

Supporting Information for:
Decomposition of the Electronic Activity in Competing
[5,6] and [6,6] Cycloaddition Reactions Between C₆₀ and
Cyclopentadiene

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Cartesian Coordinates

[5.6] path

TS

C	1.543990000	1.654243000	2.278722000
C	1.438065000	2.467130000	1.168980000
C	0.150543000	3.089907000	0.751798000
C	-1.002871000	2.540795000	1.412329000
C	-0.887409000	1.683804000	2.585044000
C	0.348821000	1.258222000	3.024109000
C	-2.159947000	2.170724000	0.710079000
C	-2.159947000	2.170724000	-0.710079000
C	-1.002871000	2.540795000	-1.412329000
C	0.150543000	3.089907000	-0.751798000
C	-2.805262000	1.063324000	-1.426605000
C	-2.014207000	0.775262000	-2.601310000
C	-0.887409000	1.683804000	-2.585044000
C	0.348821000	1.258222000	-3.024109000
C	0.529916000	-0.107886000	-3.471678000
C	-0.545515000	-0.987936000	-3.480926000
C	-1.847802000	-0.535237000	-3.034478000
C	1.831588000	-0.558838000	-3.016417000
C	2.005820000	-1.868230000	-2.592542000
C	0.881524000	-2.786657000	-2.596954000
C	-0.363992000	-2.355471000	-3.027495000
C	2.813802000	-2.150212000	-1.419168000
C	2.184859000	-3.238320000	-0.694875000
C	0.992455000	-3.630701000	-1.419615000
C	-0.149791000	-4.003754000	-0.724658000
C	-0.149791000	-4.003754000	0.724658000
C	0.992455000	-3.630701000	1.419615000
C	2.184859000	-3.238320000	0.694875000
C	2.813802000	-2.150212000	1.419168000
C	2.005820000	-1.868230000	2.592542000
C	0.881524000	-2.786657000	2.596954000
C	-0.363992000	-2.355471000	3.027495000
C	-0.545515000	-0.987936000	3.480926000
C	0.529916000	-0.107886000	3.471678000
C	1.831588000	-0.558838000	3.016417000
C	2.453667000	0.528475000	2.282458000
C	-2.014207000	0.775262000	2.601310000
C	-1.847802000	-0.535237000	3.034478000
C	3.237897000	0.258463000	1.170002000
C	3.418004000	-1.111158000	0.725990000
C	-1.453720000	-3.549098000	1.175066000
C	-1.559276000	-2.746294000	2.300473000
C	-2.473543000	-1.618137000	2.305483000

C	3.418004000	-1.111158000	-0.725990000
C	-1.559276000	-2.746294000	-2.300473000
C	-1.453720000	-3.549098000	-1.175066000
C	-2.257684000	-3.264601000	0.000000000
C	-2.473543000	-1.618137000	-2.305483000
C	-3.233784000	-1.338743000	-1.176177000
C	-3.125791000	-2.182531000	0.000000000
C	1.543990000	1.654243000	-2.278722000
C	2.453667000	0.528475000	-2.282458000
C	3.237897000	0.258463000	-1.170002000
C	-3.401849000	0.029531000	-0.732396000
C	1.438065000	2.467130000	-1.168980000
C	-3.233784000	-1.338743000	1.176177000
C	-3.401849000	0.029531000	0.732396000
C	-2.805262000	1.063324000	1.426605000
C	2.233722000	2.175708000	0.000000000
C	3.121335000	1.099979000	0.000000000
C	0.303037000	5.149613000	-1.151109000
C	0.303037000	5.149613000	1.151109000
C	-0.955903000	5.583538000	0.696295000
C	-0.955903000	5.583538000	-0.696295000
C	1.254491000	5.348829000	0.000000000
H	0.616454000	5.170093000	-2.189403000
H	-1.828116000	5.733253000	-1.321782000
H	-1.828116000	5.733253000	1.321782000
H	0.616454000	5.170093000	2.189403000
H	2.151147000	4.729241000	0.000000000
H	1.566375000	6.403444000	0.000000000

