
| 1  | -4.335554000 | 0.820769000 | -0.899650000 |
| 1  | -4.834826000 | 0.916340000 | 0.792637000  |
| 1  | -5.213331000 | 2.238527000 | -0.317867000 |
| 6  | 0.564572000  | 4.286247000 | 1.332579000  |
| 1  | 1.155391000  | 3.641560000 | 1.990273000  |
| 6  | 0.136015000  | 5.519003000 | 2.148425000  |
| 1  | -0.422612000 | 5.243533000 | 3.042916000  |
| 1  | 1.018619000  | 6.079509000 | 2.459776000  |
| 6  | 0.564572000  | 4.286247000 | 1.332579000  |
| 1  | 2.335716000  | 5.213331000 | 0.534317000  |
| 1  | 1.751522000  | 3.890562000 | -0.470988000 |
| 1  | 0.911318000  | 5.440769000 | -0.476801000 |
| 44 | -1.011180000 | 1.302416000 | 0.457916000  |
| 6  | -0.802264000 | 1.590932000 | -3.963040000 |
| 6  | -0.028186000 | 2.627730000 | -4.485232000 |
| 6  | 1.227051000  | 2.915192000 | -3.965239000 |
| 6  | 1.728165000  | 2.175323000 | -2.903132000 |
| 6  | 0.970568000  | 1.159148000 | -2.328360000 |
| 6  | -0.291742000 | 0.876123000 | -2.870234000 |
| 1  | -0.414925000 | 3.209712000 | -5.312513000 |
| 1  | 1.817481000  | 3.715559000 | -4.393479000 |
| 1  | 2.715923000  | 2.386059000 | -2.512072000 |
| 6  | -1.080558000 | -0.205921000 | -2.228632000 |
| 6  | 5.166069000  | -2.124356000 | -0.457430000 |
| 8  | 5.911024000  | -2.163124000 | 0.526705000  |
| 8  | 4.087051000  | -1.510001000 | -0.639122000 |
| 6  | 5.660236000  | -2.971693000 | -1.675951000 |
| 8  | -1.270758000 | -0.231123000 | -0.993345000 |
| 8  | -1.536514000 | -1.134840000 | -2.992987000 |
| 6  | -2.149083000 | 1.295465000  | -4.573252000 |
| 1  | -2.110845000 | 0.393942000  | -5.187298000 |
| 1  | -2.917734000 | 1.125982000  | -3.817770000 |
| 1  | -2.467645000 | 2.124102000  | -5.204625000 |
| 9  | 5.847877000  | -4.266129000 | -1.328223000 |
| 9  | 4.816735000  | -2.967615000 | -2.724871000 |
| 9  | 6.851443000  | -2.510775000 | -2.129179000 |
| 6  | 1.517055000  | 0.392421000  | -1.154003000 |
| 6  | 1.133575000  | 1.003221000  | 0.198549000  |
| 1  | 1.199981000  | -0.651061000 | -1.186338000 |
| 1  | 2.605509000  | 0.369089000  | -1.256989000 |
| 1  | 1.528914000  | 2.012356000  | 0.244056000  |
| 6  | 1.688256000  | 0.200070000  | 1.354589000  |
|   | 1   | 1.310357000 | -0.819480000 | 1.329109000 |
|---|-----|-------------|--------------|-------------|
| 1 | 1.418704000 | 0.655075000 | 2.304391000 |
| 7 | 3.202433000 | 0.042559000 | 1.755430000 |
| 6 | 3.914973000 | 1.360516000 | 1.353380000 |
| 1 | 3.544295000 | 1.971590000 | 0.426509000 |
| 1 | 3.602626000 | 2.390672000 | 2.496776000 |
| 1 | 4.629983000 | 0.879652000 | 1.206505000 |
| 1 | 5.784458000 | 0.612020000 | 0.568391000 |
| 6 | 3.440188000 | 3.941554000 | 4.695232000 |
| 1 | 3.741427000 | 2.186710000 | 2.824567000 |
| 1 | 2.409493000 | 4.154560000 | 4.023670000 |
| 6 | -1.190779000 | 3.787659000 | 3.823240000 |
| 8 | -1.082987000 | 2.824567000 | 3.406249000 |
| 8 | -1.113340000 | 4.023670000 | 4.023670000 |
| 6 | -1.444177000 | 3.787659000 | 3.406249000 |
| 9 | -0.473834000 | 2.186710000 | 2.824567000 |
| 9 | -2.615477000 | 4.154560000 | 4.023670000 |
| 9 | -1.476504000 | 3.787659000 | 3.406249000 |
| 1 | -0.917515000 | -0.564257000 | -1.605969000 |
| 6 | -4.140153000 | -1.357545000 | -1.977828000 |
| 8 | -2.959104000 | -2.184656000 | -2.460429000 |
| 1 | -1.846344000 | -2.460429000 | -2.460429000 |
| 6 | -4.918336000 | -3.355092000 | -0.676759000 |
| 9 | -4.871465000 | -4.625656000 | -0.676759000 |
| 9 | -4.382001000 | -3.071210000 | -3.071210000 |
| 9 | -6.214763000 | -3.071210000 | -3.071210000 |
|   | 0.566988000 | 0.566988000 | 0.566988000 |

