

Supporting Information

Substituent Effects on the Selectivity of the Ambimodal [6+4]/[4+2] Cycloaddition

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III. xTB_md.inp, Fetch distance data.py

I.

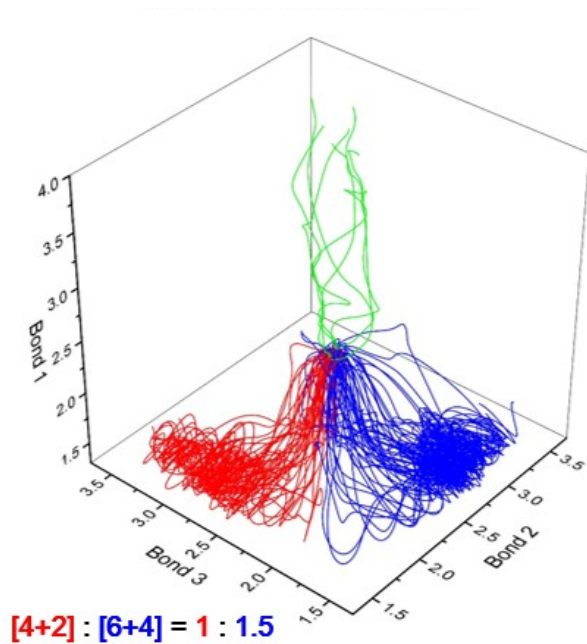


Figure S1. Trajectories distribution chart of **R1a**

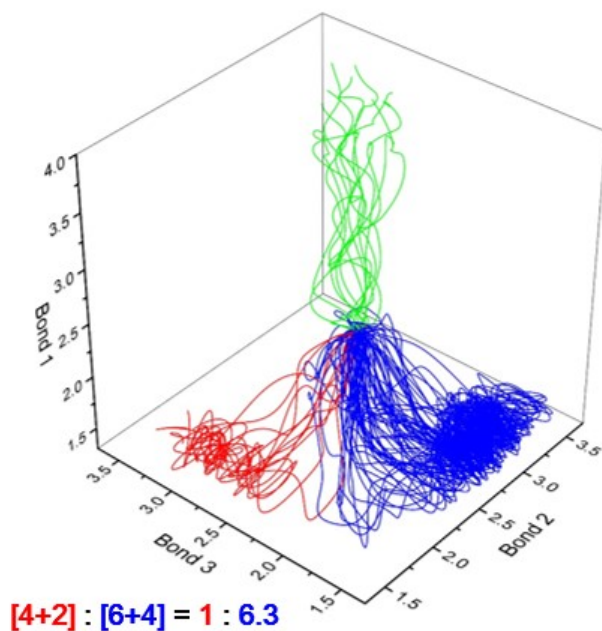


Figure S2. Trajectories distribution chart of **R1c**

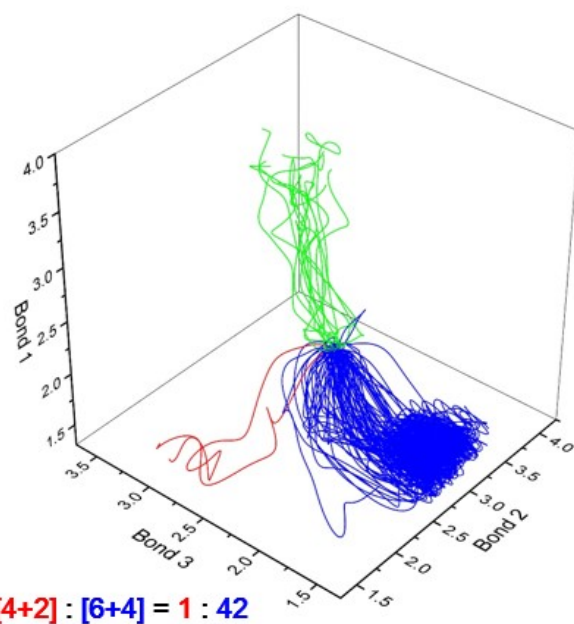


Figure S3. Trajectories distribution chart of **R2c**

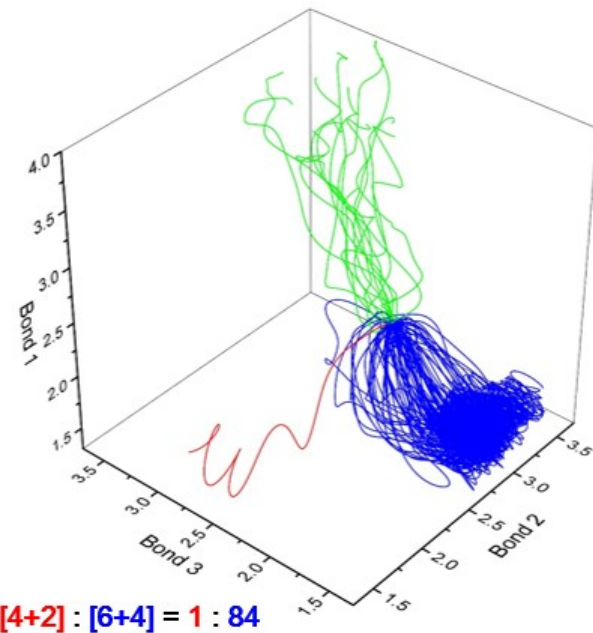
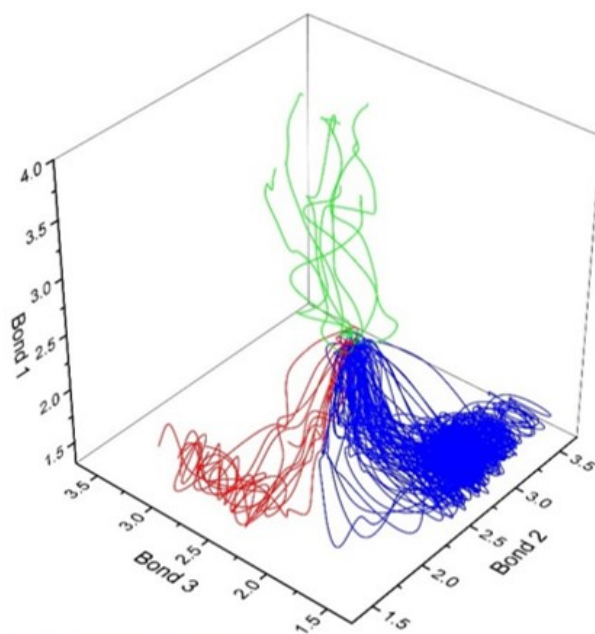
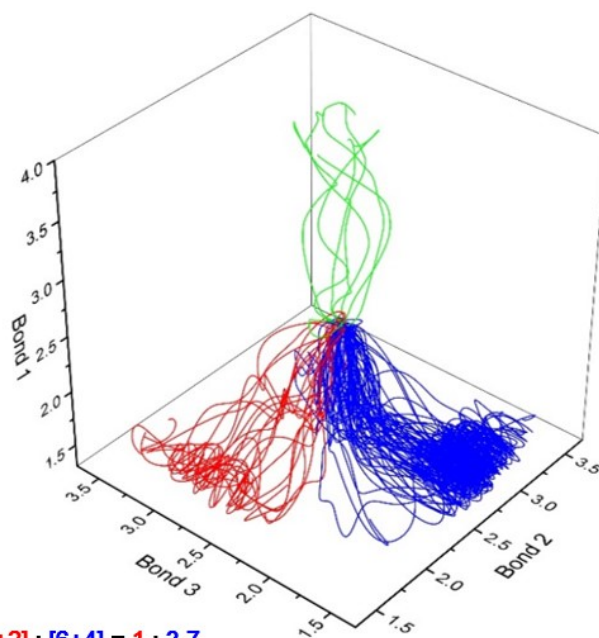


Figure S4. Trajectories distribution chart of **R2d**



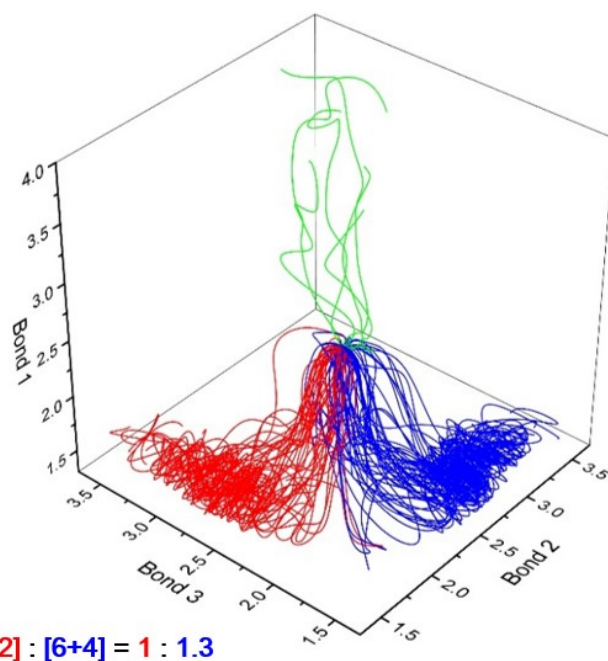
$$[4+2] : [6+4] = 1 : 7.4$$

Figure S5. Trajectories distribution chart of **R3a**



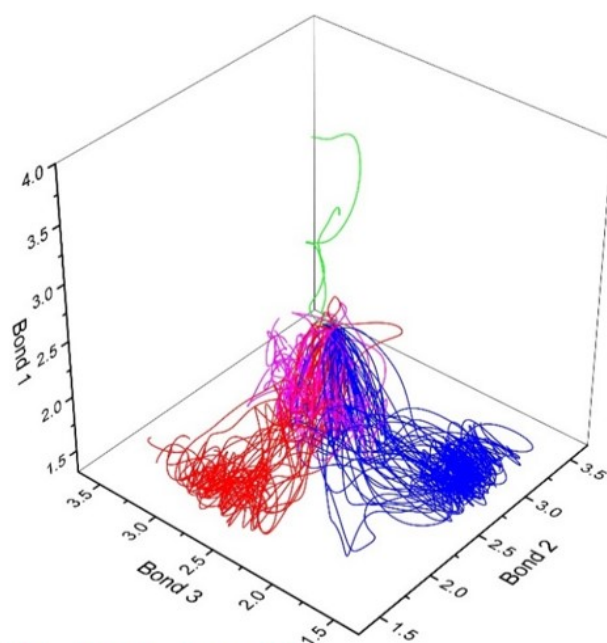
$$[4+2] : [6+4] = 1 : 3.7$$

Figure S6. Trajectories distribution chart of **R3b**



$[4+2] : [6+4] = 1 : 1.3$

Figure S7. Trajectories distribution chart of **R3c**



$[4+2] : [6+4] : \text{Hetero } [4+2] = 1 : 1.6 : 0.8$

Figure S8. Trajectories distribution chart of **R3d**

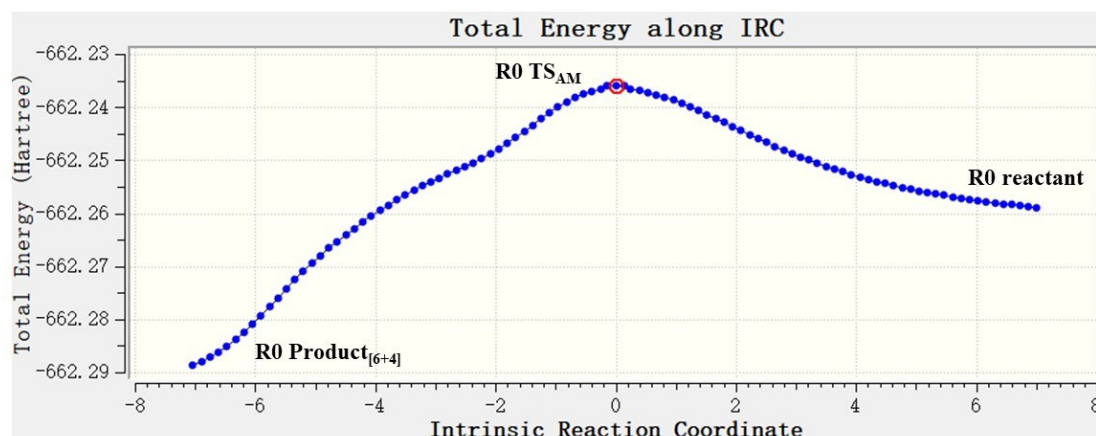


Figure S9. IRC path of **R0**

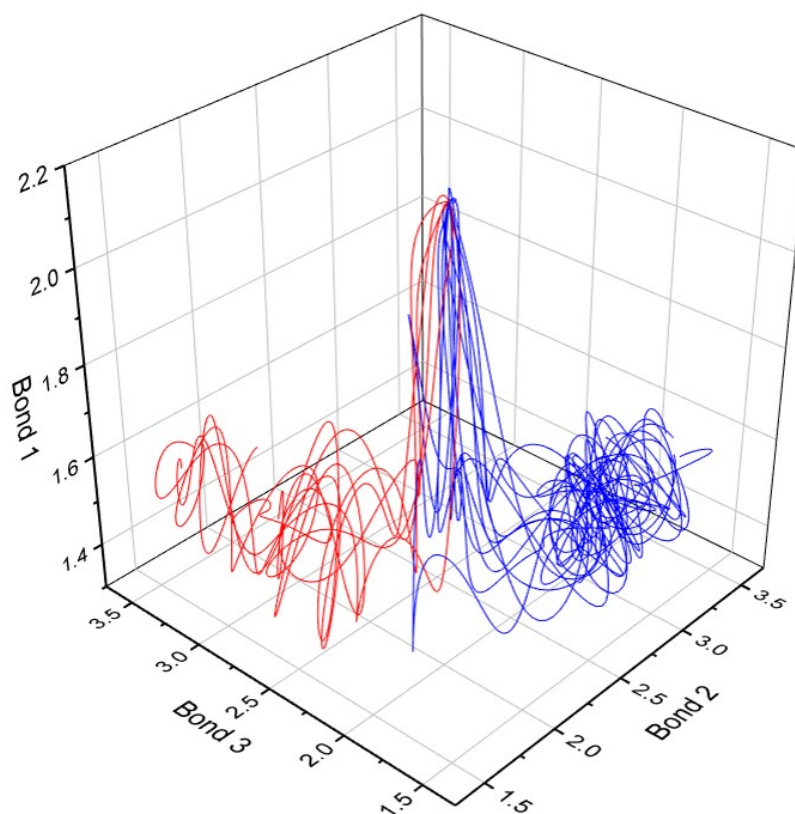


Figure S10. AIMD Trajectories of **R0**

Trajectories leading to [4+2] adduct are shown in red, trajectories leading to [6+4] adduct are shown in blue. And the ratio of [4+2] adduct : [6+4] adduct is 6:14.

