

9. Appendix

9.1 Crystallographic data

Table 1: Summary of crystallographic data and structure refinement parameters.

Compound	187
Formula	C12H20Br4O4
<i>M</i>	547.92
Crystal system	monoclinic
Space group	<i>P 1 21/n 1</i>
<i>T</i> /K	120(2)
<i>a</i> /Å	7.1207(3)
<i>b</i> /Å	10.3796(3)
<i>c</i> /Å	23.0378(9)
α /°	90
β /°	92.983(2)
γ /°	90
<i>V</i> /Å ³	1700.42(11)
<i>Z</i>	4
μ (Mo K α)/mm ⁻¹	9.475
Diffns collected	69660
Independent diffns	4579
Observed ^b diffns	4204
<i>R</i> _{int} ^c /%	0.0421
No. of parameters	191
<i>R</i> ^c obsd diffns/%	0.0239
<i>R</i> , <i>wR</i> ^c all data/%	0.0274, 0.0668
$\Delta\rho$ /e Å ⁻³	0.876, -0.680
CCDC entry	2352199

^a The range of transmission factors. ^b Diffractions with $I > 2\sigma(I)$. ^c Definitions: $R_{\text{int}} = \Sigma |F_o^2 - F_o^2(\text{mean})| / \Sigma F_o^2$, where $F_o^2(\text{mean})$ is the average intensity of symmetry-equivalent diffractions. $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$, $wR = [\Sigma \{w(F_o^2 - F_c^2)^2\} / \Sigma w(F_o^2)^2]^{1/2}$.

9.2 Computational methods

Calculations were performed using Orca 5.0.4¹⁰², Gaussian 16¹⁰⁸, Crest 2.12¹⁰³ and xTB 6.6.0¹⁰⁴ software. The relevant conformers for each product were generated by the default Crest/xTB procedure at the GFN2-xTB/ALPB (toluene) level. The corresponding transition states were found using Nudged elastic band (NEB-TS, as implemented in Orca 5.0.4)¹⁰⁵ method at

PBEh-3c¹⁰⁶ level of theory. The stationary points were reoptimized and characterized by full calculation of vibrational frequencies carried out at the M06-2X/6-311+G**/M06-2X/6-31+G* level of theory (at 298.15 K), including an implicit description of toluene solvent using conductor-like PCM (CPCM) method as implemented in Gaussian 16. Because the M06 functional is known to be more sensitive to the integration grid¹⁰⁷ a dense integration grid was used specifying the grid=ultrafine keyword.

Table 2 XYZ of ethyl propiolate (165)

6	-1.307202000	-0.778656000	0.066573000
6	-0.501443000	0.116981000	0.043564000
1	-2.021270000	-1.575451000	0.087116000
8	0.084425000	2.396020000	0.061765000
6	0.429427000	1.238181000	0.018862000
8	1.691923000	0.821158000	-0.056013000
6	2.694175000	1.860423000	-0.085169000
1	4.113225000	0.571950000	-1.074719000
1	4.831530000	1.933649000	-0.191811000
1	4.203015000	0.533901000	0.700042000
6	4.041041000	1.178399000	-0.168010000
1	2.499229000	2.500629000	-0.949935000
1	2.589371000	2.463281000	0.821051000

Table 3 XYZ of diene (176)

6	-0.294567000	0.203653000	-0.222439000
6	-0.093011000	1.016530000	0.830273000
6	-0.558367000	2.445743000	0.767922000
8	0.434977000	3.324660000	0.217921000
6	-1.787873000	2.673002000	-0.130634000
8	-3.023251000	2.660253000	0.580007000
6	-1.801733000	1.768044000	-1.339342000
6	-1.078790000	0.645147000	-1.385240000
6	1.469446000	-3.525421000	-0.282410000
1	3.103306000	-4.197663000	1.026241000
1	3.348228000	-2.716964000	-1.078910000
6	2.170541000	-4.576752000	0.590778000
1	2.426857000	-5.457097000	-0.015129000

