

Supporting Information

The Cubyl Cation Rearrangements

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Cartesian Coordinates for all optimized structures computed at the MP2/def2-TZVP level.

1

C	1.146536000	0.661953000	-0.497732000
C	0.000000000	1.296992000	0.377236000
C	-1.146536000	0.661953000	-0.497732000
C	0.000000000	0.000000000	-1.192436000
H	2.038310000	1.176819000	-0.836925000
H	0.000000000	2.342797000	0.670746000
H	-2.038310000	1.176819000	-0.836925000
C	1.123228000	-0.648496000	0.377236000
C	0.000000000	0.000000000	1.248176000
C	-1.123228000	-0.648496000	0.377236000
C	0.000000000	-1.323906000	-0.497732000
H	2.028922000	-1.171398000	0.670746000
H	0.000000000	0.000000000	2.333012000
H	-2.028922000	-1.171398000	0.670746000
H	0.000000000	-2.353637000	-0.836925000

TS₁₋₂

C	-1.288938000	0.140139000	-0.755289000
C	-0.178809000	-1.279454000	-0.106395000
C	1.026533000	-0.654744000	-0.725994000
C	0.120911000	0.528713000	-1.102788000
H	-2.149344000	0.004521000	-1.405777000
H	-0.730684000	-2.195907000	-0.293747000
H	1.759597000	-1.132961000	-1.365562000
C	-1.289885000	0.349992000	0.668454000
C	-0.066467000	-0.455664000	1.156638000
C	1.273960000	0.202073000	0.604413000
C	0.564784000	1.355577000	-0.046991000
H	-2.183101000	0.505306000	1.279180000
H	-0.112705000	-0.894462000	2.150523000
H	2.183946000	0.247548000	1.198745000
H	0.259762000	2.346152000	0.284354000

2

C	-0.509930000	1.357680000	0.168829000
C	1.358018000	-0.212038000	0.518917000
C	0.033459000	-0.843830000	0.943673000
C	-1.016773000	0.223936000	0.827820000
H	-1.089497000	2.210517000	-0.169760000
H	2.326071000	-0.286128000	0.992960000
H	-0.066057000	-1.654042000	1.657610000
C	0.870367000	1.055352000	-0.193804000
C	0.940848000	-0.311288000	-0.907309000

C	-0.379533000	-1.089391000	-0.586727000
C	-1.537819000	-0.150189000	-0.442718000
H	1.572167000	1.811511000	-0.517685000
H	1.508821000	-0.394690000	-1.823842000
H	-0.485281000	-2.085705000	-1.010294000
H	-2.318040000	0.217145000	-1.101085000

TS_{2,3}

C	0.042681000	1.459967000	-0.226335000
C	1.303436000	-0.420019000	0.592875000
C	-0.030820000	-0.345888000	1.218202000
C	-0.770372000	0.754109000	0.660339000
H	-0.315151000	2.251480000	-0.876768000
H	2.221318000	-0.806012000	1.010893000
H	-0.448055000	-1.055391000	1.924865000
C	1.214789000	0.657975000	-0.459935000
C	0.690503000	-0.818926000	-0.722332000
C	-0.855554000	-1.004017000	-0.564873000
C	-1.718447000	0.040473000	-0.208763000
H	2.070980000	0.946647000	-1.053636000
H	1.214228000	-1.445936000	-1.437579000
H	-1.225943000	-1.982407000	-0.874986000
H	-2.774664000	0.149570000	-0.427865000

3

C	-0.756218000	0.296596000	1.142253000
C	-0.756218000	-1.072533000	-0.735164000
C	-0.756218000	0.296596000	-1.142253000
C	-0.519498000	1.091614000	0.000000000
H	-0.546330000	0.632473000	2.152718000
H	-0.947757000	-1.948268000	-1.339165000
H	-0.546330000	0.632473000	-2.152718000
C	-0.756218000	-1.072533000	0.735164000
C	0.699469000	-1.013108000	0.000000000
C	1.535722000	0.291568000	0.000000000
C	0.927977000	1.506225000	0.000000000
H	-0.947757000	-1.948268000	1.339165000
H	1.255342000	-1.951779000	0.000000000
H	2.614116000	0.160571000	0.000000000
H	1.405924000	2.476252000	0.000000000

TS_{3,4}

C	0.241083000	-0.003266000	1.323190000
C	1.291640000	-0.410547000	-0.682574000
C	0.220219000	-1.336021000	-0.545326000
C	-0.553869000	-0.902165000	0.545053000
H	-0.131608000	0.541991000	2.184118000
H	2.035835000	-0.362967000	-1.465561000