II. Coordinates of the compounds

R0 reactant

$G = -661.938541$ Hartree

C	0.45498900	-1.73491100	-0.07685400
C	1.58630600	-1.45206200	0.59776400
C	-0.88875200	-1.44609300	0.40105600
C	-2.02069800	-1.77297400	-0.25381700
C	-3.01174900	1.25369400	-0.36527700
C	-3.42560400	-1.64738100	0.26547100
H	-1.92643600	-2.24128600	-1.24386500
C	2.29536500	1.35098700	-0.66862300
C	1.38192000	1.92370200	0.14112500
C	3.77903200	1.42392400	-0.51183500
C	-0.03679200	1.72321400	-0.02572200
C	-1.00480800	2.16755600	0.81178800
C	-2.41301200	1.81265800	0.70523300
C	-4.38893400	0.67405200	-0.36385300
H	-2.44100000	1.13461900	-1.29345200
C	-4.38825000	-0.84565600	-0.63588300
H	-3.41422400	-1.21699400	1.28120400
H	-3.83310900	-2.67068100	0.36847900
H	-5.41766400	-1.21929600	-0.50606900
H	-4.12968300	-1.03065900	-1.69376500
H	-5.01964900	1.16002500	-1.13129600
H	-4.86748700	0.86851800	0.61121700
C	2.96310800	-1.92321800	0.22492400
C	4.48683400	0.06191900	-0.60371400
H	4.03124600	1.91400400	0.44452100
H	4.19803400	2.06933300	-1.30836900
C	4.15060500	-0.97281800	0.48554700
H	5.57233800	0.25495600	-0.57416100
H	4.29201200	-0.38253400	-1.59688700
H	2.97481000	-2.25960100	-0.82676000
H	3.15277800	-2.83521100	0.82439900
H	4.00673900	-0.46071100	1.45442600
H	5.04196700	-1.60737500	0.61795500
H	0.52917700	-2.25936600	-1.03890900
H	-0.96548700	-0.95950900	1.38022500
H	1.71653400	2.51611200	1.00216200
H	-0.32491400	1.08650000	-0.86727300

H	-0.70926300	2.76604500	1.68119000
H	-3.01431200	1.95852200	1.61119500
H	1.50106000	-0.92220300	1.55489200
H	1.92917100	0.75724000	-1.51503700

R0 TS_{AM}

$G = -661.909703$ Hartree

Imaginary frequency: -405.61 cm^{-1}

C	-0.47321300	-1.33658100	0.13069800
C	-1.72117400	-1.22400500	-0.42287000
C	0.73142500	-0.90609600	-0.47773800
C	2.01183500	-1.05701500	0.10040300
C	2.91156500	0.73051900	0.62710900
C	3.23335300	-1.49313300	-0.68355900
H	1.98209000	-1.51279800	1.10137700
C	-2.23901400	1.20402900	0.41179400
C	-1.20571400	1.80704500	-0.25214100
C	-3.68635700	1.32135000	0.03483500
C	0.14286100	1.66758800	0.14648500
C	1.24859500	2.14307700	-0.56214300
C	2.54942200	1.71248800	-0.32770200
C	4.35995000	0.26337900	0.65240400
H	2.38518100	0.75311300	1.58595900
C	4.45611600	-1.21023500	0.18847600
H	3.28407200	-0.93406400	-1.63417600
H	3.17138200	-2.56510000	-0.94279400
H	5.40452600	-1.41356300	-0.33315900
H	4.42576300	-1.88346200	1.06239000
H	4.80364500	0.38549700	1.65334500
H	4.94556400	0.89735400	-0.03219600
C	-2.95570800	-1.88011600	0.12776500
C	-4.56230900	0.13936900	0.46780900
H	-3.77881000	1.48302900	-1.05368700
H	-4.09609700	2.23594700	0.50786600
C	-4.28245800	-1.19586300	-0.22866900
H	-5.61643500	0.41015800	0.28929100
H	-4.46684000	0.00285500	1.56097900
H	-2.86805300	-1.98539700	1.22417400
H	-3.00034200	-2.91570400	-0.26444100
H	-4.33088600	-1.05220300	-1.32402500
H	-5.10237100	-1.89041900	0.01971900
H	-0.39400300	-1.76616900	1.13889300
H	0.67403100	-0.56504400	-1.51654500

H	-1.40924100	2.30710300	-1.20777400
H	0.31661400	1.16663100	1.10042100
H	1.06372800	2.78115500	-1.43351000
H	3.31672300	2.01889100	-1.04703100
H	-1.79479400	-0.83967700	-1.44605000
H	-2.03050400	0.76706300	1.39324800

R0 Product_[6+4]

$G = -661.960086$ Hartree

C	-0.43761300	-1.14212900	0.26405800
C	-1.79781400	-0.72140400	-0.21734300
C	0.70266500	-0.89314700	-0.39403200
C	2.08964200	-0.99689800	0.16034100
C	2.68839400	0.35568500	0.71629300
C	3.16490200	-1.47401200	-0.84070400
H	2.07478600	-1.68108700	1.02656500
C	-2.13666400	0.76651400	0.23713100
C	-1.08858400	1.69597000	-0.29649300
C	-3.55669700	1.15056200	-0.20319100
C	0.11738100	1.80669200	0.28665200
C	1.35471800	2.22560300	-0.36591900
C	2.51084600	1.55221400	-0.19204100
C	4.16563800	-0.03193200	0.89418900
H	2.21312700	0.56983100	1.68735800
C	4.51152300	-0.87719700	-0.35241200
H	2.91822400	-1.09640000	-1.84609800
H	3.18475600	-2.57191600	-0.91348300
H	4.95692000	-0.24573000	-1.13709900
H	5.25598900	-1.65337800	-0.11927700
H	4.26776400	-0.64462300	1.80423800
H	4.82212100	0.84315300	1.01763000
C	-2.89862500	-1.68501700	0.25476400
C	-4.61887400	0.16019100	0.27541700
H	-3.57872400	1.20166100	-1.30772500
H	-3.78444700	2.16723500	0.15740300
C	-4.29763100	-1.26033900	-0.19267200
H	-5.61545100	0.46978300	-0.08062700
H	-4.66223500	0.17782600	1.37985200
H	-2.86935800	-1.73515700	1.35923000
H	-2.66894600	-2.70108700	-0.10616700
H	-4.35532200	-1.30118300	-1.29579700
H	-5.04984500	-1.97241100	0.18543900
H	-0.38646200	-1.54196400	1.28660000

H	0.63383600	-0.46027000	-1.39909200
H	-1.23634500	2.07793500	-1.31548200
H	0.23369100	1.35084700	1.27464800
H	1.31089000	3.03438300	-1.10397600
H	3.38333200	1.86293300	-0.77780900
H	-1.79333800	-0.70609100	-1.32222500
H	-2.09420000	0.76755900	1.34167200

R0 Product_[4+2]

$G = -661.958445$ Hartree

C	-0.42992100	-1.03306400	0.52124700
C	-1.41029000	-1.41501100	-0.30357400
C	0.67033700	-0.10790800	0.09047800
C	2.03473100	-0.41867100	0.72420800
C	3.13549800	0.57186500	0.24997400
C	2.56137000	-1.82986700	0.33139100
H	1.91616400	-0.33765700	1.81773100
C	-2.23819300	1.45075000	0.35466800
C	-1.07584800	1.65856600	-0.27179400
C	-3.60426400	1.35286700	-0.25202800
C	0.24883900	1.37963600	0.38391800
C	1.35701400	2.31444600	-0.03564000
C	2.63931400	1.94021500	-0.11388100
C	3.87743100	-0.18887400	-0.86710000
H	3.85933100	0.69177800	1.07870600
C	3.94752700	-1.61328700	-0.30949500
H	1.87250000	-2.28843700	-0.39552500
H	2.60191800	-2.51422800	1.19186400
H	4.19005700	-2.37061800	-1.07087000
H	4.73693400	-1.66317400	0.45978500
H	4.86204800	0.24514000	-1.10235400
H	3.27685600	-0.16565300	-1.79317400
C	-2.72445000	-2.03617900	0.05833200
C	-4.35938400	0.06080500	0.13797800
H	-3.54526900	1.44084500	-1.35059700
H	-4.22242700	2.20161600	0.09599600
C	-3.94260500	-1.27316300	-0.51265700
H	-5.42076700	0.22190100	-0.11554900
H	-4.33364200	-0.04920000	1.23792000
H	-2.81663700	-2.13207600	1.15400000
H	-2.77041200	-3.06329000	-0.34963900
H	-3.78887200	-1.11540500	-1.59620200
H	-4.80945500	-1.95093200	-0.43530800

H	-0.51834700	-1.22872300	1.59867700
H	0.77675600	-0.18198800	-1.00649700
H	-1.06187500	1.84324500	-1.35400300
H	0.10569400	1.46464500	1.47852100
H	1.07360300	3.34232100	-0.28482100
H	3.39411300	2.66597600	-0.43741200
H	-1.30093000	-1.16544800	-1.36779200
H	-2.19996900	1.23060100	1.43038700

R0 TS_{CP}

$G = -661.926141$ Hartree

Imaginary frequency: -374.40 cm^{-1}

C	-0.45577800	-1.18976500	0.13857700
C	-1.72556700	-1.04964700	-0.40340200
C	0.67129700	-0.51055400	-0.34207400
C	2.03097600	-0.72043500	0.25505900
C	2.93151200	0.56541000	0.53652800
C	2.96325200	-1.62276100	-0.57392000
H	1.89045300	-1.21096600	1.23370800
C	-2.19130200	1.05439600	0.41278700
C	-1.12818300	1.72213800	-0.17177100
C	-3.62440600	1.25519800	-0.00756100
C	0.20270900	1.56278000	0.24941700
C	1.32242000	2.20013100	-0.43629800
C	2.58666800	1.75154400	-0.31398400
C	4.39509900	0.07707000	0.35271700
H	2.75132600	0.83463400	1.59154600
C	4.32290700	-1.43945400	0.10086600
H	2.99831700	-1.25355700	-1.61444500
H	2.61566000	-2.66689400	-0.60546600
H	5.16746600	-1.81449800	-0.49778500
H	4.33300500	-1.98988600	1.05730700
H	5.03265300	0.33144900	1.21282100
H	4.83627500	0.57399100	-0.52657600
C	-2.91550300	-1.84032600	0.07543500
C	-4.56667000	0.11506600	0.39261900
H	-3.67113300	1.41577700	-1.09947700
H	-3.99767000	2.19117100	0.45035200
C	-4.27248100	-1.22539400	-0.28376500
H	-5.60258800	0.41387000	0.16082300
H	-4.52551300	-0.01680200	1.48969000
H	-2.84695200	-1.98833000	1.16809900
H	-2.86553600	-2.85333100	-0.36811600

H	-4.33016300	-1.09795800	-1.38058600
H	-5.06720300	-1.94247000	-0.01851200
H	-0.37418100	-1.67234900	1.12227500
H	0.66155800	-0.20314300	-1.39128200
H	-1.29553400	2.20017300	-1.14636400
H	0.36783700	1.26539400	1.28862000
H	1.09793700	3.01249900	-1.13638300
H	3.38986000	2.23293600	-0.88053300
H	-1.79415300	-0.68413300	-1.43337700
H	-2.05343100	0.69004000	1.43628200

R1a reactant

$G = -701.235002$ Hartree

C	0.40166200	-1.58409100	-0.21406500
C	1.54168300	-1.38581900	0.49093100
C	-0.96611900	-1.42563900	0.25334700
C	-2.06259200	-1.68659300	-0.48740400
C	-3.14405700	1.27986000	-0.30983100
C	-3.48275100	-1.69751500	0.00599700
H	-1.92363800	-1.98770200	-1.53537600
C	2.12706700	1.47031000	-0.77467600
C	1.24216300	1.99154300	0.09847400
C	3.61574700	1.54776600	-0.67538700
C	-0.17824200	1.77253100	-0.02253300
C	-1.12265600	2.13439300	0.87909900
C	-2.52560100	1.75351400	0.78996200
C	-4.50337600	0.66017900	-0.33182200
H	-2.59966700	1.26999900	-1.26122200
C	-4.46789400	-0.81401900	-0.78642300
H	-3.50993100	-1.42306000	1.07451000
H	-3.84695500	-2.74074100	-0.05231000
H	-5.48684500	-1.22690800	-0.69920500
H	-4.21208600	-0.86182200	-1.86016600
H	-5.17346300	1.21340200	-1.01613500
H	-4.95389400	0.72184200	0.67359300
C	2.87642600	-1.81703500	-0.08117900
C	4.33466500	0.21295000	-0.93036800
H	3.90724300	1.95169300	0.30991700
H	3.99077400	2.27132700	-1.42554500
C	4.11721000	-0.91469000	0.09291000
H	5.41584600	0.42721300	-0.97420200
H	4.06436100	-0.15647100	-1.93672300
H	2.75545000	-2.06528700	-1.14900700

H	3.11921100	-2.77546700	0.41910800
H	4.14902200	-0.49959100	1.11492000
H	4.99370500	-1.57984700	0.02529300
H	0.50418700	-1.95321900	-1.24231400
H	-1.11632900	-1.10431400	1.28829400
H	1.60359200	2.54299500	0.97568000
H	-0.48672900	1.18570500	-0.89229400
H	-0.80902300	2.67558600	1.77917800
H	-3.09786500	1.79719500	1.72496800
C	1.56561400	-0.88862700	1.90862800
H	2.09289700	-1.60333300	2.56556700
H	2.11190400	0.06611800	1.97574000
H	0.56365000	-0.71720500	2.31915800
H	1.73088600	0.91778500	-1.63538200

R1a TS_{AM}

$G = -701.204992$ Hartree

Imaginary frequency: -417.01 cm^{-1}

C	0.39916400	-1.23156300	-0.23404500
C	1.64214000	-1.15774700	0.35787800
C	-0.84085700	-0.89855000	0.35812300
C	-2.09653400	-1.00834300	-0.28566500
C	-3.03912700	0.80003300	-0.56926800
C	-3.31402300	-1.60479300	0.39448400
H	-2.02037600	-1.32378800	-1.33723800
C	2.06953100	1.31000200	-0.54267600
C	1.08671600	1.88178400	0.21749700
C	3.54290000	1.41734200	-0.28996000
C	-0.28286300	1.73309700	-0.09955500
C	-1.36323600	2.13056300	0.69160400
C	-2.66405300	1.69494200	0.46587500
C	-4.48271600	0.31938600	-0.60983000
H	-2.55020500	0.94135600	-1.53825900
C	-4.53699600	-1.21329100	-0.43295600
H	-3.39300200	-1.21337800	1.42403700
H	-3.21926500	-2.70240000	0.47322500
H	-5.48376100	-1.54029200	0.02523000
H	-4.47177300	-1.71102000	-1.41608700
H	-4.98149500	0.62440600	-1.54407400
H	-5.03524600	0.79703600	0.21522800
C	2.83435000	-1.78466200	-0.33153400
C	4.36951200	0.25717700	-0.86082900
H	3.73596700	1.53147900	0.79164300