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|   | 1   | 1.352285000 | 2.352247000 | 0.604439000 |
|---|-----|-------------|--------------|-------------|
| 6 | 1.373899000 | 3.030610000 | 0.014828000 |
| 6 | 0.428775000 | 3.136051000 | -1.018470000 |
| 6 | 0.762683000 | 2.564353000 | -0.228574000 |
| 6 | 2.034894000 | 2.026040000 | -2.516825000 |
| 6 | 3.032443000 | 2.004937000 | -1.489794000 |
| 6 | 2.667297000 | 2.477524000 | -0.221452000 |
| 1 | 1.120662000 | 3.357391000 | 1.010955000 |
| 1 | 0.028064000 | 2.544122000 | -3.077894000 |
| 1 | 2.247075000 | 1.560180000 | -3.468563000 |
| 1 | 3.352250000 | 2.352247000 | 0.604439000 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6 | 4.375647000 | 1.400676000 | -1.744119000 |
| 1 | 4.869268000 | 1.145056000 | -0.808986000 |
| 1 | 4.287604000 | 0.505326000 | -2.358028000 |
| 1 | 5.000048000 | 2.118559000 | -2.282364000 |
| 6 | -0.895386000 | 3.841375000 | -0.858216000 |
| 1 | -1.655930000 | 3.208276000 | -1.320553000 |
| 6 | -0.845430000 | 5.153261000 | -1.662715000 |
| 1 | -0.623258000 | 4.976547000 | -2.715704000 |
| 1 | -1.809703000 | 5.659200000 | -1.598412000 |
| 1 | -0.081270000 | 5.820764000 | -1.259028000 |
| 6 | -1.296392000 | 4.106838000 | 0.588440000 |
| 1 | -2.305991000 | 4.517817000 | 0.618161000 |
| 1 | -1.288359000 | 3.199914000 | 1.188751000 |
| 1 | -0.630914000 | 4.835747000 | 1.055797000 |
| 44 | 1.160224000 | 0.961981000 | -0.805455000 |
| 6 | -0.085698000 | 1.671133000 | 3.536465000 |
| 6 | -1.246663000 | 2.323390000 | 3.945031000 |
| 6 | -2.473805000 | 2.027835000 | 3.366515000 |
| 6 | -2.550098000 | 1.108957000 | 2.330622000 |
| 6 | -1.403273000 | 0.463960000 | 1.865446000 |
| 6 | -0.177287000 | 0.729193000 | 2.496413000 |
| 1 | -1.185190000 | 3.063366000 | 4.733823000 |
| 1 | -3.370217000 | 2.525683000 | 3.715221000 |
| 1 | -3.507172000 | 0.872961000 | 1.880694000 |
| 6 | 1.030460000 | -0.075967000 | 2.129587000 |
| 6 | 4.583992000 | -0.839577000 | 1.731853000 |
| 8 | 3.756123000 | -1.701572000 | 2.235283000 |
| 8 | 4.526845000 | 0.368456000 | 1.739758000 |
| 6 | 5.767034000 | -1.562727000 | 1.032471000 |
| 8 | 1.428391000 | -0.162926000 | 0.926016000 |
| 8 | 1.623565000 | -0.699294000 | 3.045506000 |
| 1 | 2.855664000 | -1.245150000 | 2.585947000 |
| 6 | 1.223272000 | 2.000685000 | 4.206431000 |
| 1 | 1.501186000 | 1.229528000 | 4.926752000 |
| 1 | 2.041655000 | 2.072584000 | 3.488813000 |
| 1 | 1.147299000 | 2.950361000 | 4.735636000 |
| 9 | 5.328035000 | -2.259323000 | -0.035707000 |
| 9 | 6.686843000 | -0.691523000 | 0.600573000 |
| 9 | 6.377354000 | -2.429251000 | 1.861699000 |
| 6 | -1.533518000 | -0.490114000 | 0.704125000 |
| 6 | -1.108085000 | 0.163734000 | -0.638513000 |
| 1 | -0.960122000 | -1.398965000 | 0.894091000 |
| 1 | -2.574659000 | -0.808730000 | 0.648216000 |
| 1 | -1.264550000 | 1.228808000 | -0.536549000 |
|   |       |       |       |       |
|---|-------|-------|-------|-------|
| 6 | -1.85531000 | -0.303206000 | -1.881487000 |       |
| 1 | -1.734819000 | -1.371825000 | -2.049118000 |       |
| 1 | -1.462036000 | 0.218710000 | -2.750650000 |       |
| 7 | -3.359664000 | -0.087593000 | -1.896086000 |       |
| 6 | -3.474649000 | 1.341403000 | -1.657085000 |       |
| 1 | -3.231154000 | 0.945109000 | -2.404370000 |       |
| 1 | -3.485984000 | 0.600492000 | -0.680136000 |       |
| 6 | -3.970258000 | -0.676018000 | -3.149870000 |       |
| 1 | -5.034583000 | -0.709209000 | -2.986405000 |       |
| 1 | -3.608511000 | -1.705330000 | -3.188063000 |       |
| 6 | -5.242775000 | 1.583784000 | -1.675822000 |       |
| 1 | -5.680639000 | 1.429151000 | -2.661056000 |       |
| 1 | -5.420101000 | 2.622762000 | -1.395467000 |       |
| 1 | -5.746652000 | 0.949237000 | -0.947699000 |       |
| 6 | -3.620466000 | 0.062616000 | -4.325320000 |       |
| 1 | -4.107377000 | -0.462026000 | -5.258372000 |       |
| 1 | -2.556145000 | 0.082930000 | -4.636561000 |       |
| 1 | -4.000756000 | 1.085914000 | -4.430943000 |       |
| 6 | 1.505848000 | -1.884292000 | -1.477638000 |       |
| 8 | 0.330239000 | -2.002806000 | -1.024349000 |       |
| 8 | 2.109713000 | -0.818015000 | -1.617325000 |       |
| 6 | 2.199762000 | -3.203279000 | -1.873343000 |       |
| 9 | 2.412425000 | -3.950933000 | -0.778576000 |       |
| 9 | 1.426229000 | -3.905040000 | -2.715648000 |       |
| 9 | 3.373879000 | -2.980798000 | -2.466146000 |       |
| 1 | 0.049395000 | -0.903150000 | -0.861920000 |       |
| 6 | -5.302181000 | -1.418822000 | 0.726796000 |       |
| 8 | -5.477165000 | -0.283231000 | 1.173488000 |       |
| 8 | -4.582816000 | -1.812958000 | -0.226355000 |       |
| 1 | -3.790938000 | -0.673695000 | -1.125330000 |       |
| 6 | -6.072161000 | -2.547877000 | 1.421271000 |       |
| 9 | -6.896557000 | -3.216134000 | 0.549249000 |       |
| 9 | -5.218645000 | -3.523444000 | 1.899122000 |       |
| 9 | -6.831384000 | -2.185139000 | 2.455936000 |       |

