Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

The 9-Homocubyl Cation Rearrangement

Revised.

Level: CCSD(T)/def2-TZVP/MP2/def2-TZVP

Isomerization of 9-homocubyl cation, 1 to 5.

1 G = -347.1415942 a.u.

C	1.529877000	0.000012000	0.217512000
C	0.555433000	-1.113411000	0.710310000
C	-0.450220000	0.000034000	1.204326000
C	0.555426000	1.113448000	0.710258000
H	2.610976000	0.000013000	0.322831000
H	0.755361000	-1.953486000	1.371334000
H	-1.009905000	0.000042000	2.134098000
H	0.755354000	1.953563000	1.371231000
C	0.758719000	-0.000028000	-1.149426000
C	-0.072116000	-1.242990000	-0.699312000
C	-1.391204000	-0.695341000	-0.223942000
C	-0.072127000	1.242953000	-0.699366000
H	1.232286000	-0.000046000	-2.126767000
H	-0.049612000	-2.165319000	-1.270388000
H	-2.190160000	-1.300307000	0.194816000
H	-0.049637000	2.165252000	-1.270489000
C	-1.391205000	0.695322000	-0.223938000
H	-2.190169000	1.300293000	0.194799000

TS_{1-3} G = -347.1349366 a.u.

C	-1.542659000	-0.000105000	-0.344651000

C	-0.837018000	1.088231000	0.539917000
C	-0.281357000	0.000224000	1.376735000
C	-0.836920000	-1.088105000	0.540251000
H	-2.587998000	-0.000198000	-0.633101000
H	-1.243263000	1.985849000	1.002685000
H	0.158602000	0.000399000	2.372442000
H	-1.243120000	-1.985582000	1.003334000
C	-0.305597000	-0.000213000	-1.297786000
C	0.313838000	1.201518000	-0.546055000
C	1.580349000	0.679240000	0.099764000
C	0.313916000	-1.201679000	-0.545692000
H	-0.324866000	-0.000372000	-2.384673000
H	0.347500000	2.166859000	-1.045273000
H	2.317857000	1.300087000	0.597096000
H	0.347631000	-2.167167000	-1.044620000
C	1.580399000	-0.679127000	0.099957000
H	2.317951000	-1.299776000	0.597473000

3 G = -347.1901895 a.u.

C	1.390107000	0.000369000	-1.204728000
C	1.298269000	-1.008306000	-0.239481000
C	1.176046000	-0.000368000	0.887463000
C	1.297634000	1.008503000	-0.238767000
H	1.460836000	0.000715000	-2.285312000
H	1.495304000	-2.074402000	-0.257597000
H	1.859286000	-0.000446000	1.733329000
H	1.495035000	2.074544000	-0.256111000
C	-1.570845000	0.703875000	-0.653321000
C	-1.571084000	-0.703327000	-0.653717000
C	-0.840147000	-1.162387000	0.439129000
C	-0.839619000	1.162103000	0.439738000
H	-2.031792000	1.332926000	-1.405243000
H	-2.032286000	-1.331795000	-1.405961000
H	-0.757904000	-2.194366000	0.757538000
H	-0.757589000	2.193807000	0.759089000
C	-0.362246000	-0.000505000	1.234099000
H	-0.599582000	-0.000731000	2.297779000

TS_{3-4} G = -347.1791743 a.u.

C	1.179784000	0.738604000	0.542353000
C	1.058191000	0.550056000	-0.951460000
C	1.222349000	-0.849926000	-0.895719000
C	1.915392000	-0.531145000	0.265736000

H	1.705817000	1.601957000	0.943219000
H	1.283380000	1.234521000	-1.763476000
H	1.236343000	-1.661657000	-1.607468000
H	2.852787000	-0.918560000	0.661477000
C	-0.719089000	-0.856049000	0.983470000
C	-0.301667000	0.572310000	1.023786000
C	-1.073120000	1.179296000	-0.123041000
C	-1.589374000	-1.051386000	-0.049054000
H	-0.397442000	-1.603021000	1.698767000
H	-0.461021000	1.046085000	1.995376000
H	-1.064377000	2.233697000	-0.370529000
H	-2.063560000	-1.989692000	-0.307151000
C	-1.802295000	0.201479000	-0.736720000
H	-2.432963000	0.337242000	-1.606326000