H	3.90938600	2.35387800	-0.75510900
C	4.20072200	-1.10039100	-0.17233800
H	5.43549900	0.53607600	-0.81316000
H	4.13371700	0.14903900	-1.93573100
H	2.60854500	-1.89943000	-1.40566900
H	2.94108800	-2.81638800	0.06147800
H	4.44898600	-0.99907700	0.89838500
H	4.96015700	-1.78642300	-0.58370000
H	0.36616800	-1.55891500	-1.28127600
H	-0.85553500	-0.66822600	1.42661600
H	1.35225900	2.35247500	1.17223000
H	-0.49931400	1.28673200	-1.07129600
H	-1.15471500	2.70312700	1.60221400
H	-3.41225100	1.91732900	1.23439600
C	1.79176800	-0.81962500	1.81614800
H	1.75137300	-1.73616400	2.43506200
H	2.75486500	-0.33475000	2.02957100
H	0.99933900	-0.14585200	2.16618800
H	1.78119800	0.89101700	-1.51163200

R1a Product_[6+4]

$G = -701.249645$ Hartree

C	0.34222500	-1.06830300	-0.35764200
C	1.71170400	-0.68247900	0.16242500
C	-0.81770800	-0.88327100	0.28673500
C	-2.18961300	-0.95405000	-0.30990700
C	-2.80118000	0.43785500	-0.74532200
C	-3.27290200	-1.54628500	0.62123800
H	-2.14623600	-1.55025100	-1.23771000
C	1.99541200	0.84149600	-0.27322800
C	0.97407100	1.74736200	0.34502500
C	3.44741100	1.25131700	0.01005900
C	-0.25200200	1.86043600	-0.19665000
C	-1.48681300	2.22573700	0.48774700
C	-2.63720300	1.55677700	0.26028200
C	-4.27366400	0.05429800	-0.96469400
H	-2.32651600	0.73981200	-1.69283200
C	-4.61749200	-0.89454400	0.20345600
H	-3.03209200	-1.29712000	1.66715700
H	-3.29331800	-2.64477900	0.55795400
H	-5.04472900	-0.32832000	1.04600500
H	-5.37537900	-1.63762100	-0.08721100
H	-4.36448100	-0.48131500	-1.92344200

H	-4.93755600	0.93090400	-1.01894600
C	2.77926100	-1.57204700	-0.51908200
C	4.45661200	0.31313500	-0.65527900
H	3.61928600	1.27418600	1.10041500
H	3.59827500	2.28480000	-0.34293200
C	4.22392300	-1.14408900	-0.25052300
H	5.48619600	0.62312500	-0.41078500
H	4.35684200	0.40190500	-1.75270300
H	2.60103700	-1.54593200	-1.60928400
H	2.62299500	-2.61845400	-0.20675100
H	4.46465700	-1.27297000	0.81864000
H	4.91308800	-1.80763200	-0.79878200
H	0.31084400	-1.37923200	-1.41104400
H	-0.79427900	-0.53530300	1.32370000
H	1.16095400	2.11060200	1.36316800
H	-0.38212400	1.43848000	-1.19707900
H	-1.44803700	2.97614400	1.28521600
H	-3.51354000	1.81078000	0.86721300
C	1.79183000	-0.83030200	1.69008400
H	1.57082900	-1.86872900	1.98083100
H	2.78860300	-0.57639400	2.07581400
H	1.07067000	-0.17980800	2.20312700
H	1.85077000	0.85485800	-1.36808500

R1a Product_[4+2]

$G = -701.253207$ Hartree

C	0.36628800	-0.81289900	-0.71683300
C	1.32607000	-1.34391700	0.06063700
C	-0.79834000	-0.00754400	-0.22594000
C	-2.12062400	-0.26319400	-0.96655900
C	-3.27421600	0.54280400	-0.32090200
C	-2.60781800	-1.71408100	-0.85572700
H	-1.98095700	0.03188900	-2.02089500
C	2.02944300	1.65797800	-0.26383100
C	0.86562900	1.76913000	0.38492600
C	3.40633100	1.50940800	0.30757200
C	-0.44246900	1.52267800	-0.31669700
C	-1.60512600	2.34666500	0.17903200
C	-2.86719500	1.90008300	0.18053400
C	-3.86598900	-0.39380400	0.78457300
H	-4.05414200	0.68552200	-1.08993100
C	-3.24407700	-1.79182400	0.54165500
H	-1.80055400	-2.44688200	-1.00604500

H	-3.37307400	-1.89875800	-1.62896900
H	-2.46631400	-1.99883200	1.29393500
H	-3.98199300	-2.60428400	0.62375500
H	-4.96436600	-0.42226000	0.71899000
H	-3.62014800	-0.01712600	1.78895100
C	2.64655500	-1.80356800	-0.50893200
C	4.20705000	0.34912000	-0.32849900
H	3.36238800	1.39171000	1.40423600
H	3.98290200	2.43444800	0.11886500
C	3.89396900	-1.10264200	0.08191200
H	5.26969800	0.52113000	-0.08735100
H	4.13797100	0.43582600	-1.42865500
H	2.64514500	-1.68534000	-1.60536400
H	2.76790900	-2.88483200	-0.30789500
H	3.86879100	-1.16957800	1.18332200
H	4.76456200	-1.70808300	-0.22241100
H	0.53886800	-0.78289600	-1.80064800
H	-0.95941600	-0.21129400	0.84328900
H	0.84394700	1.82708400	1.48077400
H	-0.28610600	1.74718500	-1.38980500
H	-1.38312400	3.35485500	0.54417100
H	-3.66564500	2.54478400	0.56516800
C	1.21459900	-1.42667100	1.56311800
H	1.72655600	-2.32550000	1.94430700
H	1.68937500	-0.55673000	2.04922900
H	0.17239500	-1.46201800	1.90696300
H	1.98485000	1.57364200	-1.35821700

R1a TS_{CP}

$G = -701.218946$ Hartree

Imaginary frequency: -340.28 cm^{-1}

C	0.40072700	-1.12524300	-0.35013500
C	1.65674000	-1.03746800	0.25427200
C	-0.78094700	-0.58492900	0.16254500
C	-2.11490900	-0.75374400	-0.50365900
C	-2.98136900	0.56202400	-0.72279300
C	-3.07051400	-1.72177300	0.26880900
H	-1.94087200	-1.16570300	-1.51074300
C	2.01617800	1.20411300	-0.41184100
C	0.95821300	1.76529100	0.28155500
C	3.46654100	1.40306000	-0.06728700
C	-0.37156900	1.60537900	-0.14158400
C	-1.53143800	2.07761500	0.59911000

C	-2.76624900	1.60021100	0.33797200
C	-4.41584000	0.01868700	-0.76059300
H	-2.68853800	0.98642100	-1.69853700
C	-4.43657200	-1.01386300	0.37232700
H	-2.66590100	-1.97216600	1.26090600
H	-3.15601900	-2.67212300	-0.28072800
H	-4.51791100	-0.49133600	1.33989000
H	-5.28753400	-1.70967300	0.31089100
H	-4.60081400	-0.47867600	-1.72783400
H	-5.17347700	0.80989900	-0.64729000
C	2.83932400	-1.69472800	-0.43061500
C	4.39841100	0.35438200	-0.68706200
H	3.59651400	1.43221600	1.02930500
H	3.78130300	2.40113100	-0.42776300
C	4.21681400	-1.07289100	-0.16468100
H	5.44376600	0.66304400	-0.51910800
H	4.25258300	0.35759400	-1.78312000
H	2.65519100	-1.72099200	-1.51828700
H	2.87689700	-2.75307300	-0.10401900
H	4.43541300	-1.09692100	0.91685600
H	4.97776200	-1.71855800	-0.63409800
H	0.38185800	-1.44955500	-1.39904500
H	-0.83943000	-0.40297200	1.23678300
H	1.13824000	2.15214700	1.29267800
H	-0.52314800	1.41054600	-1.20584900
H	-1.36982800	2.77273800	1.43050800
H	-3.62313200	1.93382000	0.93169800
C	1.77852300	-0.86790900	1.74842900
H	1.83269600	-1.86070000	2.23331900
H	2.68876800	-0.32377000	2.03644800
H	0.92511100	-0.33261500	2.18068000
H	1.82811900	0.91999200	-1.45215900

R1b reactant

$G = -701.233713$ Hartree

C	-0.47148900	-1.60376100	-0.05958500
C	-1.53783600	-1.27140900	-0.82515100
C	0.87920900	-1.29518300	-0.54534100
C	2.03751700	-1.64397100	0.04860100
C	3.07828400	1.32993400	0.39666900
C	3.41750700	-1.48892000	-0.52963600
H	2.00437000	-2.15705400	1.01738300
C	-2.24557200	1.42467500	0.77515400

C	-1.32363600	2.07784500	0.04007200
C	-3.72617300	1.55113600	0.62596000
C	0.09319500	1.83535500	0.16149000
C	1.05175200	2.37029400	-0.63267000
C	2.45799300	1.99670500	-0.59681700
C	4.44834400	0.74226400	0.29427700
H	2.53081200	1.12327500	1.32348600
C	4.43652400	-0.79816700	0.39973100
H	3.36691800	-0.96165900	-1.49741500
H	3.79868200	-2.50367900	-0.75133800
H	5.45238800	-1.16625100	0.17909900
H	4.22754900	-1.09405900	1.44335200
H	5.10677700	1.13693100	1.09017400
H	4.90041900	1.03692300	-0.66814500
C	-2.97356300	-1.67957300	-0.66083600
C	-4.44706300	0.20812600	0.41951900
H	-3.95826300	2.22984200	-0.21286900
H	-4.15001700	2.02289300	1.53342000
C	-4.05836600	-0.59362700	-0.83830400
H	-5.52888900	0.41938100	0.38343600
H	-4.29949800	-0.42517400	1.31307300
H	-3.13603500	-2.19577700	0.29806500
H	-3.15980900	-2.44719300	-1.43711900
H	-3.76500400	0.09751300	-1.64882800
H	-4.96555600	-1.10489200	-1.19868900
H	-1.65290800	2.78602100	-0.73089000
H	0.38592100	1.09668600	0.91329300
H	0.74578400	3.07132000	-1.41785400
H	3.03864600	2.22945700	-1.49816700
H	-1.89296000	0.71391400	1.53277900
H	-1.32677000	-0.71837000	-1.74894300
C	-0.58890600	-2.31446900	1.26435500
H	-1.63134800	-2.45676000	1.57487000
H	-0.10532900	-3.30543500	1.23320200
H	-0.07832600	-1.74025700	2.05608100
H	0.92612400	-0.77111800	-1.50638300

R1b TS_{AM}

$G = -701.203880$ Hartree

Imaginary frequency: -440.63 cm^{-1}

C	-0.46405000	-1.25309200	0.05161400
C	-1.67508500	-1.09657600	-0.57916800
C	0.72349900	-0.74746500	-0.56654000

C	2.04303900	-0.93675800	-0.09356900
C	2.95108500	0.74469700	0.63460700
C	3.20865800	-1.22538900	-1.02049600
H	2.10747600	-1.52787900	0.82819100
C	-2.22547400	1.29314700	0.48274800
C	-1.16874800	1.92710500	-0.10481900
C	-3.65796200	1.48609400	0.08229600
C	0.17908000	1.72326000	0.27956000
C	1.28184400	2.27732400	-0.37618700
C	2.58517400	1.83241300	-0.19862100
C	4.39652700	0.26701400	0.57702100
H	2.44438000	0.67077100	1.60142800
C	4.48500200	-1.07897000	-0.19107300
H	3.19451100	-0.51504800	-1.86510000
H	3.13245700	-2.23937700	-1.45148100
H	5.39633300	-1.14020100	-0.80612700
H	4.53250800	-1.91650600	0.52546200
H	4.82486000	0.16469100	1.58623900
H	4.99925600	1.02692700	0.05532400
C	-2.98291000	-1.74758500	-0.23028700
C	-4.56017100	0.25886600	0.26162500
H	-3.70567800	1.83600100	-0.96383700
H	-4.08442800	2.30706700	0.69263200
C	-4.23763200	-0.95217400	-0.62034100
H	-5.59884700	0.57051400	0.06029400
H	-4.54033200	-0.05404900	1.32209700
H	-3.03428500	-1.99398700	0.84265400
H	-3.02719500	-2.72289700	-0.75546700
H	-4.15514700	-0.62833200	-1.67426200
H	-5.09894200	-1.63989900	-0.58299000
H	-1.35206000	2.53078000	-1.00309300
H	0.34921400	1.13938500	1.18560700
H	1.08812300	3.00501700	-1.17223800
H	3.34659100	2.21880500	-0.88484300
H	-2.04897000	0.74242700	1.41229900
H	-1.65122900	-0.62042300	-1.56508300
C	-0.34895300	-1.88974600	1.41695800
H	-1.32692800	-2.14405300	1.84346800
H	0.25048400	-2.81474300	1.38428000
H	0.15524000	-1.21129400	2.12587500
H	0.60506300	-0.33669700	-1.57329700