1	1.928361000	-2.363419000	-2.081286000
6	2.630173000	-1.064464000	1.223316000
1	3.427286000	-1.769467000	1.489339000
1	2.987273000	-0.453777000	0.386062000
8	0.148630000	-1.066901000	-0.337169000
1	2.479930000	-0.399359000	2.080236000
1	-0.846702000	-2.995057000	2.000335000
1	0.634222000	-2.979128000	2.974443000
1	-3.001320000	-3.017213000	0.221662000
1	-0.805367000	2.806257000	1.778568000
1	-1.101374000	-0.022702000	-2.242521000
1	3.209734000	0.772791000	-2.825302000
1	-0.299201000	-1.492928000	2.769256000
14	1.072617000	-1.992582000	0.746193000
1	2.621343000	-3.996704000	-2.066082000
1	1.528085000	-4.918609000	1.411340000
6	2.394748000	-3.121312000	-1.440910000
6	0.037765000	-2.401911000	2.258029000
1	-1.705452000	3.708507000	-0.476115000
1	-0.360010000	-3.401514000	-1.479528000
1	0.406143000	-5.003712000	-1.467918000
6	0.174302000	-4.123184000	-0.851929000
1	-0.506389000	-4.450223000	-0.056036000
6	-3.334559000	1.510427000	1.356744000
6	-5.019425000	-0.703177000	-1.241109000
1	-2.501903000	1.256838000	2.026934000
1	1.609110000	2.912243000	1.875646000
6	3.435435000	1.194422000	-1.849523000
1	2.049127000	4.319934000	0.904952000
1	-5.755158000	-0.605985000	-2.034557000
6	3.994228000	2.272051000	0.651723000
6	2.457898000	1.922890000	-1.169428000
6	2.728203000	2.460888000	0.089256000
6	-3.726174000	0.294078000	0.547147000
1	-5.134971000	1.372328000	-0.668158000
1	-2.448882000	2.052153000	-2.165273000
6	-4.679425000	0.404843000	-0.469457000
6	-4.413195000	-1.938475000	-0.998349000
1	1.474639000	2.069703000	-1.606650000

6	-3.139758000	-0.945744000	0.797539000
1	5.951640000	1.408274000	0.424113000
1	-4.177717000	1.831123000	1.977280000
6	-3.477552000	-2.059604000	0.027935000
6	1.699336000	3.282319000	0.843530000
6	4.695853000	1.006051000	-1.282723000
6	4.973983000	1.550635000	-0.027757000
1	-4.672681000	-2.801503000	-1.604733000
1	5.455284000	0.438424000	-1.812776000
1	-2.389127000	-1.033058000	1.580042000
1	4.214190000	2.689231000	1.633221000
1	0.466199000	0.687810000	1.701718000

Table 4 XYZ of diene (163)

6	-1.452723000	0.915878000	2.100989000
6	-0.130886000	1.118350000	2.168437000
6	0.168938000	-0.429584000	0.274453000
8	0.915213000	-0.657634000	-0.914850000
1	0.324570000	-1.282675000	0.958807000
1	1.691351000	-5.149392000	0.552036000
14	-4.471906000	0.057695000	-0.418965000
6	2.300495000	-0.837492000	-0.660380000
6	0.694418000	0.815521000	0.951816000
1	0.352461000	1.557206000	3.036880000
1	-2.124187000	1.175592000	2.914036000
6	-2.061632000	0.348284000	0.878661000
8	2.062367000	0.632823000	1.284176000
1	0.602878000	1.654319000	0.238589000
6	-1.293915000	-0.275552000	-0.034033000
8	-3.407377000	0.506087000	0.824712000
6	2.866532000	0.382301000	0.139923000
6	4.272947000	0.147777000	0.664216000
8	2.793406000	1.463652000	-0.757555000
8	2.508460000	-1.944591000	0.183889000
6	2.953878000	-1.008250000	-2.021470000
1	4.009161000	-1.269626000	-1.904453000
1	2.448809000	-1.807942000	-2.569414000
1	2.869136000	-0.083895000	-2.592700000