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|   | 2.059388000 | 2.449569000 | -1.684584000 |       |
| 6 | 1.543770000 | 1.747546000 | -2.791411000 |       |
| 6 | 2.340555000 | 0.688970000 | -3.327967000 |       |
| 6 | 3.561439000 | 0.391487000 | -2.815995000 |       |
| 6 | 4.131080000 | 1.110236000 | -1.699538000 |       |
| 6 | 3.333525000 | 2.133305000 | -1.139077000 |       |
| 1 | 1.444523000 | 3.179703000 | -1.181813000 |       |
| 1 | 1.929193000 | 0.060210000 | -4.104332000 |       |
| 1 | 4.156820000 | -0.457322000 | -3.201102000 |       |
| 1 | 3.666708000 | 2.624382000 | -0.238033000 |       |
|   |     |             |             |             |
|---|-----|-------------|-------------|-------------|
| 6 | 5.441106000 | 0.727636000 | -1.091977000 |
| 1 | 5.471138000 | 0.984990000 | -0.035812000 |
| 1 | 5.626948000 | -0.339647000 | -1.205871000 |
| 6 | 2.641013000 | 1.265565000 | -1.608378000 |
| 1 | 0.196459000 | 2.032894000 | -3.412977000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 1 | 0.416886000 | 2.640212000 | -4.809437000 |
| 1 | 1.011051000 | 1.986760000 | -5.449448000 |
| 1 | 0.929691000 | 3.601453000 | -4.732491000 |
| 1 | -0.300225000 | 1.066374000 | -3.542962000 |
| 6 | 0.416886000 | 2.640212000 | -4.809437000 |
| 1 | -0.546032000 | 2.805624000 | -5.294624000 |
| 1 | 1.011051000 | 1.986760000 | -5.449448000 |
| 1 | -0.830105000 | 2.546730000 | -1.557914000 |
| 6 | -0.295863000 | 3.942688000 | -2.498652000 |
| 44 | 2.144950000 | 0.299130000 | -1.979680000 |
| 6 | 0.197548000 | 3.384603000 | 1.352999000 |
| 6 | -0.743590000 | 4.376355000 | 1.080426000 |
| 6 | -2.055790000 | 4.046511000 | 0.766971000 |
| 6 | -2.440023000 | 2.714855000 | 0.698623000 |
| 6 | -1.516277000 | 1.695394000 | 0.925608000 |
| 6 | -0.201118000 | 2.044878000 | 1.259276000 |
| 1 | -0.444049000 | 5.416617000 | 1.129297000 |
| 1 | -2.778813000 | 4.829630000 | 0.576083000 |
| 1 | -3.463777000 | 2.451812000 | 0.460823000 |
| 6 | 0.779591000 | 0.963799000 | 1.610733000 |
| 6 | -6.143411000 | -0.363277000 | 1.152130000 |
| 8 | -5.158332000 | 0.023412000 | 0.470497000 |
| 8 | -6.611316000 | -1.492449000 | 1.303859000 |
| 6 | -6.848925000 | 0.813184000 | 1.900989000 |
| 8 | 1.311229000 | 0.243929000 | 0.707760000 |
| 8 | 1.019964000 | 0.771812000 | 2.824585000 |
| 1 | -4.313073000 | -1.166520000 | -0.302435000 |
| 6 | 1.595961000 | 3.767414000 | 1.765240000 |
| 1 | 1.626615000 | 4.019821000 | 2.828429000 |
| 1 | 2.312448000 | 2.961793000 | 1.611325000 |
| 1 | 1.936468000 | 4.644404000 | 1.212590000 |
| 9 | -7.300474000 | 1.748120000 | 1.030884000 |
| 9 | -7.905161000 | 0.420777000 | 2.635705000 |
| 9 | -5.995005000 | 1.441326000 | 2.743675000 |
| 6 | -1.949441000 | 0.258671000 | 0.777377000 |