R1b Product_[6+4] $G = -701.255352$ Hartree

C	-0.41597700	-1.06220300	0.16790600
C	-1.76277200	-0.57406400	-0.33354600
C	0.69838600	-0.77394900	-0.53192600
C	2.12653300	-0.91884400	-0.09661400
C	2.74339200	0.31750800	0.66603200
C	3.13939900	-1.15050600	-1.23490700
H	2.21295000	-1.75908700	0.61173300
C	-2.12703500	0.85416700	0.26802200
C	-1.05095200	1.83375700	-0.09342000
C	-3.50942800	1.31027700	-0.22336900
C	0.15272800	1.82711100	0.50392700
C	1.38969600	2.33890700	-0.07810500
C	2.54640600	1.64819200	-0.02594200
C	4.22615800	-0.08980400	0.71551800
H	2.30522400	0.36477500	1.67678100
C	4.51839600	-0.72034800	-0.66909300
H	2.86289800	-0.52050200	-2.09593500
H	3.12507600	-2.19322100	-1.58680900
H	5.00120400	0.00769300	-1.33930200
H	5.21418800	-1.56845000	-0.58080800
H	4.36636600	-0.84105600	1.50882300
H	4.88955600	0.75628400	0.95146200
C	-2.90967100	-1.56716500	-0.07802900
C	-4.61281700	0.28226800	0.02409500
H	-3.44199300	1.51093400	-1.30877400
H	-3.76121100	2.27266100	0.25218200
C	-4.25428000	-1.06491300	-0.60460900
H	-5.57295700	0.65352400	-0.37094000
H	-4.75307300	0.14887400	1.11249300
H	-3.00511500	-1.74576800	1.00677000
H	-2.65366700	-2.53893400	-0.53238000
H	-4.20190700	-0.95302500	-1.70300800
H	-5.04232300	-1.80937800	-0.40300200
H	0.56318700	-0.27088600	-1.49586800
H	-1.17971900	2.38265800	-1.03575700
H	0.26460900	1.22293300	1.40932900
H	1.34228400	3.25628900	-0.67571100
H	3.41107600	2.05452800	-0.56275800
H	-2.16288200	0.73287100	1.36604700
H	-1.68177600	-0.42504000	-1.42427700
C	-0.38608900	-1.68739500	1.53844800

H	-0.88136600	-1.03566700	2.28003300
H	-0.92842900	-2.64720200	1.55977200
H	0.63534900	-1.87378000	1.89357500

R1b Product_[4+2]

$G = -701.255197$ Hartree

C	-0.40109700	-1.01008100	0.40708200
C	-1.34239800	-1.26434100	-0.51775500
C	0.70314800	-0.03494300	0.05031500
C	2.09081200	-0.38589100	0.61341300
C	3.16687600	0.62806300	0.14118000
C	2.59498100	-1.77079100	0.11266000
H	2.03166000	-0.36225300	1.71270900
C	-2.20692700	1.50206700	0.40442500
C	-1.03084700	1.76756000	-0.17223400
C	-3.55483300	1.49573400	-0.24851400
C	0.28642300	1.42327200	0.46749000
C	1.39073000	2.39340600	0.12416000
C	2.66718400	2.02974700	-0.04503200
C	3.79049300	-0.03710400	-1.10163500
H	3.96176600	0.65807500	0.91092300
C	3.89752300	-1.50458800	-0.67482400
H	1.83356000	-2.22642000	-0.53954500
H	2.75596400	-2.47710300	0.94100100
H	4.03399100	-2.19575300	-1.52070700
H	4.77313200	-1.62607300	-0.01503600
H	4.75408200	0.41027900	-1.39222400
H	3.10597600	0.06938900	-1.96087500
C	-2.68427000	-1.91722900	-0.37510800
C	-4.31349000	0.15746800	-0.09537700
H	-3.46223700	1.75437700	-1.31745100
H	-4.18847800	2.27863400	0.20871400
C	-3.84508100	-1.05589900	-0.92369400
H	-5.36332600	0.35312200	-0.37164600
H	-4.33829500	-0.12109200	0.97441000
H	-2.89363200	-2.19025300	0.67160000
H	-2.68949600	-2.86624900	-0.94348100
H	-3.59459800	-0.72245200	-1.94759100
H	-4.71498000	-1.72471500	-1.03650900
H	0.78723500	-0.01574200	-1.04963400
H	-0.99871500	2.07292700	-1.22639500
H	0.14096700	1.42764000	1.56459500
H	1.10488900	3.44380900	0.00540300

H	3.41247600	2.78753400	-0.31197800
H	-2.19882600	1.16355900	1.44971000
H	-1.16152300	-0.85551600	-1.51990300
C	-0.48019300	-1.46436400	1.83878800
H	-0.41544700	-0.60892500	2.53357200
H	-1.40998700	-2.00588800	2.05727900
H	0.35964500	-2.13341300	2.09101700

R1b TS_{CP}

$G = -701.219853$ Hartree

Imaginary frequency: -375.33 cm^{-1}

C	-0.47814700	-1.15800500	0.10913400
C	-1.72639300	-0.93568600	-0.47607400
C	0.64385200	-0.48901100	-0.42497900
C	2.06620500	-0.76085000	-0.01448200
C	2.86318900	0.38908600	0.72082700
C	3.00126700	-1.11082800	-1.19630400
H	2.07696900	-1.60483900	0.69222700
C	-2.15674600	1.16236800	0.38889900
C	-1.03416700	1.81800700	-0.08821500
C	-3.54487100	1.46908900	-0.11324500
C	0.26400100	1.54813900	0.37319600
C	1.44923100	2.21682100	-0.15197200
C	2.68253000	1.70438100	0.02831300
C	4.29842000	-0.14965200	0.67269900
H	2.49345600	0.45969900	1.75827000
C	4.44381000	-0.78115200	-0.73152900
H	2.72728100	-0.49323400	-2.06579400
H	2.87913500	-2.16059400	-1.50398100
H	4.91853900	-0.07364800	-1.42890100
H	5.08867100	-1.67261200	-0.70614500
H	4.41965000	-0.92297500	1.44811800
H	5.04941500	0.62979300	0.87383500
C	-3.00280400	-1.66114400	-0.13310000
C	-4.57363600	0.35788900	0.11613600
H	-3.49767500	1.71518200	-1.18896900
H	-3.90738500	2.38628600	0.38947900
C	-4.27285900	-0.95187500	-0.61524100
H	-5.56562000	0.72613500	-0.19467200
H	-4.65004300	0.15405700	1.20029200
H	-3.08113700	-1.82824000	0.95376100
H	-2.96746500	-2.67013500	-0.58794100
H	-4.19303300	-0.75552000	-1.70026700

H	-5.12886800	-1.63574200	-0.49027200
H	0.53095300	-0.12045900	-1.44723800
H	-1.13097800	2.39312200	-1.01880700
H	0.35499000	1.12436500	1.37776000
H	1.30733200	3.12011600	-0.75549400
H	3.55621400	2.20185800	-0.40440500
H	-2.10293000	0.73124000	1.39439700
H	-1.70696100	-0.53012000	-1.49221200
C	-0.34945400	-1.84808400	1.44720000
H	0.02508500	-1.15174200	2.21908300
H	-1.30351100	-2.25441700	1.80456000
H	0.36735800	-2.68452600	1.40574400

R1c reactant

$G = -701.234285$ Hartree

C	0.47050400	-1.58532800	-0.24599400
C	1.64790700	-1.50710000	0.40194600
C	-0.86492900	-1.41534900	0.33830600
C	-1.95151300	-1.56436100	-0.45840600
C	-2.93205500	1.35939900	-0.45911700
C	-3.40766600	-1.59569000	-0.08744400
H	-1.75736600	-1.76314200	-1.52111300
C	2.38918000	1.44090900	-0.60147700
C	1.44819700	1.97201900	0.20468600
C	3.86596400	1.48611900	-0.37466700
C	0.03472100	1.80826300	-0.03074600
C	-0.95300600	2.20909300	0.80572900
C	-2.35920100	1.86643900	0.65040300
C	-4.31191100	0.78953800	-0.52962300
H	-2.33863400	1.28842200	-1.37791300
C	-4.31284700	-0.69439100	-0.94894400
H	-3.55674600	-1.35715500	0.97702500
H	-3.75730700	-2.63819600	-0.21479400
H	-5.34979500	-1.06762700	-0.90747200
H	-4.00190100	-0.77720900	-2.00607400
H	-4.92759200	1.35081700	-1.25737200
H	-4.80555800	0.89477000	0.45164000
C	2.98240300	-1.88093200	-0.18151800
C	4.58919900	0.15764500	-0.64464800
H	4.07536300	1.82761800	0.65399500
H	4.31323800	2.24616500	-1.04521700
C	4.21129300	-1.04368100	0.23905600
H	5.67025100	0.34351000	-0.52804500

H	4.44962300	-0.12101000	-1.70533800
H	2.91542900	-1.92811300	-1.28260400
H	3.18232800	-2.92109200	0.14146600
H	4.09166500	-0.71271300	1.28679400
H	5.07925400	-1.72291700	0.24293400
H	1.75337100	2.49641800	1.11923900
H	-0.23165500	1.22918300	-0.91973200
H	-0.67454000	2.74753400	1.71893700
H	-2.97950100	1.96766800	1.54944900
H	2.05433700	0.91719400	-1.50522600
H	1.65689500	-1.24767500	1.46645100
H	0.48469000	-1.83927100	-1.31379800
C	-0.95429200	-1.13926900	1.81555000
H	-0.57346200	-1.99480700	2.39891200
H	-0.34245400	-0.26396200	2.08018400
H	-1.98162800	-0.93435000	2.13911900

R1c TS_{AM}

$G = -701.206650$ Hartree

Imaginary frequency: -442.83 cm^{-1}

C	0.48001000	-1.24875900	-0.21289500
C	1.75058200	-1.21505200	0.29792400
C	-0.73238000	-0.89476200	0.44408600
C	-1.96851000	-0.99829700	-0.25641000
C	-2.82473800	0.80243700	-0.71183300
C	-3.24231200	-1.54393600	0.36108600
H	-1.83995500	-1.36177900	-1.28531100
C	2.31905200	1.22697800	-0.44270800
C	1.28499200	1.85893700	0.19437900
C	3.76055500	1.29987400	-0.03098900
C	-0.05584400	1.74641300	-0.23385600
C	-1.16273200	2.22933100	0.46413400
C	-2.46377300	1.78822600	0.24395000
C	-4.28243700	0.36768200	-0.77660500
H	-2.29818800	0.84821900	-1.67041500
C	-4.39027000	-1.15575400	-0.56916500
H	-3.40260700	-1.11496100	1.36372900
H	-3.17522300	-2.63979700	0.48450600
H	-5.37646400	-1.44758900	-0.17500300
H	-4.26321500	-1.68119700	-1.53172900
H	-4.74918700	0.67106300	-1.72804600
H	-4.83725300	0.87924000	0.02663100
C	2.94420000	-1.83840000	-0.37230200

C	4.62477400	0.14292300	-0.54547600
H	3.83556800	1.37220800	1.06857200
H	4.19139900	2.24358700	-0.42073100
C	4.30281600	-1.24242500	0.02254500
H	5.68046300	0.37319300	-0.32402300
H	4.54891700	0.10497700	-1.64797100
H	2.82175300	-1.81039700	-1.47021600
H	2.96433300	-2.91419600	-0.10708900
H	4.37163000	-1.20894800	1.12572100
H	5.09261900	-1.93843000	-0.30646700
H	1.47691300	2.35650400	1.15384500
H	-0.22325400	1.22542600	-1.17819700
H	-0.97855000	2.87384600	1.33089700
H	-3.23183300	2.10176400	0.95919800
H	2.12285200	0.80597600	-1.43347100
H	1.89078400	-0.94736400	1.34927200
H	0.37393900	-1.55852700	-1.26111300
C	-0.77538200	-0.60139400	1.91655400
H	-1.06248800	-1.50096600	2.49066100
H	0.18798200	-0.24614500	2.30404200
H	-1.53255400	0.17016300	2.12818700

R1c Product_[6+4]

$G = -701.253589$ Hartree

C	0.41263800	-0.99527300	-0.27569000
C	1.82326600	-0.68328100	0.12962600
C	-0.70758900	-0.85825700	0.46203400
C	-2.05742100	-0.88595000	-0.22252600
C	-2.61951600	0.51504700	-0.72912600
C	-3.24979600	-1.47313400	0.54232500
H	-1.94166600	-1.48312900	-1.14319500
C	2.22095600	0.79384300	-0.30389500
C	1.22219900	1.76355400	0.25371700
C	3.66997100	1.09307400	0.10076100
C	0.01078800	1.89578600	-0.31474200
C	-1.21018000	2.34909700	0.33793700
C	-2.38434200	1.70300700	0.17844700
C	-4.13641900	0.23562800	-0.95186400
H	-2.12446100	0.72288500	-1.69040100
C	-4.42722600	-1.17752500	-0.39136100
H	-3.38372100	-0.94692300	1.50242000
H	-3.12766500	-2.54462100	0.76656700
H	-5.40565600	-1.24195600	0.10872200

H	-4.43569300	-1.91747800	-1.20870700
H	-4.40956300	0.31158500	-2.01484500
H	-4.73737300	0.99220200	-0.42432300
C	2.83502100	-1.68335700	-0.45462000
C	4.65757100	0.07021500	-0.46447000
H	3.73514800	1.09606800	1.20480300
H	3.93815300	2.11066900	-0.22820400
C	4.27669000	-1.35579500	-0.05973300
H	5.68240500	0.30506300	-0.13215600
H	4.66244800	0.14466000	-1.56731700
H	2.74427300	-1.67571000	-1.55678600
H	2.56852200	-2.70234400	-0.12938600
H	4.38461000	-1.46300100	1.03518300
H	4.97014800	-2.08343800	-0.51322700
H	1.40090700	2.15139100	1.26502600
H	-0.12617400	1.42917400	-1.29512500
H	-1.14115000	3.15326500	1.07907600
H	-3.23822700	2.03744800	0.77805500
H	2.15451800	0.81262900	-1.40749500
H	1.91433100	-0.71512300	1.22772500
C	-0.70439200	-0.59237900	1.94284500
H	-1.25714700	0.33122100	2.17560100
H	-1.21061500	-1.41073300	2.48213900
H	0.30708000	-0.49599800	2.35480600
H	0.28325300	-1.20358800	-1.34693800

R1c Product_[4+2]

$G = -701.244772$ Hartree

C	0.50529400	-1.03142100	-0.41632300
C	1.54160000	-1.44096800	0.32173800
C	-0.61010000	-0.13250500	0.06447200
C	-1.91636500	-0.44194900	-0.71472700
C	-3.05502200	0.59672700	-0.47738800
C	-2.55356100	-1.82342600	-0.39510400
H	-1.63747000	-0.40580800	-1.77986400
C	2.28313700	1.42297700	-0.43990300
C	1.15694900	1.69867700	0.22689400
C	3.68606600	1.37705900	0.08292400
C	-0.19004800	1.35426200	-0.34352400
C	-1.30518200	2.31588900	-0.00698300
C	-2.59439800	1.96149000	-0.05493900
C	-4.05566800	-0.11282500	0.45636600
H	-3.58063000	0.72015000	-1.44414900