H	-0.186572000	-1.919079000	-1.363889000
C	1.365342000	0.380556000	0.544959000
C	0.350141000	1.072651000	-0.493007000
C	-1.175442000	0.934826000	-0.482691000
C	-1.764030000	-0.159123000	0.070349000
H	2.209557000	0.987219000	0.842569000
H	0.750796000	2.004190000	-0.900502000
H	-1.719057000	1.718509000	-1.002226000
H	-2.809463000	-0.431331000	0.025775000

4

C	0.768418000	-0.551041000	0.000000000
C	-0.341981000	-0.079541000	2.012667000
C	-0.341981000	1.120496000	1.242707000
C	0.217984000	0.833371000	0.000000000
H	1.871066000	-0.543823000	0.000000000
H	-0.767333000	-0.178830000	3.002909000
H	-0.849528000	2.039977000	1.514044000
C	0.239539000	-1.094932000	1.286410000
C	0.239539000	-1.094932000	-1.286410000
C	-0.341981000	-0.079541000	-2.012667000
C	-0.341981000	1.120496000	-1.242707000
H	0.388654000	-2.112366000	1.627576000
H	0.388654000	-2.112366000	-1.627576000
H	-0.767333000	-0.178830000	-3.002909000
H	-0.849528000	2.039977000	-1.514044000

TS₁₋₁

C	0.000000000	0.745468000	0.959312000
C	1.227370000	0.772308000	0.062775000
C	1.227370000	-0.772308000	0.062775000
C	0.000000000	-0.745468000	0.959312000
H	0.000000000	0.000000000	2.045079000
H	2.036731000	1.494215000	0.045878000
H	2.036731000	-1.494215000	0.045878000
C	-1.227370000	0.772308000	0.062775000
C	0.000000000	0.757536000	-0.968789000
C	0.000000000	-0.757536000	-0.968789000
C	-1.227370000	-0.772308000	0.062775000
H	-2.036731000	1.494215000	0.045878000
H	0.000000000	1.441902000	-1.810737000
H	0.000000000	-1.441902000	-1.810737000
H	-2.036731000	-1.494215000	0.045878000

TS_{4,4}

C	-0.723771000	0.005072000	-0.310466000
C	-0.026682000	-2.127951000	0.166574000
C	1.132994000	-1.358201000	0.000289000
C	0.737853000	-0.016173000	-0.300937000
H	0.014219000	-0.010225000	-1.416604000
H	-0.043246000	-3.193811000	0.351044000
H	2.152029000	-1.718780000	0.071628000
C	-1.161344000	-1.325307000	-0.015625000
C	-1.122171000	1.349858000	-0.026137000
C	0.035433000	2.120748000	0.149068000
C	1.172165000	1.316346000	-0.011194000
H	-2.191204000	-1.656479000	0.041320000
H	-2.141917000	1.711352000	0.028479000
H	0.049868000	3.188132000	0.324700000
H	2.201310000	1.647670000	0.056736000

TS_{1,2'}

H	2.381201000	-0.952550000	-0.909084000
C	1.570438000	-0.523572000	-0.327337000
C	-0.396767000	-0.521238000	-0.902941000
H	1.773474000	1.728837000	0.121163000
H	-0.423021000	1.630705000	-1.587947000
C	1.119165000	0.869581000	0.024629000
C	-0.194593000	0.938638000	-0.783969000
C	0.512110000	-1.091808000	0.430545000
C	-1.619468000	-0.660128000	-0.249485000
H	0.308334000	-2.125256000	0.691800000
H	-2.184147000	-1.519448000	0.092431000
C	0.168308000	0.259983000	1.150457000
C	-1.213642000	0.644687000	0.413531000
H	0.381410000	0.382298000	2.211041000
H	-1.910555000	1.358558000	0.848002000

2'

H	2.103551000	0.133227000	-1.731476000
C	1.584921000	0.003611000	-0.789900000
C	-1.341201000	0.252893000	-0.815826000
H	1.378142000	1.865806000	0.483753000
H	-1.121947000	2.163483000	0.154755000
C	0.872625000	0.983135000	0.100798000
C	-0.635910000	1.247635000	-0.175308000
C	1.327475000	-1.055952000	0.007152000
C	-1.558594000	-0.962640000	-0.415156000
H	1.565414000	-2.111317000	-0.044112000
H	-1.889034000	-1.949332000	-0.690568000
C	0.553995000	-0.239683000	1.008450000
C	-0.994790000	-0.222072000	0.780632000

H	0.809770000	-0.220141000	2.066071000
H	-1.697028000	0.076710000	1.556525000