4 G = -347.1965766 a.u.

C	1.021116000	-1.076204000	0.033120000
C	1.223358000	-0.000077000	1.057436000
C	1.020942000	1.076271000	0.033462000
C	2.034020000	0.000144000	-0.193696000
H	1.320940000	-2.099392000	0.224047000
H	1.504859000	-0.000261000	2.096613000
H	1.320525000	2.099494000	0.224567000
H	3.097594000	0.000261000	-0.364363000
C	-0.253986000	0.765687000	-0.799264000
C	-0.253890000	-0.765648000	-0.799314000
C	-1.414050000	-1.118362000	0.027291000
C	-1.414246000	1.118269000	0.027162000
H	-0.228415000	1.252039000	-1.777495000
H	-0.228606000	-1.251852000	-1.777634000
H	-1.690117000	-2.142803000	0.264581000
H	-1.690553000	2.142679000	0.264310000
C	-2.050883000	-0.000087000	0.547798000
H	-2.880509000	-0.000113000	1.241401000

TS_{4-5} G = -347.1741435 a.u.

C	0.855064000	-0.888324000	0.158698000
C	1.153486000	0.384497000	0.936918000
C	2.197688000	0.827478000	0.123182000
C	2.241327000	-0.489081000	-0.299159000
H	0.817020000	-1.834363000	0.700350000
H	0.946264000	0.629522000	1.977846000
H	2.856138000	1.682929000	0.105472000
H	3.091646000	-1.116489000	-0.559082000

C	-0.597752000	0.842956000	-0.807575000
C	-0.379720000	-0.642469000	-0.723983000
C	-1.549258000	-1.108251000	0.099364000
C	-1.702419000	1.165887000	-0.079276000
H	-0.005102000	1.529275000	-1.397739000
H	-0.302338000	-1.146858000	-1.691963000
H	-1.717900000	-2.145151000	0.359456000
H	-2.097343000	2.165687000	0.050025000
C	-2.287948000	-0.041857000	0.483310000
H	-3.171194000	-0.069569000	1.106755000

5 G = -347.1915609 a.u.

C	-0.778881000	-0.771788000	-0.536322000
C	-0.778831000	0.771401000	-0.536792000
C	-2.189096000	0.672105000	-0.000473000
C	-2.189191000	-0.671810000	-0.000047000
H	-0.550117000	-1.393493000	-1.399551000
H	-0.549537000	1.392729000	-1.400145000
H	-2.893280000	1.439112000	0.295704000
H	-2.893527000	-1.438517000	0.296565000
C	0.297516000	0.763631000	0.684631000
C	0.297538000	-0.763884000	0.684428000
C	1.548773000	-1.121975000	0.057232000
C	1.548561000	1.122126000	0.057672000
H	-0.040178000	1.346509000	1.538881000
H	-0.039382000	-1.346789000	1.538992000
H	1.826944000	-2.146817000	-0.172060000
H	1.826643000	2.147089000	-0.171196000
C	2.264591000	0.000163000	-0.346303000
H	3.186564000	0.000363000	-0.911353000

Isomerization of 9-homocubyl cation

$TS_{1\text{-}1}$ G = -347.1353837 a.u.

C	-0.863174000	-0.958225000	0.780991000
C	-0.863174000	-0.958225000	-0.780991000
C	-0.874434000	0.600898000	-0.810558000
C	-0.874434000	0.600898000	0.810558000
H	-1.469546000	-1.552730000	1.460255000
H	-1.469546000	-1.552730000	-1.460255000
H	-1.539478000	1.278177000	-1.336712000

H	-1.539478000	1.278177000	1.336712000
C	0.697089000	-0.922746000	0.784754000
C	0.697089000	-0.922746000	-0.784754000
C	0.697089000	0.561258000	-1.191338000
C	0.697089000	0.561258000	1.191338000
H	1.321973000	-1.631667000	1.319180000
H	1.321973000	-1.631667000	-1.319180000
H	0.967711000	0.943276000	-2.167997000
H1	0.967711000	0.943276000	2.167997000
C	0.810983000	1.352622000	0.000000000
H	0.693958000	2.435935000	0.000000000

$TS_{1\text{-}1'}$ G = -347.1238723 a.u.