C	-4.03691500	-1.55351700	-0.06593200
H	-2.04975400	-2.28622100	0.46573700
H	-2.43774900	-2.52878300	-1.23109700
H	-4.45658400	-2.28089500	0.64607400
H	-4.64545100	-1.61276500	-0.98440200
H	-5.05622700	0.34744700	0.43516200
H	-3.69916900	-0.07608300	1.49857600
C	2.83437700	-2.01366100	-0.17662300
C	4.44831900	0.09758500	-0.33048400
H	3.69343200	1.48920600	1.18078900
H	4.25890100	2.23309500	-0.32112600
C	4.07936400	-1.24579700	0.32942400
H	5.51543100	0.27662200	-0.11574900
H	4.38431500	-0.01246800	-1.42889500
H	2.83922800	-2.05942600	-1.27943600
H	2.93539400	-3.05587800	0.17945300
H	3.98995800	-1.10153300	1.42205400
H	4.94642100	-1.91377100	0.19218700
H	1.20378000	2.00694700	1.27841000
H	-0.07768600	1.33412200	-1.44323100
H	-1.02640700	3.33459000	0.28088200
H	-3.37163700	2.69204400	0.19584400
H	2.18033600	1.10238600	-1.48540800
H	1.51859500	-1.26528800	1.40272100
C	-0.79545000	-0.20902100	1.58803300
H	-1.60345000	0.45059700	1.92538300
H	-1.02236700	-1.23394300	1.91319700
H	0.11669600	0.10406100	2.11382800
H	0.54769700	-1.17586000	-1.50448200

R1c TS_{CP}

$G = -701.218198$ Hartree

Imaginary frequency: -336.14 cm^{-1}

C	0.48472400	-1.14757200	-0.20070400
C	1.77182600	-1.08976200	0.29942700
C	-0.64574400	-0.52287000	0.36863100
C	-1.97245700	-0.71042500	-0.32981500
C	-2.85528800	0.58346200	-0.68293600
C	-2.97669100	-1.64313700	0.37602900
H	-1.75177100	-1.17410000	-1.30452400
C	2.25046900	1.09424700	-0.44764500
C	1.17761900	1.75508800	0.11890300
C	3.67926900	1.25612900	-0.00151000

C	-0.14299100	1.58044500	-0.33255200
C	-1.28030500	2.26569600	0.25835400
C	-2.54263900	1.81826200	0.10305400
C	-4.32537500	0.11303900	-0.53965300
H	-2.63471800	0.79329900	-1.74396100
C	-4.27570900	-1.41474600	-0.39669700
H	-3.11188800	-1.33493500	1.42602000
H	-2.63599100	-2.69031200	0.37983700
H	-5.16542100	-1.82904300	0.10257500
H	-4.20539100	-1.89280800	-1.38922400
H	-4.95736200	0.44645200	-1.37678700
H	-4.75544700	0.54725100	0.37848100
C	2.93774100	-1.82697300	-0.30515800
C	4.61068000	0.13880400	-0.48550300
H	3.72213000	1.33669500	1.09927600
H	4.06581600	2.21875800	-0.38824900
C	4.30766800	-1.25245100	0.07652300
H	5.64926700	0.40706500	-0.22934000
H	4.57082800	0.09708900	-1.58967800
H	2.83313700	-1.86200400	-1.40452600
H	2.90171200	-2.88081100	0.03224400
H	4.38618100	-1.22261800	1.17907200
H	5.09115800	-1.94970700	-0.26440100
H	1.32585600	2.26376800	1.08044700
H	-0.27382400	1.20986600	-1.35203500
H	-1.08188700	3.11170300	0.92546400
H	-3.36781800	2.33396000	0.60424600
H	2.12232800	0.72172700	-1.46897400
H	1.90941900	-0.80036300	1.34471100
C	-0.68623400	-0.27457100	1.85869000
H	-1.50024600	0.41125400	2.12879700
H	-0.85690000	-1.22257400	2.39820500
H	0.25355700	0.15362100	2.23143200
H	0.36789500	-1.52922100	-1.22371700

R1d reactant

$G = -701.230011$ Hartree

C	0.32778600	1.75712800	0.26419500
C	1.51609700	1.59354000	-0.34872000
C	-0.96770900	1.55228500	-0.36314400
C	-2.15175200	1.79826500	0.23111700
C	-3.01213400	-1.14096700	0.20697300
C	-3.51185700	1.71159200	-0.40487000

H	-2.14259700	2.14282400	1.27492000
C	2.55378300	-1.40285400	0.33165200
C	1.48858100	-1.73086100	-0.42372100
C	3.95336000	-1.25304600	-0.17641100
C	0.10309200	-1.78967300	0.02345800
C	-0.87056100	-1.85373700	-0.93048500
C	-2.30322500	-1.64805500	-0.82544300
C	-4.42510900	-0.66569700	0.09466600
H	-2.52035900	-0.92101000	1.15474300
C	-4.53327100	0.85097700	0.36800800
H	-3.41999700	1.34929500	-1.44305600
H	-3.92061800	2.73763600	-0.47113500
H	-5.55678000	1.17851700	0.12053000
H	-4.40858600	1.03784000	1.44976100
H	-5.08223400	-1.19330900	0.81078500
H	-4.81126700	-0.88791900	-0.91469900
C	2.84727600	1.99072500	0.23393100
C	4.64574200	0.05642200	0.23308100
H	3.96797900	-1.35673900	-1.27530000
H	4.56735200	-2.08578300	0.21870000
C	4.11202000	1.35953500	-0.38248400
H	5.71046200	-0.03422000	-0.04167300
H	4.63070500	0.14595500	1.33514100
H	2.84314000	1.84367500	1.32855300
H	2.93748500	3.08518200	0.09406100
H	3.95856800	1.21881600	-1.46803600
H	4.92050400	2.10383500	-0.29602900
H	1.64605200	-1.88584900	-1.49816900
H	-0.51801500	-1.98044300	-1.96051900
H	-2.85186200	-1.80723600	-1.76240300
H	2.41564800	-1.20731700	1.40069400
H	1.52087800	1.24589100	-1.38912500
H	0.31380400	2.11345000	1.30323000
C	-0.18370700	-1.69289700	1.49664400
H	0.64571600	-2.10253500	2.09003700
H	-0.32447800	-0.64197000	1.80341600
H	-1.09400300	-2.24673100	1.76336600
H	-0.95796500	1.19204700	-1.39848100

R1d TS_{AM}

$G = -701.197148$ Hartree

Imaginary frequency: -430.33 cm^{-1}

C	-0.46090300	-1.36107000	0.27287300
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C	-1.73449300	-1.26436500	-0.25192500
C	0.72413900	-1.05382800	-0.41775700
C	2.02446500	-1.16413100	0.12518500
C	2.97341700	0.67594100	0.40104700
C	3.20073400	-1.71050000	-0.65782500
H	2.03278700	-1.50375200	1.17145500
C	-2.31566200	1.11783900	0.12272200
C	-1.21906200	1.66777200	-0.49961500
C	-3.69889100	1.11066900	-0.46718000
C	0.07426100	1.72870400	0.06834800
C	1.17472000	1.97141000	-0.78097200
C	2.48818000	1.56708300	-0.59288000
C	4.41833800	0.21397000	0.29178000
H	2.57363700	0.75723600	1.41093600
C	4.47573400	-1.31440600	0.08488200
H	3.19475800	-1.29188300	-1.67966300
H	3.12508600	-2.80792500	-0.75977300
H	5.39014500	-1.62092500	-0.44738800
H	4.48960200	-1.82908600	1.06146300
H	5.00118900	0.51033300	1.17931500
H	4.88406500	0.71115800	-0.57424900
C	-2.94745500	-1.87380300	0.40023500
C	-4.64248900	0.06916200	0.14318100
H	-3.64236700	0.97884000	-1.56257000
H	-4.14633800	2.11206500	-0.31222800
C	-4.28989400	-1.38903200	-0.15801700
H	-5.66612100	0.26607000	-0.21693800
H	-4.67278600	0.21514300	1.23881400
H	-2.90950500	-1.71233900	1.49289400
H	-2.90139700	-2.97227900	0.26440800
H	-4.29601200	-1.54368600	-1.25278800
H	-5.08987900	-2.03369500	0.24292700
H	-1.30089400	1.90304400	-1.56825800
H	0.93254500	2.37495700	-1.77135900
H	3.16628000	1.75610300	-1.43307000
H	-2.26239000	0.92131000	1.19676600
H	-1.82024400	-1.05762800	-1.32383100
H	-0.36302000	-1.68527700	1.31795400
C	0.23087800	1.60602600	1.56686300
H	-0.63467600	2.05943300	2.07253900
H	0.29675700	0.56494400	1.91613200
H	1.12902200	2.13772000	1.90921000
H	0.63365200	-0.79452200	-1.47836700

R1d Product_[6+4] $G = -701.250772$ Hartree

C	-0.42883600	-1.18234700	0.34838200
C	-1.80338600	-0.86822600	-0.17629600
C	0.69684100	-0.96747000	-0.34557200
C	2.09004200	-0.99572900	0.19684900
C	2.79423700	0.41948600	0.36828500
C	3.10907700	-1.79078200	-0.63149300
H	2.05883200	-1.44096900	1.20710600
C	-2.17269300	0.65949900	0.04711100
C	-1.09273100	1.48717000	-0.57364600
C	-3.57301000	0.94697400	-0.51431200
C	0.03726200	1.87207200	0.05462100
C	1.23777800	2.12202000	-0.77488400
C	2.41117000	1.47162500	-0.65550600
C	4.31718600	0.08633500	0.32122900
H	2.52515000	0.79384600	1.36463200
C	4.44407300	-1.42327200	0.01992300
H	3.07941600	-1.44318400	-1.67996700
H	2.90046400	-2.87192400	-0.63568300
H	5.31755600	-1.65975000	-0.60698500
H	4.55739400	-1.99302800	0.95745800
H	4.82302800	0.35878100	1.25962600
H	4.80113600	0.67495000	-0.47352900
C	-2.89270800	-1.76815400	0.42489700
C	-4.64025200	0.02761200	0.08349500
H	-3.54775500	0.81694000	-1.61217100
H	-3.82828000	2.00402100	-0.33335500
C	-4.28514000	-1.44695500	-0.12218500
H	-5.62632900	0.25174200	-0.35615200
H	-4.72796100	0.23192400	1.16636100
H	-2.89006400	-1.63948000	1.52335900
H	-2.63875900	-2.82432300	0.23604500
H	-4.31048000	-1.67821400	-1.20275400
H	-5.04000300	-2.09541200	0.35271500
H	-1.10577500	1.52429500	-1.67118500
H	1.11468400	2.79197400	-1.63424800
H	3.17578500	1.70082100	-1.40666200
H	-2.19615200	0.82232800	1.13780100
H	-1.79746800	-1.01589500	-1.27186500
H	-0.36014900	-1.46830100	1.40702600
H	0.60977600	-0.66123600	-1.39456900
C	0.16845700	1.87855900	1.56062100

H	0.40198000	0.88006600	1.96386200
H	0.96792300	2.56352500	1.87902500
H	-0.76815700	2.20601900	2.03500400

R1d Product_[4+2]

$G = -701.248636$ Hartree

C	0.43697400	1.06289900	0.62153500
C	1.42144300	1.52415700	-0.15757900
C	-0.65159500	0.18541400	0.07550000
C	-2.04674100	0.46320500	0.65047700
C	-3.12851000	-0.47194300	0.02864000
C	-2.53014500	1.90983700	0.34331900
H	-2.00932600	0.30499200	1.73936800
C	2.27272200	-1.39484800	0.04425400
C	1.06796100	-1.49195300	-0.52562800
C	3.58655600	-1.17004100	-0.64203300
C	-0.24750800	-1.34662600	0.21039700
C	-1.33622400	-2.16419700	-0.45649100
C	-2.60992500	-1.76301000	-0.53533600
C	-3.88463300	0.42081800	-0.97718900
H	-3.85235800	-0.72752200	0.82579400
C	-3.93990200	1.76987300	-0.25684400
H	-1.85462800	2.37178600	-0.39462300
H	-2.50750100	2.55739400	1.23242500
H	-4.21232200	2.60957000	-0.91492600
H	-4.69686900	1.72547800	0.54527400
H	-4.87332300	0.01785900	-1.24788900
H	-3.29788300	0.50925800	-1.90831200
C	2.73673400	2.10861300	0.25677700
C	4.37466200	0.03565200	-0.07657000
H	3.44103300	-1.05314800	-1.72983800
H	4.22773700	-2.06119600	-0.50730100
C	3.94153000	1.46307300	-0.46538000
H	5.41986900	-0.07932500	-0.40996600
H	4.40775600	-0.04588600	1.02571600
H	2.86382600	2.03829800	1.35085100
H	2.75725900	3.18675700	0.00940700
H	3.76124900	1.49957800	-1.55571800
H	4.81062200	2.11945700	-0.28991700
H	0.99328100	-1.46787000	-1.62069300
H	-1.04392200	-3.13710100	-0.86561900
H	-3.34774200	-2.40996100	-1.02380800
H	2.33306400	-1.37820700	1.13807200

H	1.31253500	1.37827200	-1.24073500
H	0.50990100	1.16631700	1.71161700
H	-0.70764700	0.36492300	-1.01196000
C	-0.14267000	-1.77579900	1.68751800
H	-1.12138600	-1.70686200	2.18177100
H	0.19587900	-2.82060000	1.75698700
H	0.56651600	-1.15300300	2.25181700

R1d TS_{CP}

$G = -701.216657$ Hartree

Imaginary frequency: -403.53 cm^{-1}

C	-0.45172000	-1.20597200	0.31311900
C	-1.71510800	-1.14025700	-0.27092300
C	0.66300500	-0.55886900	-0.22879600
C	2.03467000	-0.72131800	0.36134400
C	3.04256000	0.49605000	0.20903200
C	2.80190400	-1.92662100	-0.23896500
H	1.91179400	-0.91115300	1.43997700
C	-2.24701800	0.99275600	0.13907600
C	-1.11720300	1.59418600	-0.39992300
C	-3.61237800	1.09274700	-0.49634300
C	0.16355800	1.55128600	0.18847600
C	1.28345100	2.13819900	-0.58171200
C	2.54769500	1.68211000	-0.56832100
C	4.33727600	-0.11220000	-0.38158800
H	3.26981600	0.83279000	1.23655100
C	4.27832700	-1.59680500	-0.01489800
H	2.59870600	-1.98539300	-1.32229500
H	2.47691100	-2.88053300	0.20335400
H	4.96373800	-2.22147000	-0.60877700
H	4.54094000	-1.73824200	1.04841100
H	5.24338800	0.39887700	-0.02083000
H	4.32120700	-0.00856500	-1.48035700
C	-2.91533800	-1.87402400	0.27441000
C	-4.61106600	0.05163400	0.02098700
H	-3.52020500	1.01648600	-1.59469500
H	-4.02365500	2.10035100	-0.29792500
C	-4.24947700	-1.39801400	-0.31067500
H	-5.60934800	0.27624000	-0.39029300
H	-4.70129800	0.15964400	1.11769900
H	-2.93378100	-1.79223000	1.37602800
H	-2.80284200	-2.95268100	0.05478600
H	-4.21885300	-1.51957300	-1.40915100