1	4.977512000	0.062197000	-0.167556000
1	4.570682000	0.988231000	1.296533000
1	4.299401000	-0.765299000	1.258721000
6	3.240244000	2.723985000	-0.268362000
6	2.053118000	-3.203726000	-0.299722000
1	4.337260000	2.739956000	-0.230958000
6	2.724219000	3.788494000	-1.216467000
1	2.858196000	2.884581000	0.747486000
1	1.630504000	3.780258000	-1.242656000
1	3.058543000	4.778352000	-0.891643000
1	3.095832000	3.611044000	-2.229921000
6	2.018930000	-4.157666000	0.878082000
1	1.056020000	-3.092338000	-0.743770000
1	2.736631000	-3.573335000	-1.075220000
1	3.013056000	-4.249410000	1.325286000
1	1.327010000	-3.795492000	1.644243000
1	-1.688771000	-0.757041000	-0.922800000
6	-6.128318000	0.652487000	0.205821000
1	-6.385822000	0.167874000	1.153492000
1	-6.118140000	1.735248000	0.369032000
1	-6.919611000	0.425409000	-0.517183000
1	-5.311159000	-2.104018000	-1.262718000
1	-3.553992000	-2.187499000	-1.084811000
6	-4.470539000	-1.806120000	-0.624820000
1	-4.595389000	-2.300677000	0.344731000
1	-3.924533000	2.014284000	-1.840847000
6	-3.995616000	0.933552000	-2.005243000
1	-3.039420000	0.589700000	-2.411158000
1	-4.764375000	0.760057000	-2.767487000

Table 5 XYZ of DA product (167)

6	-0.147196000	-3.424440000	-1.893268000
6	-0.493886000	-2.427526000	-0.800396000
8	-1.809777000	-2.573723000	-0.323377000
6	-2.848005000	-2.607170000	-1.296459000
6	-4.163032000	-2.443570000	-0.561020000
6	0.408435000	-2.616177000	0.492282000
6	-0.053251000	-3.774613000	1.359241000

8	1.707337000	-2.816500000	-0.014814000
6	2.756509000	-2.958410000	0.940303000
6	4.061143000	-2.649540000	0.231767000
8	0.384106000	-1.465698000	1.340867000
6	0.697112000	-0.324416000	0.557140000
6	-0.457314000	-0.132498000	-0.405934000
8	-0.337783000	-1.134682000	-1.404558000
6	-0.488516000	1.362447000	-0.837677000
6	-1.051499000	1.998677000	0.443490000
8	-2.219766000	2.687269000	0.383864000
14	-3.744052000	1.940053000	0.350434000
6	-3.947571000	1.059872000	-1.294303000
6	-3.851225000	0.750738000	1.793365000
6	-4.952188000	3.352920000	0.510840000
6	-0.321399000	1.772762000	1.539174000
6	0.977517000	1.029463000	1.259529000
1	-0.334991000	-4.446505000	-1.552594000
1	0.902341000	-3.322690000	-2.164927000
1	-0.760329000	-3.223396000	-2.775182000
1	-2.826900000	-3.566086000	-1.829752000
1	-2.697975000	-1.804512000	-2.029713000
1	-4.179105000	-1.500299000	-0.007068000
1	-4.307310000	-3.262513000	0.149850000
1	-4.996380000	-2.445264000	-1.270488000
1	-1.069564000	-3.599677000	1.709897000
1	0.609936000	-3.858139000	2.224236000
1	-0.019975000	-4.710029000	0.794211000
1	2.761124000	-3.983733000	1.332001000
1	2.594070000	-2.267561000	1.775632000
1	4.204361000	-3.320996000	-0.620015000
1	4.902775000	-2.775019000	0.919509000
1	4.062676000	-1.617978000	-0.133945000
1	1.589956000	-0.571956000	-0.023938000
1	-1.389210000	-0.328703000	0.135421000
1	-0.597327000	2.111844000	2.531219000
1	-3.198039000	0.272696000	-1.436223000
1	-3.851713000	1.770263000	-2.123355000
1	-4.936623000	0.591600000	-1.363061000
1	-4.835225000	0.268027000	1.821821000