C	0.000000000	0.779162000	-1.352924000
C	0.000000000	-0.779162000	-1.352924000
C	-1.064894000	-0.786826000	-0.221079000
C	-1.064894000	0.786826000	-0.221079000
C	1.064894000	0.786826000	-0.221079000
C	1.064894000	-0.786826000	-0.221079000
H	0.000000000	-1.441677000	-2.211882000
H	0.000000000	1.441677000	-2.211882000
H	2.002061000	-1.338328000	-0.228612000
H	2.002061000	1.338328000	-0.228612000
H	-2.002061000	1.338328000	-0.228612000
H	-2.002061000	-1.338328000	-0.228612000
C	0.000000000	1.158108000	0.904644000
C	0.000000000	-1.158108000	0.904644000
H	0.000000000	0.000000000	2.844149000
C	0.000000000	0.000000000	1.753095000
H	0.000000000	2.155159000	1.330372000
H	0.000000000	-2.155159000	1.330372000

$TS_{1\text{-}2}$ G = -347.1267805 a.u.

C	-0.675830000	0.576168000	1.245813000
C	-0.746802000	-0.898750000	0.788272000
C	-0.746802000	-0.898750000	-0.788272000
C	-0.675830000	0.576168000	-1.245813000
H	-1.134062000	1.037360000	2.112703000
H	-1.374216000	-1.607228000	1.319870000
H	-1.374216000	-1.607228000	-1.319870000
C	0.817429000	0.563459000	0.974100000
C	0.817429000	-0.963747000	0.766115000
C	0.817429000	-0.963747000	-0.766115000
C	0.817429000	0.563459000	-0.974100000

H	1.566500000	1.261056000	1.331157000
H	1.413152000	-1.583308000	1.432684000
H	1.413152000	-1.583308000	-1.432684000
H	1.566500000	1.261056000	-1.331157000
H	-1.134062000	1.037360000	-2.112703000
C	-0.526843000	1.341504000	0.000000000
H	-0.328400000	2.409657000	0.000000000

2 G = -347.1432428 a.u.

C	0.723920000	1.246987000	0.553439000
C	0.785870000	0.776272000	-0.902255000
C	0.785870000	-0.776272000	-0.902255000
C	0.723920000	-1.246987000	0.553439000
H	1.448078000	1.747928000	1.187197000
H	1.379342000	1.351547000	-1.607560000
H	1.379342000	-1.351547000	-1.607560000
C	-0.723920000	1.246987000	0.553439000
C	-0.785870000	0.776272000	-0.902255000
C	-0.785870000	-0.776272000	-0.902255000
C	-0.723920000	-1.246987000	0.553439000
H	-1.448078000	1.747928000	1.187197000
H	-1.379342000	1.351547000	-1.607560000
H	-1.379342000	-1.351547000	-1.607560000
H	-1.448078000	-1.747928000	1.187197000
H	1.448078000	-1.747928000	1.187197000
C	0.000000000	0.000000000	1.281721000
H	0.000000000	0.000000000	2.362715000

Automerization of 3

TS_{3-3} G = -347.1881865 a.u.

C	-1.415223000	-0.680791000	-0.888764000
C	-1.415219000	0.680798000	-0.888761000
C	-1.131282000	0.754013000	0.567479000
C	-1.131286000	-0.754014000	0.567474000
H	-1.548373000	-1.437096000	-1.652962000
H	-1.548364000	1.437107000	-1.652955000
H	-1.640128000	1.393542000	1.282738000
H	-1.640129000	-1.393548000	1.282731000
C	1.228756000	-1.131465000	-0.206463000
C	1.583181000	-0.000003000	-0.942332000

C	1.228761000	1.131462000	-0.206464000
C	0.556409000	-0.748497000	0.993163000
H	1.346582000	-2.156881000	-0.541577000
H	2.039628000	-0.000004000	-1.923000000
H	1.346592000	2.156877000	-0.541579000
H	0.640577000	-1.325938000	1.907823000
C	0.556409000	0.748498000	0.993162000
H	0.640584000	1.325939000	1.907821000