RC

C	1.547053000	1.637316000	2.296458000
C	1.441369000	2.446811000	1.174537000
C	0.137224000	2.899698000	0.725322000
C	-1.003647000	2.521914000	1.419120000
C	-0.892612000	1.675413000	2.592068000
C	0.353732000	1.243861000	3.022892000
C	-2.196786000	2.130532000	0.694209000
C	-2.196786000	2.130532000	-0.694209000
C	-1.003647000	2.521914000	-1.419120000
C	0.137224000	2.899698000	-0.725322000
C	-2.824379000	1.040001000	-1.419145000
C	-2.018508000	0.759615000	-2.593190000
C	-0.892612000	1.675413000	-2.592068000
C	0.353732000	1.243861000	-3.022892000
C	0.532183000	-0.124962000	-3.470728000
C	-0.543790000	-1.001093000	-3.471178000
C	-1.847840000	-0.548698000	-3.022481000
C	1.836285000	-0.577488000	-3.022244000

C	2.006953000	-1.885986000	-2.593420000
C	0.881607000	-2.802564000	-2.593872000
C	-0.365070000	-2.369643000	-3.022244000
C	2.813047000	-2.165579000	-1.419287000
C	2.185634000	-3.254915000	-0.693761000
C	0.991961000	-3.648498000	-1.419648000
C	-0.149223000	-4.024455000	-0.725707000
C	-0.149223000	-4.024455000	0.725707000
C	0.991961000	-3.648498000	1.419648000
C	2.185634000	-3.254915000	0.693761000
C	2.813047000	-2.165579000	1.419287000
C	2.006953000	-1.885986000	2.593420000
C	0.881607000	-2.802564000	2.593872000
C	-0.365070000	-2.369643000	3.022245000
C	-0.543790000	-1.001093000	3.471178000
C	0.532183000	-0.124962000	3.470728000
C	1.836285000	-0.577488000	3.022244000
C	2.463478000	0.511665000	2.296332000
C	-2.018508000	0.759615000	2.593190000
C	-1.847840000	-0.548698000	3.022481000
C	3.234417000	0.244394000	1.174171000
C	3.413037000	-1.124388000	0.725722000
C	-1.453301000	-3.571827000	1.174181000
C	-1.558801000	-2.763193000	2.296551000
C	-2.475292000	-1.637720000	2.296822000
C	3.413038000	-1.124388000	-0.725722000
C	-1.558801000	-2.763193000	-2.296551000
C	-1.453301000	-3.571827000	-1.174181000
C	-2.259223000	-3.291932000	0.000000000
C	-2.475292000	-1.637720000	-2.296822000
C	-3.245399000	-1.369816000	-1.174214000
C	-3.134972000	-2.215663000	0.000000000
C	1.547053000	1.637316000	-2.296458000
C	2.463478000	0.511665000	-2.296332000
C	3.234417000	0.244394000	-1.174171000
C	-3.424545000	-0.001047000	-0.725842000
C	1.441369000	2.446811000	-1.174537000
C	-3.245399000	-1.369816000	1.174214000
C	-3.424545000	-0.001047000	0.725842000
C	-2.824379000	1.040001000	1.419145000
C	2.248173000	2.166758000	0.000000000
C	3.124228000	1.090474000	0.000000000
C	0.361307000	6.117319000	-1.177000000
C	0.361307000	6.117319000	1.177000000
C	-0.906805000	6.190197000	0.734570000
C	-0.906805000	6.190197000	-0.734570000
C	1.293444000	6.071103000	0.000000000
H	0.689494000	6.094226000	-2.209066000

H	-1.799037000	6.234795000	-1.348812000
H	-1.799037000	6.234795000	1.348812000
H	0.689494000	6.094225000	2.209066000
H	1.913866000	5.162427000	0.000000000
H	1.993230000	6.918385000	0.000000000