1	-3.711029000	1.286579000	2.738940000
1	-3.091445000	-0.037960000	1.740824000
1	-4.809961000	3.882514000	1.458518000
1	-5.984597000	2.987979000	0.476346000
1	-4.819382000	4.071608000	-0.304691000
6	1.678922000	1.756536000	0.110263000
1	-1.124548000	1.543691000	-1.705568000
6	0.930513000	1.883484000	-0.993113000
1	1.623264000	0.919703000	2.131277000
1	1.288820000	2.310217000	-1.923562000
6	3.114574000	2.094190000	0.210409000
8	3.564864000	2.775536000	-0.852962000
8	3.813092000	1.783894000	1.155028000
6	4.966566000	3.104074000	-0.862458000
1	5.716196000	1.093746000	-0.596806000
1	5.480595000	1.573114000	-2.295508000
1	6.854287000	2.212599000	-1.371366000
6	5.802042000	1.918476000	-1.308734000
1	5.042242000	3.934455000	-1.566050000
1	5.254424000	3.446138000	0.134346000

Table 6 XYZ of DA product (175)

6	2.287931000	-0.448919000	1.025161000
6	1.115745000	-1.414523000	1.004397000
6	0.422093000	-1.175802000	-0.365469000
8	-0.664019000	-2.080629000	-0.444049000
6	-0.036646000	0.298339000	-0.449719000
8	0.479202000	0.860025000	-1.641261000
6	0.440876000	1.039082000	0.839395000
6	1.941851000	0.840094000	0.939525000
6	5.374411000	-0.105807000	-0.989542000
1	3.295814000	0.302186000	-1.579613000
1	4.451989000	-2.014005000	-1.546631000
6	4.288775000	0.760292000	-1.646295000
1	4.522983000	0.901794000	-2.711512000
1	6.204609000	-2.115091000	-1.287071000
6	5.194271000	1.293378000	1.795887000
1	4.855805000	2.158178000	1.216060000

1	4.618783000	1.260569000	2.727681000
8	3.508852000	-1.024636000	1.071251000
1	6.245553000	1.462167000	2.057797000
1	6.032268000	-1.660782000	2.697320000
1	5.968630000	-2.610432000	1.203251000
1	0.148984000	2.090167000	0.830722000
1	1.138664000	-1.370925000	-1.176469000
1	1.443971000	-2.450226000	1.096417000
1	-6.700311000	-1.367964000	-0.998355000
1	7.230902000	-1.383199000	1.423318000
14	5.045851000	-0.329345000	0.861212000
1	5.569263000	-1.356836000	-2.755996000
1	4.224588000	1.756499000	-1.190458000
6	5.400774000	-1.479281000	-1.676678000
6	6.177173000	-1.616492000	1.612397000
1	-1.133735000	0.318341000	-0.479220000
1	7.555124000	-0.003095000	-0.719934000
1	6.965254000	0.693387000	-2.235748000
6	6.739353000	0.579198000	-1.166147000
1	6.753480000	1.580566000	-0.718503000
6	-0.100082000	2.114935000	-1.995265000
6	-3.840978000	2.353774000	-1.297734000
1	-5.801606000	-2.341603000	-3.104546000
1	-1.186729000	-2.954493000	-2.228853000
6	-4.753067000	-1.153163000	-0.099896000
1	-1.023338000	-1.192403000	-2.281186000
1	-5.437266000	1.473833000	-2.446638000
6	-3.753659000	-2.235341000	-2.455714000
6	-3.377518000	-1.334994000	-0.253199000
6	-2.867093000	-1.872013000	-1.437011000
6	-1.599633000	2.018909000	-2.158154000
1	-1.465275000	0.892493000	-3.986845000
1	-0.341111000	-1.709578000	2.738748000
6	-2.462366000	2.542054000	-1.192023000
6	-4.366145000	1.637397000	-2.371641000
1	-2.991675000	0.085977000	5.331332000
6	-2.135692000	1.308703000	-3.236915000
1	-4.500771000	2.752551000	-0.532181000
1	-2.696013000	-1.073517000	0.553241000