| 6 | -1.991614000 | -0.165668000 | -0.698568000 |
| 1 | -1.268330000 | -0.405969000 | 1.311258000 |
| 1 | -2.938282000 | 0.137019000 | 1.219260000 |
| 1 | -2.685456000 | 0.474108000 | -1.248348000 |
Table S5. Electronic energies (in a.u.), solution entropies (in cal·mol⁻¹·K⁻¹) and Gibbs free-energies (in a.u.) of all the main stationary points, determined at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.
|   |        |        |        |        |
|---|--------|--------|--------|--------|
| INT-1 | -6303.95796 | 226.757 | -6303.60545 |
| TS-2  | -6303.92896 | 225.797 | -6303.57303 |
| INT-2  | -6303.93768 | 230.69 | -6303.58746 |
| TS-3  | -6303.91067 | 223.538 | -6303.56471 |
| INT-3  | -6303.92226 | 229.918 | -6303.57303 |
| HOTFA | -527.00041 | 61.923 | -526.98609 |
| R2    | -330.63146 | 80.729 | -330.44954 |
| INT-3-1 | -5776.89785 | 185.246 | -5776.57848 |
| INT-3-2  | -6634.60761 | 282.261 | -6634.05428 |
| TS-4  | -6634.57786 | 281.877 | -6634.02474 |
| INT-4  | -6634.60475 | 292.471 | -6634.0522 |
| INT-4-1  | -6634.60818 | 273.039 | -6634.04938 |
| TS-5  | -6634.58751 | 278.777 | -6634.03277 |
| NHR2  | -213.88665 | 61.101 | -213.7605 |
| INT-5  | -6420.70854 | 234.784 | -6420.29613 |
| TS-5  | -6634.56748 | 289.917 | -6634.01812 |
| INT-5  | -6420.68143 | 250.611 | -6420.27346 |
| INT-3-2-NA | -6107.57254 | 238.872 | -6107.0515 |
| TS-4-NA  | -6107.53957 | 239.803 | -6107.01995 |
| INT-4-NA  | -6107.56684 | 243.151 | -6107.04582 |
| INT-4-1-NA | -6107.5917 | 224.629 | -6107.06415 |
| TS-5-NA  | -6107.53465 | 230.265 | -6107.013 |
| INT-5-NA  | -6107.54848 | 233.942 | -6107.02716 |
| TS-allyl | -6634.55017 | 297.361 | -6634.00422 |
| INT-allyl | -6420.65948 | 250.201 | -6420.25284 |
| TS-6  | -6420.67879 | 239.69 | -6420.26944 |
| INT-6  | -6420.69617 | 250.562 | -6420.28919 |
| TS-7  | -6420.68349 | 243.825 | -6420.27505 |
| INT-7  | -6420.71091 | 245.747 | -6420.30127 |
| TS-8  | -6420.69059 | 247.576 | -6420.28227 |
| P  | -577.08101 | 95.513 | -576.90991 |
| TS-BHE-1 | -6634.58085 | 279.636 | -6634.02797 |
| INT-BHE-1 | -6634.58586 | 288.258 | -6634.03378 |
| Ru(0)  | -5844.71004 | 181.04 | -5844.47263 |
| P' | -789.76307 | 134.601 | -789.47175 |
| TS-BHE-2  | -6634.58245 | 284.005 | -6634.03295 |
| INT-BHE-2  | -6634.58844 | 281.12 | -6634.0365 |
| P''  | -789.77112 | 128.875 | -789.47771 |
| pre-1  | -6634.56752 | 241.653 | -6634.01016 |
| TS-prot-1 | -6634.55358 | 237.930 | -6633.99928 |
| INT-prot-1 | -6634.60865 | 241.015 | -6634.05003 |
| pre-2  | -6634.57970 | 239.545 | -6634.01642 |
Table S6. Imaginary frequencies (in cm$^{-1}$) of the main transition states, determined at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.