PC

C	1.555196000	1.705230000	2.273634000
C	1.452918000	2.521842000	1.171093000
C	0.188803000	3.304815000	0.814760000
C	-0.995151000	2.616441000	1.431452000
C	-0.879964000	1.745362000	2.606119000
C	0.352876000	1.311864000	3.033315000
C	-2.107877000	2.234759000	0.724918000
C	-2.107877000	2.234759000	-0.724918000
C	-0.995151000	2.616441000	-1.431452000
C	0.188803000	3.304815000	-0.814760000
C	-2.774174000	1.122420000	-1.433847000
C	-2.002737000	0.833817000	-2.615332000
C	-0.879964000	1.745362000	-2.606119000
C	0.352876000	1.311864000	-3.033315000
C	0.531683000	-0.055597000	-3.474992000
C	-0.544614000	-0.936609000	-3.489966000
C	-1.844322000	-0.480435000	-3.046503000
C	1.829088000	-0.509782000	-3.013436000
C	2.003671000	-1.819694000	-2.593085000
C	0.877824000	-2.736284000	-2.599223000
C	-0.365316000	-2.303940000	-3.033170000
C	2.812257000	-2.105489000	-1.419822000
C	2.179458000	-3.189426000	-0.696287000
C	0.986857000	-3.578840000	-1.419985000
C	-0.156712000	-3.947879000	-0.724243000
C	-0.156712000	-3.947879000	0.724243000
C	0.986857000	-3.578840000	1.419985000
C	2.179458000	-3.189426000	0.696287000
C	2.812257000	-2.105489000	1.419822000
C	2.003671000	-1.819694000	2.593085000
C	0.877824000	-2.736284000	2.599223000
C	-0.365316000	-2.303940000	3.033170000
C	-0.544614000	-0.936609000	3.489966000
C	0.531683000	-0.055597000	3.474992000
C	1.829088000	-0.509782000	3.013436000
C	2.450742000	0.575229000	2.275264000
C	-2.002737000	0.833817000	2.615332000
C	-1.844322000	-0.480435000	3.046503000
C	3.241451000	0.300388000	1.166703000
C	3.421085000	-1.069303000	0.726123000
C	-1.458680000	-3.488621000	1.175773000

C	-1.562048000	-2.690000000	2.304208000
C	-2.470094000	-1.557228000	2.311884000
C	3.421085000	-1.069303000	-0.726123000
C	-1.562048000	-2.690000000	-2.304208000
C	-1.458680000	-3.488621000	-1.175772000
C	-2.260709000	-3.199865000	0.000000000
C	-2.470094000	-1.557228000	-2.311884000
C	-3.224093000	-1.270063000	-1.178243000
C	-3.120968000	-2.112401000	0.000000000
C	1.555196000	1.705230000	-2.273634000
C	2.450742000	0.575229000	-2.275264000
C	3.241451000	0.300388000	-1.166703000
C	-3.371186000	0.097359000	-0.737017000
C	1.452918000	2.521842000	-1.171093000
C	-3.224093000	-1.270063000	1.178243000
C	-3.371186000	0.097359000	0.737017000
C	-2.774174000	1.122420000	1.433847000
C	2.222538000	2.211430000	0.000000000
C	3.121274000	1.135608000	0.000000000
C	0.280849000	4.853054000	-1.125202000
C	0.280849000	4.853054000	1.125202000
C	-1.035766000	5.454721000	0.668145000
C	-1.035766000	5.454721000	-0.668145000
C	1.211857000	5.333022000	0.000000000
H	0.583213000	5.048657000	-2.155087000
H	-1.855436000	5.720275000	-1.325271000
H	-1.855436000	5.720275000	1.325271000
H	0.583213000	5.048657000	2.155087000
H	2.196550000	4.857967000	0.000000000
H	1.323748000	6.419173000	0.000000000

[6.6] path

TS			
C	-2.391177000	1.962693000	0.732004000
C	-1.283435000	2.427708000	1.415077000
C	-0.136869000	3.038321000	0.719331000
C	-3.482221000	0.018784000	0.000000000
C	-3.064810000	0.761178000	1.175221000
C	-2.617653000	0.079569000	2.301765000
C	1.053459000	2.516403000	1.416745000
C	2.193254000	2.143544000	0.734072000
C	-3.433273000	-1.368152000	0.000000000
C	0.637582000	1.768331000	2.578551000
C	3.075196000	-1.842242000	1.174837000
C	2.621981000	-1.167273000	2.299446000
C	1.466900000	-1.664513000	3.025877000