H	-5.05479300	-2.06105100	0.04712100
H	-1.16110400	1.88360900	-1.45842600
H	1.03829500	2.96572900	-1.25765400
H	3.28832400	2.19132600	-1.19504500
H	-2.26779000	0.82514700	1.21962300
H	-1.74681600	-0.95425200	-1.34978600
H	-0.38026400	-1.57368900	1.34550100
H	0.64782400	-0.35857700	-1.30380100
C	0.29185800	1.54185800	1.70185000
H	1.31811600	1.33393200	2.02975100
H	0.01875100	2.53365000	2.10211100
H	-0.36702800	0.79915800	2.17121600

R1e reactant

$G = -701.234169$ Hartree

C	-0.25503500	-1.96347400	-0.10994800
C	-1.41018500	-1.63111800	-0.71829000
C	1.06579900	-1.52228500	-0.53243900
C	2.21714800	-1.89519800	0.06056400
C	3.03624100	1.17681300	0.55479600
C	3.61148000	-1.60378100	-0.41771400
H	2.15231500	-2.52852600	0.95674800
C	-2.18198800	1.00850200	0.86525400
C	-1.38670900	1.75983700	0.06525400
C	-3.67372900	0.93688600	0.91206900
C	0.05201400	1.57582900	0.18711100
C	1.02033500	2.16148100	-0.55676800
C	2.43796000	1.83382700	-0.45801200
C	4.43964400	0.66327100	0.52188500
H	2.45193900	0.92814600	1.44827500
C	4.51210600	-0.87654700	0.60410100
H	3.57467900	-1.03226200	-1.36044400
H	4.08698600	-2.57221500	-0.66130400
H	5.56232000	-1.17956600	0.45794600
H	4.24071800	-1.20520200	1.62306900
H	5.02788300	1.08000900	1.36047500
H	4.92972800	0.99952700	-0.40787500
C	-2.75049300	-2.23926300	-0.42177200
C	-4.22089600	-0.50056600	0.89574200
H	-4.12831200	1.50823700	0.08749900
H	-4.02569600	1.41856800	1.84518600
C	-3.97841500	-1.30765600	-0.39487400
H	-5.30769900	-0.43979200	1.07193600

H	-3.81099500	-1.05733300	1.75786300
H	-2.70002500	-2.81464300	0.51926600
H	-2.93936400	-2.98891300	-1.21524600
H	-3.93895200	-0.62254400	-1.26124900
H	-4.86224800	-1.94419600	-0.56351700
H	0.74080200	2.87638800	-1.33660400
H	3.05326300	2.10793400	-1.32421000
H	-1.67334200	0.34503200	1.57370500
H	-1.37147900	-0.93491200	-1.56558200
H	-0.28792300	-2.65428100	0.74311400
H	1.10819300	-0.87189600	-1.41342900
H	0.35525300	0.82910900	0.92565300
C	-1.89846500	2.72351400	-0.97342500
H	-1.50834500	3.73846900	-0.79045600
H	-1.55683600	2.43091300	-1.98078100
H	-2.99372300	2.78352100	-0.99124700

R1e TS_{AM}

$G = -701.204734$ Hartree

Imaginary frequency: -434.58 cm^{-1}

C	0.33675100	-1.51456500	0.05287600
C	1.60336400	-1.37943000	0.55018100
C	-0.83661900	-0.92982000	0.59434300
C	-2.12807800	-1.13802600	0.05812500
C	-2.94914400	0.51217800	-0.83825500
C	-3.36334400	-1.35319400	0.90953500
H	-2.12186600	-1.79114300	-0.82711900
C	2.15506100	0.93317700	-0.64133500
C	1.17964000	1.66183700	-0.00545500
C	3.63534600	0.98849000	-0.40178100
C	-0.17454000	1.47748600	-0.41396900
C	-1.29726600	2.08724100	0.14931600
C	-2.59939900	1.64800900	-0.06781600
C	-4.40874100	0.07660100	-0.83319500
H	-2.38653400	0.34769200	-1.76216600
C	-4.57267700	-1.23292700	-0.01835500
H	-3.39697700	-0.59591300	1.71186600
H	-3.33818000	-2.34237600	1.40020000
H	-5.52827700	-1.25785700	0.52834400
H	-4.57680200	-2.10094600	-0.69942600
H	-4.79207100	-0.05414800	-1.85729100
H	-5.01297800	0.87260800	-0.37011700
C	2.78059100	-2.17282000	0.05808900

C	4.39071500	-0.29758700	-0.76037800
H	3.85622600	1.25511100	0.64460600
H	4.05483800	1.81353100	-1.01169800
C	4.14925000	-1.48924200	0.17183000
H	5.46989500	-0.07043800	-0.75749400
H	4.14576700	-0.58997500	-1.79811200
H	2.60545300	-2.48416400	-0.98732700
H	2.83207900	-3.11403200	0.64128600
H	4.30915000	-1.16815900	1.21792800
H	4.92356300	-2.24825600	-0.03042400
H	-1.14888900	2.87044500	0.89811200
H	-3.38739500	2.09977800	0.54470100
H	1.85167900	0.38397700	-1.53712600
H	1.73743100	-0.83798700	1.49317700
H	0.21085000	-2.10353600	-0.86623400
H	-0.75027500	-0.42045100	1.55918100
H	-0.32443100	0.83345600	-1.28120700
C	1.46369500	2.52611200	1.19935500
H	1.08106800	3.54915900	1.05194800
H	0.96321300	2.12715300	2.09841400
H	2.53583000	2.60536300	1.41732000

R1e Product_[6+4]

$G = -701.256537$ Hartree

C	0.32189900	-1.33449900	-0.05821600
C	1.70930900	-0.87220500	0.28832500
C	-0.79738000	-0.90859300	0.54186800
C	-2.18872500	-1.09522000	0.02182300
C	-2.74211500	0.09591500	-0.85288600
C	-3.28456500	-1.27913800	1.09212200
H	-2.19548600	-1.96989800	-0.65191900
C	2.05076300	0.51139500	-0.42099800
C	1.03943100	1.55762500	-0.00569700
C	3.51244600	0.90509300	-0.15637900
C	-0.14377000	1.58693000	-0.65568300
C	-1.40516500	2.15244600	-0.17869600
C	-2.56769100	1.47158100	-0.24909500
C	-4.22323800	-0.30076100	-0.97177800
H	-2.23808800	0.06810900	-1.83308200
C	-4.61233800	-0.82067200	0.43217800
H	-3.04894400	-0.64655200	1.96322700
H	-3.32247400	-2.31696100	1.45633500
H	-5.08059700	-0.02111500	1.02724200

H	-5.35156200	-1.63346400	0.36867800
H	-4.31968300	-1.11011000	-1.71296800
H	-4.85888800	0.52997100	-1.31488700
C	2.75614300	-1.93737500	-0.08006200
C	4.50196400	-0.18764800	-0.56145900
H	3.64639300	1.11554000	0.91859500
H	3.73454500	1.84595400	-0.68722400
C	4.19578600	-1.49256600	0.17447700
H	5.53452000	0.14076300	-0.35707900
H	4.43710700	-0.35903800	-1.65151600
H	2.63939200	-2.18009900	-1.15269300
H	2.53379900	-2.86617000	0.47082900
H	4.34748600	-1.34172800	1.25901900
H	4.89732300	-2.28639300	-0.13128600
H	-1.40038300	3.12412000	0.32593100
H	-3.46106200	1.93468800	0.18520400
H	1.93663200	0.33131000	-1.50437000
H	1.76568500	-0.68355400	1.37566500
H	0.23223700	-1.94831100	-0.96549900
H	-0.70555200	-0.27057600	1.42877800
C	1.28271700	2.30054700	1.27941000
H	1.47778400	1.59998400	2.11157000
H	2.16851200	2.95340300	1.20928300
H	0.42616400	2.92352800	1.56736100
H	-0.22768200	0.94947400	-1.54071500

R1e Product_[4+2]

$G = -701.255638$ Hartree

C	0.34236800	-1.22588200	-0.46460200
C	1.32952700	-1.51873700	0.38790200
C	-0.73798800	-0.23353100	-0.15067600
C	-2.10497200	-0.59962000	-0.75047700
C	-3.18899900	0.45563600	-0.40360000
C	-2.65413400	-1.94295800	-0.18653000
H	-1.98179900	-0.65457500	-1.84510700
C	2.17258800	1.22629500	-0.60588600
C	1.03911500	1.55002800	0.03831000
C	3.58235100	1.15715400	-0.10055000
C	-0.28323300	1.19710800	-0.62041500
C	-1.38883400	2.19739800	-0.38889900
C	-2.67819300	1.85968400	-0.27257700
C	-3.89630700	-0.12494500	0.83679100
H	-3.93682400	0.45061900	-1.21960200

C	-4.00219300	-1.61357800	0.49154000
H	-1.94247000	-2.35244900	0.54734800
H	-2.76279900	-2.70800600	-0.96969500
H	-4.20820900	-2.25097500	1.36515800
H	-4.83310400	-1.76151600	-0.21886100
H	-4.86737500	0.35243500	1.04235500
H	-3.26148200	0.02332400	1.72763900
C	2.61464500	-2.22363500	0.08039100
C	4.26886300	-0.19893500	-0.38400300
H	3.63736300	1.37777400	0.97760400
H	4.18776800	1.93584100	-0.60155700
C	3.87332000	-1.41728400	0.47422000
H	5.35221500	-0.04504100	-0.24452500
H	4.14216000	-0.45088800	-1.45305300
H	2.65794100	-2.48930600	-0.98999200
H	2.65483200	-3.17647500	0.64073800
H	3.78197500	-1.10278100	1.53033700
H	4.72296900	-2.12036000	0.45013300
H	-1.10059200	3.25194500	-0.32786600
H	-3.42659000	2.64179400	-0.10145000
H	2.06090600	0.86621500	-1.63656600
H	1.25046800	-1.13030500	1.41252600
H	0.40780000	-1.56913200	-1.50624200
H	-0.85386900	-0.17971100	0.94576600
C	0.97675500	2.03325700	1.46113400
H	0.36570900	1.35609000	2.08313300
H	1.96956600	2.11597500	1.92275600
H	0.49425300	3.02277400	1.52559000
H	-0.09888900	1.13200600	-1.70900100

R1e TS_{CP}

$G = -701.220880$ Hartree

Imaginary frequency: -377.11 cm^{-1}

C	0.34001400	-1.36097200	-0.00669300
C	1.63773300	-1.19407900	0.44766800
C	-0.74957800	-0.57564500	0.40363400
C	-2.13480600	-0.86356700	-0.10398200
C	-2.94891400	0.31637100	-0.78305600
C	-3.12339900	-1.37594800	0.95563400
H	-2.04709400	-1.64522600	-0.87841300
C	2.11324000	0.81360100	-0.59272700
C	1.08895900	1.56508100	-0.02487900
C	3.57294000	0.97131400	-0.25419200

C	-0.23638900	1.35586600	-0.48141100
C	-1.40064300	2.11356200	-0.02629800
C	-2.65797800	1.65248900	-0.17050800
C	-4.43730500	-0.11443300	-0.65596500
H	-2.64015400	0.34510200	-1.84225300
C	-4.45905400	-1.39663000	0.20892100
H	-3.15624300	-0.65814900	1.79445100
H	-2.83227400	-2.35427100	1.36859000
H	-5.33248000	-1.44470500	0.87728400
H	-4.49882100	-2.29059400	-0.43560100
H	-4.90178500	-0.28183400	-1.63916900
H	-5.01556900	0.68677600	-0.16986200
C	2.76810500	-2.08307200	-0.00639400
C	4.44002200	-0.22805800	-0.65056700
H	3.69990000	1.16382800	0.82412900
H	3.95816100	1.87529400	-0.76533000
C	4.16922900	-1.48996400	0.17140400
H	5.50183500	0.04857300	-0.54092500
H	4.28970300	-0.44986200	-1.72316800
H	2.61241600	-2.35944700	-1.06450200
H	2.72047200	-3.03211100	0.56153900
H	4.33159800	-1.26241700	1.24121300
H	4.91366000	-2.25978800	-0.09216100
H	-1.24132700	3.06529000	0.48905000
H	-3.49741500	2.24853100	0.20083900
H	1.91497600	0.37274800	-1.57431200
H	1.78019500	-0.70848200	1.41965400
H	0.19622800	-1.98654900	-0.89843600
H	-0.69783100	-0.12481200	1.39896200
C	1.34995100	2.32449200	1.25441700
H	1.55862800	1.63019200	2.09047700
H	2.22467000	2.98699400	1.16557800
H	0.49450800	2.94035500	1.55896300
H	-0.32871500	0.91210100	-1.47663300

R1f reactant

$G = -701.234351$ Hartree

C	0.28139100	1.76338300	0.08152100
C	1.38442200	1.55895400	-0.66376500
C	-1.07696900	1.50200700	-0.37049200
C	-2.19058800	1.73347800	0.35243400
C	-3.10513900	-1.30632500	0.18078600
C	-3.60830200	1.63498300	-0.13910700

H	-2.07277100	2.09441300	1.38399600
C	2.25585200	-1.31818900	0.52722800
C	1.30777300	-1.72941400	-0.35092600
C	3.71164900	-1.34477700	0.14580800
C	-0.11705600	-1.63391700	-0.16010200
C	-1.05391300	-1.97886600	-1.07783100
C	-2.47752900	-1.70444400	-0.94380000
C	-4.49784700	-0.76951600	0.23902900
H	-2.54398800	-1.27883700	1.12206900
C	-4.53229100	0.70977200	0.68070300
H	-3.61648500	1.32853600	-1.19897100
H	-4.03996100	2.65313700	-0.11003600
H	-5.57312500	1.06721000	0.60856500
H	-4.26014800	0.78149100	1.74896800
H	-5.11605300	-1.35369800	0.94572000
H	-4.97148100	-0.86413100	-0.75309900
C	2.77548100	2.00153800	-0.30906900
C	4.43582600	0.01241600	0.20918700
H	3.81796600	-1.75999700	-0.87001200
H	4.24698400	-2.03576800	0.82548700
C	3.95268600	1.10776900	-0.75736400
H	5.49959900	-0.18477300	-0.00593000
H	4.41522700	0.40333200	1.24156400
H	2.84495200	2.20814800	0.77362200
H	2.92182700	2.98426200	-0.79807000
H	3.71755100	0.65804800	-1.73923700
H	4.81081600	1.77541300	-0.93794800
H	0.39004200	2.19325000	1.08607200
H	-1.18307400	1.12115800	-1.39270000
H	1.64307100	-2.10916600	-1.32339700
H	-0.45849500	-1.16158400	0.76257100
H	-0.72084200	-2.41076200	-2.02850100
H	-3.06567100	-1.75627400	-1.86839200
H	1.26009900	1.12181800	-1.66256900
C	1.95277800	-0.81397400	1.91131000
H	0.92258000	-1.01820500	2.22724600
H	2.63205100	-1.28108000	2.64520500
H	2.10999000	0.27479400	1.98450300