6	-3.511237000	1.116803000	-3.344323000
6	-1.380747000	-2.031563000	-1.666817000
6	-5.630270000	-1.508791000	-1.122291000
6	-5.125748000	-2.053259000	-2.304116000
1	-2.052374000	3.076180000	-0.336731000
1	-3.363423000	-2.663879000	-3.377302000
1	-3.917594000	0.553430000	-4.179503000
1	0.154955000	2.878812000	-1.248446000
1	0.381800000	2.386520000	-2.938167000
6	0.097705000	-0.999884000	2.045859000
6	-0.255463000	0.287600000	1.955188000
1	-2.825785000	1.711197000	4.619411000
6	-1.348293000	0.930687000	2.713136000
8	-1.769988000	2.044680000	2.469042000
8	-1.840820000	0.148930000	3.685096000
6	-2.983835000	0.652994000	4.399376000
1	-4.380398000	-0.632719000	3.374668000
1	-5.121184000	0.766772000	4.178388000
1	-4.224408000	0.993868000	2.663407000
6	-4.254866000	0.430513000	3.600460000
1	-5.140292000	-0.732579000	0.823949000
1	2.628945000	1.675521000	0.881074000

Table 7 XYZ of DA reaction intermediate

6	-0.670530000	-4.061902000	-1.724950000
6	-0.550606000	-3.234987000	-0.457229000
8	-1.422779000	-3.653312000	0.562047000
6	-2.806031000	-3.704879000	0.227888000
6	-3.583609000	-3.813391000	1.524668000
6	0.874764000	-3.301013000	0.181184000
6	1.201441000	-4.653687000	0.786896000
8	1.741222000	-2.934658000	-0.854859000
6	3.129890000	-2.834123000	-0.535378000
6	3.779427000	-1.994400000	-1.616876000
8	0.953334000	-2.363272000	1.254247000
6	0.692567000	-1.049307000	0.796288000
6	-0.710026000	-0.977691000	0.219636000
8	-0.845553000	-1.894923000	-0.841847000

6	-0.982737000	0.445679000	-0.280478000
6	-0.781304000	1.388558000	0.849020000
8	-1.387746000	2.510623000	0.918045000
14	-2.615193000	3.336383000	-0.046533000
6	-2.160498000	3.300729000	-1.848223000
6	-4.204970000	2.448148000	0.360856000
6	-2.522527000	5.042444000	0.686070000
6	0.140383000	1.093658000	1.913364000
6	0.837745000	-0.065209000	1.899482000
1	-0.597143000	-5.126992000	-1.489037000
1	0.122571000	-3.785982000	-2.420065000
1	-1.636226000	-3.868432000	-2.198960000
1	-3.001407000	-4.574197000	-0.412980000
1	-3.087686000	-2.799598000	-0.325080000
1	-3.397123000	-2.941064000	2.158327000
1	-3.285487000	-4.710133000	2.075524000
1	-4.656452000	-3.872737000	1.318516000
1	0.436135000	-4.934430000	1.511123000
1	2.167344000	-4.598301000	1.295747000
1	1.258304000	-5.412128000	0.001739000
1	3.568110000	-3.839872000	-0.493490000
1	3.250397000	-2.361325000	0.447273000
1	3.626991000	-2.452082000	-2.598971000
1	4.855163000	-1.914411000	-1.432114000
1	3.352558000	-0.986511000	-1.620001000
1	1.422457000	-0.775196000	0.017666000
1	-1.423263000	-1.236470000	1.018345000
1	0.272483000	1.844416000	2.685169000
1	-2.369623000	2.336837000	-2.320831000
1	-1.099876000	3.525992000	-1.996337000
1	-2.754352000	4.067266000	-2.361360000
1	-5.045462000	2.972337000	-0.108240000
1	-4.378383000	2.433678000	1.441643000
1	-4.212938000	1.416458000	-0.005246000
1	-2.711157000	5.020990000	1.763964000
1	-3.266921000	5.698006000	0.221473000
1	-1.533000000	5.479556000	0.516654000
6	1.151575000	1.357458000	-1.504642000
1	-2.025421000	0.516127000	-0.615205000