| Names         | I. F. | Names         | I. F. |
|---------------|-------|---------------|-------|
| TS-1          | -87 i | TS-2          | -73 i |
| TS-3          | -1467 i | TS-4          | -313 i |
| TS-5          | -201 i | TS-6          | -37 i |
| TS-7          | -98 i | TS-8          | -94 i |
| TS-4-NA       | -306 i | TS-5-NA       | -305 i |
| TS-allyl      | -10 i | TS-BHE-1      | -667 i |
| TS-BHE-2      | -647 i | TS-prot-1     | -1022 i |
| TS-prot-2     | -1111 i | TS-prot-3    | -1147 i |
Figure S1. Catalyst’s Generation and Characterization

**Figure S2** provides two reaction channels corresponding to the C–C bond coupling happening at the two olefinic carbon centers, respectively. The first channel leads to the correct product as observed experimentally. The second pathway starts from INT-3-2a, a conformational isomer of INT-3-2, and involves the four-center transition state TS-4a leading to INT-4a and INT-4-1a. Free-energy computations reveal that the two pathways involve the free-energy barriers of 18.5 and 22.7 kcal/mol, respectively. Obviously, the former path corresponding to the C–C bond coupling at the terminal olefinic carbon is kinetically more competitive, which is in
good agreement with the experimental observation. Additionally, the thermodynamic aspect favors the former pathway as well. The steric repulsion between the secondary amide group and the phenyl group should be responsible for the observed regioselectivity.