R1f TS_{AM}

$G = -701.203191$ Hartree

Imaginary frequency: -416.82 cm^{-1}

C	0.33416200	1.39750500	0.15362200
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C	1.53860000	1.36334800	-0.48897500
C	-0.89068500	0.97311700	-0.42930000
C	-2.15523000	1.03137300	0.20160400
C	-3.03767200	-0.81249800	0.44263600
C	-3.39033700	1.58741800	-0.48253100
H	-2.09915300	1.34117800	1.25636200
C	2.15491200	-1.18594200	0.30523300
C	1.10940100	-1.63997000	-0.45996000
C	3.56403700	-1.23001900	-0.23725300
C	-0.25717800	-1.59512100	-0.09413600
C	-1.32422100	-1.99518700	-0.90375100
C	-2.64168700	-1.64079900	-0.63872200
C	-4.49520300	-0.38156200	0.51696500
H	-2.52910700	-0.97254500	1.39855300
C	-4.60289100	1.14984200	0.33737300
H	-3.44888200	1.19799800	-1.51403700
H	-3.33425100	2.68805400	-0.55613000
H	-5.55805600	1.44257300	-0.12644900
H	-4.56173200	1.64982300	1.32056600
H	-4.96097900	-0.69830700	1.46398200
H	-5.05168700	-0.88045600	-0.29256900
C	2.81425600	1.98093000	0.00129100
C	4.47422300	-0.04003300	0.10522800
H	3.52916700	-1.36054500	-1.33170700
H	4.05153600	-2.14125800	0.16436900
C	4.09956000	1.31180100	-0.51167400
H	5.49122300	-0.29727500	-0.23555600
H	4.55193800	0.06885700	1.20093000
H	2.81860900	2.02762200	1.10548700
H	2.83779800	3.03754000	-0.33163800
H	4.02738900	1.20161400	-1.60954700
H	4.93899800	2.00503700	-0.33500200
H	0.30298600	1.75027700	1.19298300
H	-0.87245600	0.75337000	-1.50181800
H	1.33353100	-1.94008500	-1.49087400
H	-0.49505100	-1.26337200	0.91513700
H	-1.09761600	-2.49004600	-1.85460700
H	-3.39003100	-1.85647000	-1.40892600
H	1.54692700	1.02081300	-1.52989500
C	2.02791400	-0.90270000	1.77703700
H	0.99183700	-0.93707600	2.13215000
H	2.60284500	-1.65480100	2.34893800
H	2.44246200	0.07847200	2.05119400

R1f Product_[6+4] $G = -701.249722$ Hartree

C	-0.29842800	-1.17668300	0.34031700
C	-1.64160800	-0.80462600	-0.22147400
C	0.85058900	-0.96262000	-0.31603300
C	2.23457700	-0.98674200	0.25064000
C	2.82033900	0.43761600	0.60657200
C	3.31316200	-1.59180200	-0.67635900
H	2.22280600	-1.54293000	1.20409000
C	-2.03630300	0.71460200	0.12869600
C	-0.98061000	1.57907900	-0.52015100
C	-3.41452100	1.00637400	-0.50886400
C	0.23230600	1.78760100	0.01953700
C	1.45226700	2.12429200	-0.70982900
C	2.61855800	1.49312100	-0.45945000
C	4.30372100	0.09779400	0.82450400
H	2.34907700	0.78008300	1.54211700
C	4.65293200	-0.90806600	-0.29477500
H	3.05480400	-1.37480500	-1.72530400
H	3.35027400	-2.68759700	-0.58246000
H	5.07669900	-0.38488000	-1.16630700
H	5.41556400	-1.62987800	0.03455600
H	4.41982600	-0.38086800	1.81018000
H	4.94875900	0.98995300	0.81953700
C	-2.75500900	-1.78273200	0.18577000
C	-4.51286400	0.01415600	-0.11963000
H	-3.29468600	0.98598900	-1.60704800
H	-3.71559900	2.03584700	-0.25085700
C	-4.10286000	-1.42410200	-0.44358700
H	-5.44724300	0.27283000	-0.64480200
H	-4.73661400	0.09988300	0.95756000
H	-2.84741600	-1.79978300	1.28601700
H	-2.45644500	-2.80196700	-0.10972800
H	-4.02589900	-1.53784300	-1.54049800
H	-4.88040200	-2.13199300	-0.11149800
H	-0.26696900	-1.50861400	1.38643700
H	0.78764400	-0.61504400	-1.35384200
H	-1.13806400	1.81253500	-1.58132500
H	0.38429900	1.48273000	1.05682900
H	1.38852900	2.82028500	-1.55373200
H	3.47998500	1.72525300	-1.09584700
H	-1.56511600	-0.82903200	-1.32257400
C	-2.09663400	0.92607400	1.64977000

H	-2.31454300	1.98095300	1.87673900
H	-2.87831400	0.31174400	2.11714500
H	-1.14864800	0.66713000	2.14069400

R1f Product_[4+2]

$G = -701.252780$ Hartree

C	0.21247900	1.05088300	0.64715400
C	1.13224700	1.55976000	-0.17960300
C	-0.87941400	0.15515100	0.13966700
C	-2.22436800	0.27069000	0.87105500
C	-3.30006000	-0.60664000	0.18371000
C	-2.83312300	1.67831300	0.80956000
H	-2.06914500	-0.05151300	1.91532400
C	2.13443400	-1.36209000	0.05334400
C	0.92786200	-1.44419600	-0.53417600
C	3.38770600	-1.09092200	-0.74423300
C	-0.39179000	-1.34128300	0.17684500
C	-1.47597800	-2.23551700	-0.37664700
C	-2.77141400	-1.89792000	-0.37545600
C	-3.97372900	0.32051600	-0.88250800
H	-4.06461700	-0.85383100	0.94158300
C	-3.46435500	1.75352100	-0.58971500
H	-2.09334600	2.47222000	0.99398200
H	-3.61599100	1.76800300	1.58209400
H	-2.69922600	2.04429300	-1.32681300
H	-4.26290300	2.50842800	-0.65184600
H	-5.07025800	0.25881900	-0.80849200
H	-3.70802800	0.00297400	-1.90207900
C	2.46378000	2.15711000	0.15855100
C	4.17727300	0.17022200	-0.31757300
H	3.14334800	-1.02431400	-1.81747500
H	4.07845300	-1.94783400	-0.63011400
C	3.62415100	1.56337500	-0.67431400
H	5.16709200	0.09457800	-0.79889700
H	4.38182300	0.12947600	0.76624400
H	2.67318100	2.05725300	1.23774700
H	2.44302200	3.24261900	-0.05326200
H	3.33252200	1.57372700	-1.74081500
H	4.47044100	2.26657500	-0.59512300
H	0.35811400	1.10307100	1.73435700
H	-1.03789600	0.38761100	-0.92756200
H	0.87905100	-1.37235800	-1.62800200
H	-0.24546000	-1.59987500	1.24030100

H	-1.16429500	-3.20129900	-0.78766700
H	-3.50750300	-2.58846800	-0.80263100
H	0.94857400	1.45070800	-1.25714100
C	2.33299000	-1.43212500	1.54698100
H	3.28077500	-1.94034000	1.79050200
H	2.38747700	-0.42403100	1.99294700
H	1.52264300	-1.96958100	2.05697200

R1f TS_{CP}

$G = -701.218477$ Hartree

Imaginary frequency: -348.85 cm^{-1}

C	0.34198900	1.27141600	0.28053600
C	1.56938500	1.18386200	-0.36166000
C	-0.81524400	0.67620200	-0.23576400
C	-2.16444300	0.78597500	0.41018600
C	-2.98238400	-0.56348000	0.59017300
C	-3.14540900	1.73076600	-0.35782300
H	-2.02099700	1.18474200	1.42767300
C	2.07861300	-1.04874400	0.20138900
C	0.97910100	-1.56666000	-0.48027300
C	3.45230000	-1.17199200	-0.43006800
C	-0.34399800	-1.50714800	-0.02246900
C	-1.48877700	-1.97917800	-0.79171000
C	-2.73694400	-1.55153700	-0.51177900
C	-4.43302200	-0.06908000	0.65569600
H	-2.66851900	-1.01293900	1.54808600
C	-4.49978100	0.99557800	-0.44640800
H	-2.75422100	1.97842200	-1.35597000
H	-3.24121100	2.68465500	0.18362700
H	-4.59598900	0.50037900	-1.42666500
H	-5.36309600	1.67085200	-0.34334000
H	-4.62385900	0.39258400	1.63928200
H	-5.16606700	-0.88062600	0.52559400
C	2.81495100	1.90030500	0.08211900
C	4.47078900	-0.08465100	-0.06256700
H	3.34074800	-1.21065600	-1.52711000
H	3.87832000	-2.15064600	-0.13288100
C	4.10515400	1.32967900	-0.51966400
H	5.43994500	-0.36000000	-0.51111100
H	4.63963500	-0.08379300	1.02814300
H	2.87652000	1.91073800	1.18506800
H	2.73518500	2.96311000	-0.21719300
H	4.01384800	1.33963400	-1.62153400

H	4.94093200	2.00745900	-0.27812000
H	0.31925200	1.64150200	1.31383400
H	-0.83895600	0.51156000	-1.31597400
H	1.12594000	-1.81714500	-1.53884000
H	-0.50941400	-1.40130100	1.05061000
H	-1.30632600	-2.63157500	-1.65270800
H	-3.58328500	-1.88446000	-1.12090700
H	1.54991400	0.92010200	-1.42376600
C	2.06409400	-0.92423300	1.70571100
H	2.48531300	-1.84137500	2.15800700
H	2.67486700	-0.08416500	2.06442900
H	1.05327700	-0.78954600	2.10802100

R2a reactant

$G = -740.525994$ Hartree

C	-0.51927800	1.32478400	-0.70497100
C	-1.69220400	1.41201800	-0.04980100
C	0.82010300	1.23089300	-0.11374500
C	1.89865800	1.19425800	-0.93473000
C	2.84276900	-1.66396000	-0.34136500
C	3.35557300	1.27503100	-0.57363300
H	1.70194900	1.18183000	-2.01532500
C	-2.47782100	-1.64403100	-0.32121300
C	-1.52433700	-1.99336500	0.56574300
C	-3.94886500	-1.59699400	-0.05899600
C	-0.11621300	-1.93259000	0.26045600
C	0.89073600	-2.16179400	1.13783800
C	2.29836300	-1.91283200	0.86692700
C	4.23161900	-1.15896200	-0.56419200
H	2.21903100	-1.76200500	-1.23700200
C	4.24645200	0.21983100	-1.25637100
H	3.49935200	1.23234900	0.51746100
H	3.71799600	2.27317400	-0.88622200
H	5.28779400	0.58104600	-1.29335600
H	3.92607100	0.10653200	-2.30776300
H	4.80931700	-1.86401900	-1.19069800
H	4.75724600	-1.08919600	0.40347700
C	-3.02178400	1.69731200	-0.69111300
C	-4.66041400	-0.36835500	-0.64616500
H	-4.13811500	-1.66094600	1.02672200
H	-4.42331500	-2.49397400	-0.50373700
C	-4.26715700	1.01051900	-0.08984700
H	-5.74239300	-0.50700400	-0.48216200

H	-4.52564500	-0.36310700	-1.74349800
H	-2.96997600	1.50383600	-1.77701100
H	-3.18699000	2.78837100	-0.59787200
H	-4.16077800	0.95206800	1.00886600
H	-5.12280200	1.68254600	-0.26669200
H	-1.81178400	-2.27493900	1.58679900
H	0.13246200	-1.58979000	-0.74800500
H	0.63168200	-2.46412800	2.15889300
H	2.95111200	-1.84920400	1.74623300
H	-2.15856400	-1.36298500	-1.33223200
H	-1.69952600	1.37149300	1.04494900
H	-0.54105900	1.36330000	-1.80195200
C	0.95581300	1.27944400	1.39116900
H	0.12244200	0.72595100	1.84887300
H	1.86529300	0.74000300	1.69279300
C	0.99496100	2.71079300	1.94164600
H	0.09091400	3.27069100	1.65576100
H	1.06389700	2.71413700	3.04157200
H	1.86255200	3.26196000	1.54531200

R2a TS_{AM}

$G = -740.498387$ Hartree

Imaginary frequency: -449.81 cm^{-1}

C	0.51331500	-0.99670800	-0.67091100
C	1.77719200	-1.11853000	-0.15263900
C	-0.69701200	-0.80638000	0.05116100
C	-1.93052400	-0.70373600	-0.65611000
C	-2.75776700	1.16431100	-0.63389500
C	-3.22244400	-1.37237600	-0.22297100
H	-1.79405300	-0.78570300	-1.74357700
C	2.37985400	1.40612400	-0.19176400
C	1.34306400	1.86509200	0.57801200
C	3.81402800	1.34140800	0.24681700
C	0.01019800	1.89971900	0.11745900
C	-1.10298000	2.19209400	0.90813200
C	-2.40397000	1.85197200	0.55724700
C	-4.21902300	0.78768900	-0.83504100
H	-2.21282000	1.45631800	-1.53716900
C	-4.34819200	-0.73473100	-1.03557800
H	-3.39717500	-1.22061700	0.85484400
H	-3.17253600	-2.46238200	-0.39331200
H	-5.34459600	-1.10428900	-0.74635200
H	-4.20917400	-0.99186500	-2.10009300