6	-0.069815000	0.845864000	-1.501620000
1	1.555849000	-0.288783000	2.685566000
1	-0.604380000	0.620355000	-2.426891000
6	2.001627000	1.725721000	-0.434207000
8	1.715000000	2.988691000	0.051329000
8	2.955872000	1.083453000	0.021460000
6	2.629345000	3.524245000	1.009109000
1	4.414711000	3.309687000	-0.181451000
1	3.584945000	4.870235000	-0.384043000
1	4.526917000	4.548575000	1.087695000
6	3.866230000	4.098703000	0.339070000
1	2.063798000	4.304976000	1.525947000
1	2.901192000	2.745141000	1.728287000

Table 8 XYZ of transition state (163 → intermediate)

6	-0.564024000	-3.934769000	-1.746303000
6	-0.527152000	-3.111867000	-0.470542000
8	-1.444218000	-3.560383000	0.497061000
6	-2.810164000	-3.614954000	0.099772000
6	-3.645057000	-3.742148000	1.358876000
6	0.865726000	-3.156700000	0.246611000
6	1.153651000	-4.493296000	0.907573000
8	1.784998000	-2.834450000	-0.762318000
6	3.150615000	-2.682590000	-0.377381000
6	3.881797000	-2.088833000	-1.563678000
8	0.902615000	-2.190431000	1.293924000
6	0.635817000	-0.888664000	0.790773000
6	-0.766429000	-0.875030000	0.225642000
8	-0.835719000	-1.776538000	-0.863121000
6	-1.176617000	0.526879000	-0.182487000
6	-1.013567000	1.468200000	0.851428000
8	-1.644893000	2.620909000	0.920955000
14	-3.001812000	3.224961000	0.039732000
6	-2.590882000	3.281606000	-1.782586000
6	-4.456814000	2.114771000	0.423963000
6	-3.206610000	4.929094000	0.761975000
6	0.008515000	1.260670000	1.859271000
6	0.781528000	0.154849000	1.848658000

1	-0.456138000	-4.997589000	-1.513153000
1	0.242556000	-3.623625000	-2.409868000
1	-1.518969000	-3.777873000	-2.254581000
1	-2.971848000	-4.477970000	-0.558934000
1	-3.072078000	-2.704762000	-0.454689000
1	-3.493956000	-2.874712000	2.008468000
1	-3.365208000	-4.642116000	1.914101000
1	-4.707065000	-3.807118000	1.103827000
1	0.349896000	-4.748580000	1.598342000
1	2.090904000	-4.427045000	1.465766000
1	1.246572000	-5.275417000	0.149430000
1	3.569767000	-3.659860000	-0.104588000
1	3.220361000	-2.016178000	0.491045000
1	3.799688000	-2.746580000	-2.434414000
1	4.941101000	-1.957303000	-1.322385000
1	3.460514000	-1.109485000	-1.806245000
1	1.360735000	-0.670915000	-0.005655000
1	-1.452084000	-1.224722000	1.014768000
1	0.149852000	2.049508000	2.591368000
1	-2.715397000	2.312545000	-2.276521000
1	-1.561126000	3.618234000	-1.942740000
1	-3.261255000	3.993644000	-2.278374000
1	-5.360354000	2.515900000	-0.049531000
1	-4.634632000	2.070394000	1.503580000
1	-4.317645000	1.092429000	0.057911000
1	-3.360549000	4.879904000	1.844714000
1	-4.071819000	5.432787000	0.317399000
1	-2.320742000	5.542891000	0.569177000
6	1.229577000	1.476594000	-1.334655000
1	-2.117764000	0.570448000	-0.729709000
6	0.022888000	1.122474000	-1.502837000
1	1.578321000	0.026151000	2.578046000
1	-0.627598000	1.038940000	-2.364067000
6	2.305911000	1.694308000	-0.430590000
8	2.309963000	2.964785000	0.057728000
8	3.175441000	0.875534000	-0.143889000
6	3.380259000	3.295329000	0.951920000
1	5.011965000	2.766164000	-0.360545000
1	4.472960000	4.456442000	-0.503241000