**Figure S2.** Migratory insertion pathways and free-energy variations (in kcal/mol), calculated at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory.
Discussion on the Explicit Solvation Effect

![Diagram showing solvation effect](image)

**Figure S3.** The solvent-containing structures involved in the product separation step and the relative free-energies values (in kcal/mol), determined at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory for simplicity.

We have tested the explicit solvation effect of TCE (see **Figure S3**). The last step of the main pathway, \( \text{INT-7} \rightarrow P + \text{CAT} \), has the free-energy change of +3.1 kcal/mol, indicating that the product may not easily separate from \( \text{INT-7} \), possibly due to the presence of an intramolecular hydrogen bond in \( \text{INT-7} \). The difficulty in the product separation might lead to the deactivation of the catalyst. However, a TCE molecule is able to form a hydrogen bond with the product carboxyl group, and the participation of only one TCE makes the final step near free-energy neutral (\( \Delta G = 0.5 \) kcal/mol), which facilitates the separation of the product from the ruthenium center. We also found that the explicit solvation effect of TCE may help to control the correct reaction direction, because the protonation of the side product (\( \text{C}_2\text{H}_5\text{NH} \)) by HOTFA could be effectively prevented, as follows.

The catalytic reaction produces the secondary amine (\( \text{C}_2\text{H}_5\text{NH} \)), which could be protonated by HOTFA and thus might prevent the protonation of \( \text{R2} \) by HOTFA. DFT calculations predict that protonation of (\( \text{C}_2\text{H}_5\text{NH} \)) by HOTFA is 0.6 kcal/mol more favorable thermodynamically than that of \( \text{R2} \) by HOTFA. If the explicit solvation effect of TCE is considered (TCE forms an H-bond with each amine), however, the former process is computed to be 0.7 kcal/mol less favorable thermodynamically than the latter process. Since the protonation of \( \text{R2} \) is crucial for
promoting the β-amide elimination step, this solvation effect should be important for controlling the correct reaction direction. The present arguments on the solvent effect are only for qualitative reference.

In addition, we tested the explicit solvation effect on the C-H activation process. We attempted to introduce one or two TCE molecules to form H-bonds with the oxygen atoms, but we found that the relative free energies varied not evidently (see Figure S4).

**Figure S4.** The solvent-containing structures involved in the C-H activation process and the relative free-energies values (in kcal/mol), determined at the B3LYP+IDSCRF/DZVP level of theory for simplicity.
**Figure S5.** The transition states of C-H activation induced by an internal base (TS-3) and an external base (TS-3-R2 and TS-3-OTFA) and the rate-determining free-energy barriers, calculated at the B3LYP-D3+IDSCRF/TZP-DKH(-dfg) level of theory. Hydrogen atoms are omitted for the sake of clarity.

**Figure S6.** Mechanism for the generation of a ruthenium-(η3-allyl) complex proposed in the literature, with the key bond lengths (in Å) free-energy parameters (in kcal/mol) calculated at the B3LYP+D3-IDSCRF/TZP-DKH(-dfg) level of theory. Hydrogen atoms are omitted for the sake of clarity.