C	0.817098000	-2.812839000	2.595173000
C	1.293093000	-3.518235000	1.420050000
C	3.489895000	-1.096809000	0.000000000
C	3.429685000	0.289542000	0.000000000
C	2.956295000	0.997312000	1.175805000
C	2.565576000	0.282214000	2.303834000
C	0.695439000	-0.521025000	3.474684000
C	-0.690315000	-0.574765000	3.473983000
C	-1.370474000	-1.774875000	3.025355000
C	-0.633455000	-2.869473000	2.594936000
C	-1.053293000	-3.609765000	1.419843000
C	0.137564000	-4.011487000	0.693799000
C	-2.191441000	-3.222725000	0.726198000
C	-2.960792000	-2.078398000	1.174707000
C	-2.560858000	-1.369782000	2.299027000
C	1.378029000	0.679575000	3.023307000
C	-1.463619000	0.569306000	3.021425000
C	2.397181000	-3.042830000	0.726141000
C	-0.296007000	5.209210000	1.154817000
C	0.964901000	5.590570000	0.702394000
C	-1.248804000	5.350493000	0.000000000
H	-2.107010000	4.675223000	0.000000000
H	-1.630137000	6.383419000	0.000000000
H	1.838204000	5.731345000	1.328286000
H	-0.609168000	5.209086000	2.192987000
C	-0.810400000	1.712404000	2.578717000
C	-2.391177000	1.962693000	-0.732004000
C	-1.283435000	2.427708000	-1.415077000
C	-0.136869000	3.038321000	-0.719331000
C	-3.064810000	0.761178000	-1.175221000
C	-2.617653000	0.079569000	-2.301765000
C	1.053459000	2.516403000	-1.416745000
C	2.193254000	2.143544000	-0.734072000
C	0.637582000	1.768331000	-2.578551000
C	3.075196000	-1.842242000	-1.174837000
C	2.621981000	-1.167273000	-2.299446000
C	1.466900000	-1.664513000	-3.025877000
C	0.817098000	-2.812839000	-2.595173000
C	1.293093000	-3.518235000	-1.420050000
C	2.956295000	0.997312000	-1.175805000
C	2.565576000	0.282214000	-2.303834000
C	0.695439000	-0.521025000	-3.474684000
C	-0.690315000	-0.574765000	-3.473983000
C	-1.370474000	-1.774875000	-3.025355000
C	-0.633455000	-2.869473000	-2.594936000
C	-1.053293000	-3.609765000	-1.419843000
C	0.137564000	-4.011487000	-0.693799000
C	-2.191441000	-3.222725000	-0.726198000

C	-2.960792000	-2.078398000	-1.174707000
C	-2.560858000	-1.369782000	-2.299027000
C	1.378029000	0.679575000	-3.023307000
C	-1.463619000	0.569306000	-3.021425000
C	2.397181000	-3.042830000	-0.726141000
C	-0.296007000	5.209210000	-1.154817000
C	0.964901000	5.590570000	-0.702394000
H	1.838204000	5.731345000	-1.328286000
H	-0.609168000	5.209086000	-2.192987000
C	-0.810400000	1.712404000	-2.578717000

RC

C	-2.395085000	1.967489000	0.726521000
C	-1.285411000	2.431411000	1.418388000
C	-0.129317000	2.919082000	0.692609000
C	-3.494576000	0.025188000	0.000000000
C	-3.074885000	0.767209000	1.175031000
C	-2.619009000	0.090036000	2.298255000
C	1.061149000	2.519168000	1.418680000
C	2.201904000	2.142580000	0.727521000
C	-3.439996000	-1.361211000	0.000000000
C	0.641111000	1.782130000	2.593678000
C	3.076802000	-1.838734000	1.174433000
C	2.622546000	-1.162283000	2.297492000
C	1.466094000	-1.655782000	3.023601000
C	0.815047000	-2.803168000	2.594059000
C	1.290648000	-3.510495000	1.419516000
C	3.496943000	-1.096519000	0.000000000
C	3.445265000	0.289793000	0.000000000
C	2.970208000	0.997671000	1.175350000
C	2.568698000	0.287728000	2.299649000
C	0.696077000	-0.511266000	3.473461000
C	-0.690720000	-0.564008000	3.473137000
C	-1.371434000	-1.763695000	3.023286000
C	-0.635198000	-2.858477000	2.593841000
C	-1.055805000	-3.599820000	1.419283000
C	0.134574000	-4.002826000	0.693649000
C	-2.193791000	-3.214072000	0.725718000
C	-2.963983000	-2.068976000	1.174286000
C	-2.562056000	-1.359742000	2.297185000
C	1.378755000	0.689386000	3.025509000
C	-1.462366000	0.581375000	3.024486000
C	2.395631000	-3.038891000	0.725714000
C	-0.326057000	5.833027000	1.175460000
C	0.944505000	5.902753000	0.732298000
C	-1.260668000	5.818577000	0.000000000
H	-1.934418000	4.950639000	0.000000000