1	5.432591000	3.944497000	0.900250000
6	4.653216000	3.634946000	0.196401000
1	3.010435000	4.158474000	1.509836000
1	3.539573000	2.462831000	1.643514000

Table 9 XYZ of transition state (intermediate → 167)

6	-0.448966000	-3.814654000	-1.736592000
6	-0.488402000	-2.929769000	-0.503680000
8	-1.508179000	-3.292823000	0.395526000
6	-2.836199000	-3.301093000	-0.118454000
6	-3.783683000	-3.278162000	1.065072000
6	0.836918000	-2.999143000	0.342333000
6	0.964774000	-4.292211000	1.129827000
8	1.858221000	-2.832756000	-0.604887000
6	3.194358000	-2.729616000	-0.113850000
6	4.077091000	-2.382714000	-1.294689000
8	0.870019000	-1.952939000	1.313658000
6	0.709089000	-0.685739000	0.674360000
6	-0.674130000	-0.672854000	0.075717000
8	-0.713537000	-1.603624000	-0.986959000
6	-1.082047000	0.739896000	-0.329837000
6	-1.142912000	1.560221000	0.872347000
8	-1.984065000	2.557960000	1.029878000
14	-3.427627000	2.960412000	0.167926000
6	-2.991582000	3.349908000	-1.608130000
6	-4.599430000	1.513108000	0.341009000
6	-4.023663000	4.467843000	1.082789000
6	-0.105504000	1.407066000	1.825252000
6	0.857164000	0.452994000	1.638352000
1	-0.377229000	-4.865935000	-1.444908000
1	0.408023000	-3.549960000	-2.355093000
1	-1.363050000	-3.668974000	-2.318149000
1	-2.994274000	-4.203698000	-0.722600000
1	-2.990990000	-2.424902000	-0.760688000
1	-3.638659000	-2.368019000	1.655258000
1	-3.608097000	-4.141537000	1.713348000
1	-4.821403000	-3.308395000	0.719371000
1	0.096602000	-4.423528000	1.775370000

1	1.862548000	-4.250667000	1.751159000
1	1.044002000	-5.142695000	0.447438000
1	3.498590000	-3.682840000	0.337220000
1	3.249256000	-1.944723000	0.649934000
1	4.008261000	-3.155112000	-2.066997000
1	5.119385000	-2.304915000	-0.969963000
1	3.774083000	-1.419243000	-1.711807000
1	1.477149000	-0.613916000	-0.101773000
1	-1.376687000	-1.006237000	0.853202000
1	-0.011221000	2.157398000	2.603976000
1	-2.837132000	2.454772000	-2.219063000
1	-2.085131000	3.962737000	-1.660464000
1	-3.808697000	3.922511000	-2.062611000
1	-5.562605000	1.759901000	-0.120195000
1	-4.780513000	1.291301000	1.398169000
1	-4.226992000	0.602171000	-0.139330000
1	-4.192486000	4.243370000	2.140782000
1	-4.966377000	4.827147000	0.655965000
1	-3.290784000	5.278495000	1.016868000
6	1.279237000	1.641991000	-0.938159000
1	-2.013184000	0.728712000	-0.899174000
6	0.044913000	1.471962000	-1.262932000
1	1.740570000	0.446543000	2.274657000
1	-0.421149000	1.792649000	-2.195040000
6	2.547479000	1.657402000	-0.354432000
8	2.835919000	2.852794000	0.252389000
8	3.362509000	0.725586000	-0.393051000
6	4.149306000	2.972770000	0.808351000
1	5.253087000	2.500587000	-0.985684000
1	4.897789000	4.232391000	-0.778039000
1	6.159941000	3.459488000	0.203564000
6	5.177640000	3.311674000	-0.257192000
1	4.062068000	3.779015000	1.540670000
1	4.410720000	2.046217000	1.326853000

Table 10 XYZ of transition state (176 → 175)

6	2.049029000	-0.481791000	0.980829000
6	1.203284000	-1.338541000	0.298276000

6	0.247475000	-0.770288000	-0.717334000
8	-0.744419000	-1.745700000	-0.971670000
6	-0.350187000	0.590757000	-0.297636000
8	-0.146835000	1.496527000	-1.387210000
6	0.310014000	1.164787000	0.935621000
6	1.569289000	0.806678000	1.326511000
6	5.128326000	-0.460309000	-0.600828000
1	3.315587000	0.609583000	-1.244011000
1	3.601446000	-1.945065000	-1.109268000
6	4.404960000	0.661038000	-1.363473000
1	4.622829000	0.580822000	-2.438035000
1	5.154050000	-2.657383000	-0.635022000
6	4.920621000	1.380102000	1.893472000
1	4.291814000	2.088168000	1.344249000
1	4.653516000	1.433607000	2.954860000
8	3.187039000	-0.967065000	1.542499000
1	5.960530000	1.714241000	1.795243000
1	5.477968000	-1.591618000	3.281540000
1	5.823155000	-2.553445000	1.834750000
1	-0.137485000	2.067229000	1.348140000
1	0.818915000	-0.587841000	-1.644147000
1	1.554125000	-2.348195000	0.096197000
1	-6.776780000	-2.408310000	-1.094475000
1	6.873359000	-1.190290000	2.266293000
14	4.757084000	-0.377946000	1.256668000
1	4.976835000	-1.895291000	-2.224267000
1	4.732093000	1.654154000	-1.034123000
6	4.688366000	-1.818473000	-1.166347000
6	5.835216000	-1.539165000	2.247477000
1	-1.428572000	0.465173000	-0.129476000
1	7.206366000	-1.119364000	-0.334125000
1	6.884134000	-0.303093000	-1.871928000
6	6.645326000	-0.300066000	-0.799133000
1	7.018059000	0.645033000	-0.384233000
6	-1.098087000	2.560329000	-1.441463000
6	-4.715550000	1.362952000	-1.660480000
1	-5.884142000	-2.646473000	-3.403033000
1	-1.205303000	-2.076472000	-2.955563000
6	-4.860177000	-1.888815000	-0.252230000

1	-1.474906000	-0.420398000	-2.387643000
1	-5.794474000	0.796182000	-3.433838000
6	-3.867574000	-2.152549000	-2.837027000
6	-3.507044000	-1.667248000	-0.504122000
6	-3.002837000	-1.792181000	-1.801200000
6	-2.431257000	2.106521000	-1.989024000
1	-1.748198000	2.125211000	-4.031600000
1	-0.162762000	-2.742389000	1.802258000
6	-3.505353000	1.828551000	-1.141042000
6	-4.857455000	1.170342000	-3.031350000
1	-1.476532000	2.251616000	5.286042000
6	-2.583995000	1.912474000	-3.367648000
1	-5.538442000	1.134445000	-0.989578000
1	-2.836904000	-1.394097000	0.306928000
6	-3.787394000	1.444926000	-3.887533000
6	-1.557765000	-1.477983000	-2.103981000
6	-5.722559000	-2.235530000	-1.292440000
6	-5.221596000	-2.369150000	-2.587623000
1	-3.391367000	1.956031000	-0.065899000
1	-3.479696000	-2.257073000	-3.848658000
1	-3.894616000	1.295518000	-4.958363000
1	-1.227801000	3.009070000	-0.447609000
1	-0.647712000	3.310104000	-2.097414000
6	-0.259399000	-1.671962000	1.796584000
6	-0.825966000	-0.639550000	2.178546000
1	-2.402564000	2.541269000	3.791189000
6	-1.704179000	0.364923000	2.710206000
8	-2.674047000	0.807218000	2.116908000
8	-1.318478000	0.782352000	3.927053000
6	-2.134691000	1.796277000	4.544439000
1	-3.076831000	0.428969000	5.922820000
1	-3.932140000	1.969454000	5.708819000
1	-4.012987000	0.732508000	4.438910000
6	-3.365482000	1.189164000	5.191423000
1	-5.241426000	-1.784362000	0.760104000
1	2.103153000	1.381165000	2.078251000