H	-1.907215000	6.707965000	0.000000000
H	1.836536000	5.935264000	1.347531000
H	-0.653269000	5.811645000	2.208128000
C	-0.810172000	1.727130000	2.594305000
C	-2.395085000	1.967489000	-0.726521000
C	-1.285411000	2.431411000	-1.418388000
C	-0.129317000	2.919082000	-0.692609000
C	-3.074885000	0.767209000	-1.175031000
C	-2.619009000	0.090036000	-2.298255000
C	1.061149000	2.519168000	-1.418680000
C	2.201904000	2.142580000	-0.727521000
C	0.641111000	1.782130000	-2.593678000
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C	2.622546000	-1.162283000	-2.297492000
C	1.466094000	-1.655782000	-3.023601000
C	0.815047000	-2.803168000	-2.594059000
C	1.290648000	-3.510495000	-1.419516000
C	2.970208000	0.997671000	-1.175350000
C	2.568698000	0.287728000	-2.299649000
C	0.696077000	-0.511266000	-3.473461000
C	-0.690720000	-0.564008000	-3.473137000
C	-1.371434000	-1.763695000	-3.023286000
C	-0.635198000	-2.858477000	-2.593841000
C	-1.055805000	-3.599820000	-1.419283000
C	0.134574000	-4.002826000	-0.693649000
C	-2.193791000	-3.214072000	-0.725718000
C	-2.963983000	-2.068976000	-1.174286000
C	-2.562056000	-1.359742000	-2.297185000
C	1.378755000	0.689386000	-3.025509000
C	-1.462366000	0.581375000	-3.024486000
C	2.395631000	-3.038891000	-0.725714000
C	-0.326057000	5.833027000	-1.175460000
C	0.944505000	5.902753000	-0.732298000
H	1.836536000	5.935264000	-1.347531000
H	-0.653269000	5.811645000	-2.208128000
C	-0.810172000	1.727130000	-2.594305000

PC

C	-2.387439000	2.013780000	0.740985000
C	-1.301557000	2.489438000	1.430661000
C	-0.161731000	3.284066000	0.800887000
C	-3.470263000	0.068370000	0.000000000
C	-3.056179000	0.810488000	1.175166000
C	-2.620576000	0.127081000	2.306707000
C	1.036569000	2.591197000	1.435272000
C	2.157298000	2.210150000	0.741201000
C	-3.429731000	-1.318031000	0.000000000
C	0.622971000	1.825667000	2.578170000

C	3.069013000	-1.772182000	1.175559000
C	2.615263000	-1.100986000	2.302682000
C	1.463821000	-1.604610000	3.029930000
C	0.818171000	-2.755237000	2.597287000
C	1.296074000	-3.455998000	1.420988000
C	3.477099000	-1.023481000	0.000000000
C	3.399361000	0.361280000	0.000000000
C	2.923774000	1.066008000	1.175060000
C	2.548931000	0.347715000	2.307210000
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C	-0.697018000	-0.523733000	3.479685000
C	-1.373281000	-1.725419000	3.030023000
C	-0.632385000	-2.817093000	2.597179000
C	-1.049336000	-3.555792000	1.420796000
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C	-2.188375000	-3.169926000	0.726714000
C	-2.959054000	-2.028961000	1.175674000
C	-2.563510000	-1.321770000	2.302905000
C	1.365473000	0.738239000	3.027890000
C	-1.473868000	0.617528000	3.026285000
C	2.397841000	-2.974520000	0.726730000
C	-0.257051000	4.832037000	1.121762000
C	1.051706000	5.446577000	0.668166000
C	-1.200895000	5.291704000	0.000000000
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H	-0.559127000	5.020148000	2.153066000
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C	-1.301557000	2.489438000	-1.430661000
C	-0.161731000	3.284066000	-0.800887000
C	-3.056179000	0.810488000	-1.175166000
C	-2.620576000	0.127081000	-2.306707000
C	1.036569000	2.591197000	-1.435272000
C	2.157298000	2.210150000	-0.741201000
C	0.622971000	1.825667000	-2.578170000
C	3.069013000	-1.772182000	-1.175559000
C	2.615263000	-1.100986000	-2.302682000
C	1.463821000	-1.604610000	-3.029930000
C	0.818171000	-2.755237000	-2.597287000
C	1.296074000	-3.455998000	-1.420988000
C	2.923774000	1.066008000	-1.175060000
C	2.548931000	0.347715000	-2.307210000
C	0.687933000	-0.464912000	-3.479912000
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C	-1.373281000	-1.725419000	-3.030023000
C	-0.632385000	-2.817093000	-2.597179000

C	-1.049336000	-3.555792000	-1.420796000
C	0.142350000	-3.952467000	-0.693854000
C	-2.188375000	-3.169926000	-0.726714000
C	-2.959054000	-2.028961000	-1.175674000
C	-2.563510000	-1.321770000	-2.302905000
C	1.365473000	0.738239000	-3.027890000
C	-1.473868000	0.617528000	-3.026285000
C	2.397841000	-2.974520000	-0.726730000
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