H	-4.66224100	1.33721700	-1.68159000
H	-4.78436500	1.08053400	0.06456600
C	2.97240700	-1.56592600	-0.94873200
C	4.67790900	0.35842500	-0.55151000
H	3.86809300	1.10774100	1.32492700
H	4.26029200	2.34999500	0.13890300
C	4.33181400	-1.12449500	-0.38951500
H	5.73109900	0.50471700	-0.25848900
H	4.62264500	0.62491200	-1.62322400
H	2.87112400	-1.24198800	-2.00041400
H	2.96993800	-2.67350400	-0.98160800
H	4.38300900	-1.39559300	0.68133200
H	5.11832800	-1.71620000	-0.88721500
H	1.52507300	2.07905100	1.63919100
H	-0.14812600	1.66191400	-0.93582400
H	-0.92514800	2.57213600	1.92023000
H	-3.18111500	1.97134000	1.31987100
H	2.19852900	1.27947500	-1.26334200
H	1.90183200	-1.14206000	0.93371100
H	0.41820700	-1.02054700	-1.76472000
C	-0.71683000	-0.92693700	1.55589800
H	0.17844900	-0.44900700	1.98079600
H	-1.57625500	-0.35902900	1.94613400
C	-0.79076100	-2.38161300	2.04251200
H	0.07901100	-2.95600500	1.68695300
H	-0.80572900	-2.43031500	3.14345900
H	-1.69397200	-2.88865700	1.67057700

R2a Product_[6+4]

$G = -740.545337$ Hartree

C	0.43854200	-0.71532300	-0.67017100
C	1.83925400	-0.55209500	-0.15827800
C	-0.69867200	-0.74706300	0.05242400
C	-2.02652300	-0.57638600	-0.64396300
C	-2.64061400	0.90182300	-0.62432200
C	-3.19935800	-1.46350900	-0.20490400
H	-1.85852700	-0.78902800	-1.71261600
C	2.27484300	0.97626800	-0.22196900
C	1.29034300	1.79675000	0.55640900
C	3.72397300	1.13887400	0.25422300
C	0.06935300	2.06932700	0.06133800
C	-1.12526400	2.33427900	0.85188100
C	-2.32074100	1.77676400	0.56861900

C	-4.17219800	0.66908200	-0.78509700
H	-2.23981100	1.40350100	-1.51939700
C	-4.38345600	-0.84715300	-0.95328300
H	-3.35932800	-1.38700100	0.88412300
H	-3.03339100	-2.52602700	-0.44188600
H	-5.36369100	-1.18322100	-0.58154300
H	-4.32686400	-1.12848100	-2.01855900
H	-4.59472800	1.24656500	-1.62110300
H	-4.68985300	1.01263800	0.12486900
C	2.84647000	-1.41551500	-0.93636000
C	4.70053000	0.24999900	-0.51813800
H	3.77125800	0.88636500	1.32993100
H	4.01776000	2.19837700	0.17177300
C	4.28448500	-1.22123000	-0.45206100
H	5.72393400	0.38008500	-0.12887900
H	4.72524800	0.57248200	-1.57513200
H	2.78141600	-1.15399100	-2.00888500
H	2.55242700	-2.47511300	-0.85847800
H	4.36602400	-1.57491500	0.59208200
H	4.97331300	-1.84423500	-1.04646900
H	1.48387600	1.92714600	1.62935400
H	-0.09594600	1.87159200	-1.00178100
H	-1.01199500	2.89138900	1.78870700
H	-3.13758700	1.94279200	1.27975000
H	2.21927600	1.26280600	-1.28855100
H	1.88993400	-0.84583700	0.90290300
C	-0.70176900	-0.88654900	1.55965400
H	-1.63622800	-0.47357200	1.96604600
H	0.10423800	-0.27740900	1.99594900
H	0.34142700	-0.63929700	-1.76195800
C	-0.54674700	-2.34363500	2.01552100
H	-0.57398400	-2.42288600	3.11453600
H	-1.35137100	-2.97730300	1.61093500
H	0.40846100	-2.76566900	1.66513800

R2a Product_[4+2]

$G = -740.530372$ Hartree

C	0.53080600	-0.90257600	-0.65140700
C	1.58832200	-1.35792300	0.02903300
C	-0.57036400	-0.04362400	-0.07096400
C	-1.84158400	-0.14227400	-0.96159300
C	-2.96404100	0.85119700	-0.56284800
C	-2.54367700	-1.52501300	-1.02717500

H	-1.48937000	0.12501900	-1.97047500
C	2.39082000	1.50253400	-0.28131100
C	1.25583600	1.70596100	0.39746800
C	3.78489900	1.36578200	0.24910800
C	-0.08034500	1.47663700	-0.24788200
C	-1.17671600	2.43007400	0.17020200
C	-2.47561300	2.13990000	0.03175700
C	-3.93422600	0.02159400	0.30179900
H	-3.51544100	1.10280700	-1.49012800
C	-3.94997500	-1.35018300	-0.39233000
H	-1.94909400	-2.29485900	-0.52009600
H	-2.63542300	-1.85501400	-2.07274500
H	-4.20929400	-2.16773600	0.29800800
H	-4.71852900	-1.35110300	-1.18200700
H	-4.93392300	0.47871000	0.37058900
H	-3.54716300	-0.06219100	1.32825500
C	2.86787300	-1.90551600	-0.52907700
C	4.53996200	0.15456600	-0.34239900
H	3.77656700	1.31195100	1.35138900
H	4.37048500	2.26699900	-0.01379600
C	4.13138100	-1.26601100	0.09223000
H	5.60436300	0.27727800	-0.07993300
H	4.49952800	0.21802900	-1.44560500
H	2.88828700	-1.80304600	-1.62792200
H	2.92349400	-2.98992500	-0.31741700
H	4.03882700	-1.29526100	1.19376000
H	4.98003200	-1.92829300	-0.14845000
H	1.28599500	1.87336800	1.48078400
H	0.07249500	1.59916400	-1.33527100
H	-0.87295100	3.39348200	0.59210100
H	-3.23425400	2.86505100	0.34644900
H	2.30109200	1.32844000	-1.36195400
H	1.58829200	-1.26196300	1.12009400
C	-0.78305900	-0.29899500	1.44362700
H	-1.50740800	0.43396300	1.82279300
H	0.16081800	-0.04234800	1.94790200
H	0.54513000	-0.96962800	-1.74761500
C	-1.19253700	-1.69947000	1.90671600
H	-1.10666600	-1.76726100	3.00336200
H	-2.23239200	-1.94511300	1.65386000
H	-0.55008100	-2.48047500	1.47434200

R2a TS_{CP} $G = -740.508677$ HartreeImaginary frequency: -306.90 cm^{-1}

C	0.51251200	-0.94684400	-0.59420800
C	1.79232800	-1.03676000	-0.08716500
C	-0.61937500	-0.47539300	0.11147100
C	-1.93970500	-0.45464700	-0.62742500
C	-2.78007300	0.91600500	-0.67553200
C	-2.99934100	-1.48922700	-0.20017300
H	-1.70829700	-0.67351600	-1.68243400
C	2.29960000	1.29797500	-0.27608200
C	1.23233100	1.78358900	0.44810800
C	3.73071100	1.32545100	0.18726400
C	-0.09307000	1.72836100	-0.02605200
C	-1.22449200	2.24576500	0.72291800
C	-2.48879300	1.88021200	0.42913800
C	-4.26377500	0.47334000	-0.74360700
H	-2.48823400	1.39150900	-1.62763300
C	-4.25029800	-1.04701700	-0.95881200
H	-3.18491500	-1.42117600	0.88435800
H	-2.68694000	-2.52144700	-0.42111600
H	-5.17258800	-1.53848300	-0.61209100
H	-4.13634700	-1.28486000	-2.03062300
H	-4.82733100	1.01112900	-1.52100600
H	-4.75331300	0.69814400	0.21858600
C	2.96105900	-1.60458100	-0.84713600
C	4.64452300	0.34229300	-0.55401900
H	3.77698100	1.14125700	1.27527700
H	4.13206800	2.34654900	0.03816900
C	4.32992400	-1.13984000	-0.33402200
H	5.68737400	0.53170300	-0.24938700
H	4.59940600	0.56258100	-1.63660500
H	2.85987700	-1.37398300	-1.92292100
H	2.92602500	-2.70880700	-0.77389700
H	4.40187700	-1.36899400	0.74533300
H	5.11301300	-1.74207500	-0.82423100
H	1.38824600	2.03275300	1.50578600
H	-0.22547600	1.63760900	-1.10653800
H	-1.02352600	2.87066800	1.59971300
H	-3.32146000	2.24384600	1.03907200
H	2.16024200	1.18095600	-1.35544600
H	1.92751600	-0.99578500	0.99674900
C	-0.65096200	-0.62108800	1.62623200

H	-1.54105400	-0.10925900	2.01954800
H	0.21207300	-0.09676900	2.06378900
H	0.39998300	-1.06665400	-1.67994400
C	-0.63315100	-2.07572800	2.11778400
H	0.27693100	-2.59554900	1.78203400
H	-0.65958800	-2.11193700	3.21918900
H	-1.49225500	-2.65060200	1.74418800

R2b reactant

$G = -779.817319$ Hartree

C	-0.52232700	0.99456400	-0.94649500
C	-1.69971900	1.18842200	-0.32351500
C	0.81710300	0.98800500	-0.34821800
C	1.88981100	0.79994900	-1.15746900
C	2.77326300	-1.96653000	-0.17960200
C	3.35023900	0.89198100	-0.81279600
H	1.68706800	0.62311600	-2.22232100
C	-2.54156700	-1.84041700	-0.09809600
C	-1.58303800	-2.06177900	0.82392700
C	-4.00861400	-1.72546300	0.16598900
C	-0.17865000	-2.07593800	0.49734100
C	0.83755800	-2.19512500	1.38560100
C	2.24549500	-2.02546300	1.06019900
C	4.17064700	-1.53808900	-0.49130200
H	2.13071300	-2.17300800	-1.04287000
C	4.20882300	-0.26362700	-1.36064900
H	3.49845600	0.97813700	0.27500200
H	3.73714800	1.83452300	-1.24556000
H	5.25764000	0.06388600	-1.45485300
H	3.87252900	-0.50669100	-2.38465100
H	4.71583200	-2.33717300	-1.02737200
H	4.71733100	-1.35580900	0.44965600
C	-3.02051300	1.38421800	-1.01473800
C	-4.70725400	-0.60315300	-0.61651100
H	-4.18599400	-1.60001100	1.24834900
H	-4.50166300	-2.67714200	-0.11453600
C	-4.28267200	0.84257700	-0.30991700
H	-5.78936000	-0.69040300	-0.42089700
H	-4.58600700	-0.78908600	-1.69961900
H	-2.97039800	1.00298400	-2.04990100
H	-3.15998500	2.47833400	-1.11499400
H	-4.17927100	0.97603800	0.78252600
H	-5.12238100	1.49198500	-0.60694400

H	-1.86161600	-2.17353700	1.87952000
H	0.06103700	-1.89474700	-0.55434900
H	0.58990100	-2.33623200	2.44375000
H	2.91693100	-1.85696000	1.91112700
H	-2.22972200	-1.73016300	-1.14386200
H	-1.71666600	1.32208200	0.76280200
H	-0.53943300	0.85581000	-2.03556700
C	0.98358300	1.26052900	1.13107500
H	0.07125600	0.96562700	1.67049000
H	1.77803800	0.60582500	1.51969800
C	1.33366300	2.72058800	1.47204700
H	1.52030800	2.78730600	2.55864100
H	2.28809000	2.98170900	0.98337100
C	0.27138300	3.74453600	1.07552900
H	0.58516200	4.76561700	1.34581000
H	0.07936500	3.72429100	-0.00824000
H	-0.68758800	3.54499900	1.58139200

R2b TS_{AM}

$G = -779.789731$ Hartree

Imaginary frequency: -437.09 cm^{-1}

C	-0.50543000	0.63863200	-0.90363200
C	-1.78336100	0.81595900	-0.42722000
C	0.70758100	0.63961900	-0.16580000
C	1.93586300	0.38477400	-0.84546300
C	2.73958200	-1.46707300	-0.45152400
C	3.24597500	1.09726700	-0.56775600
H	1.79087800	0.24135000	-1.92529300
C	-2.38112600	-1.59295100	0.04149000
C	-1.35011700	-1.91066500	0.89362800
C	-3.81588200	-1.44506800	0.46096300
C	-0.02258000	-2.04790900	0.45105800
C	1.09621500	-2.17110100	1.27722900
C	2.39285500	-1.90030100	0.85548400
C	4.20169300	-1.15808100	-0.73930200
H	2.17866900	-1.92213200	-1.27366300
C	4.34712800	0.28791300	-1.25066500
H	3.43682200	1.15538800	0.51619800
H	3.21564700	2.13358000	-0.94831300
H	5.35343600	0.69203500	-1.05821200
H	4.19213300	0.32379500	-2.34307700
H	4.62834000	-1.87664600	-1.45824300
H	4.77463900	-1.26681000	0.19590700

C	-2.96278400	1.10850400	-1.31526600
C	-4.68745300	-0.66376700	-0.52773900
H	-3.86881700	-0.98251300	1.46264100
H	-4.25345100	-2.45633500	0.57775300
C	-4.33424500	0.81624300	-0.69434900
H	-5.73901300	-0.74063400	-0.20411600
H	-4.63722700	-1.15861700	-1.51525300
H	-2.85800900	0.57140500	-2.27553300
H	-2.93595200	2.18489600	-1.57690000
H	-4.39509900	1.31786900	0.28922400
H	-5.10826100	1.28875500	-1.32206000
H	-1.53579800	-1.90459200	1.97546800
H	0.13478600	-2.01118200	-0.62855900
H	0.92753300	-2.34493800	2.34571900
H	3.17626700	-1.86669600	1.62034800
H	-2.20383600	-1.70849400	-1.03182500
H	-1.92102400	1.06577400	0.62744800
H	-0.40403200	0.44125000	-1.97936500
C	0.74568100	1.04089800	1.28863900
H	-0.19099300	0.74581400	1.78581100
H	1.54497600	0.46225800	1.77987600
C	0.99796300	2.54110100	1.54856700
H	1.12694400	2.67782500	2.63682800
H	1.95648600	2.83721000	1.09320700
C	-0.10274300	3.47581900	1.04992600
H	0.14146800	4.52674500	1.27373200
H	-0.24633900	3.38487200	-0.03749400
H	-1.07007700	3.24988800	1.52812600

R2b Product_[6+4]

$G = -779.837968$ Hartree

C	-0.47684300	0.11215000	-1.03842900
C	-1.86884900	0.24187200	-0.49431600
C	0.67485400	0.45490000	-0.42813800
C	1.98630300	-0.05391000	-0.97402100
C	2.58035900	-1.35857600	-0.26163500
C	3.17863800	0.91119100	-1.01968400
H	1.80103400	-0.36962500	-2.01393600
C	-2.32906500	-1.12653200	0.17262200
C	-1.34226100	-1.50575900	1.23599500
C	-3.77088900	-1.01359900	0.68409200
C	-0.13491200	-2.00635300	0.91676400
C	1.06938900	-1.89188500	1.72844900

C	2.26774300	-1.55909300	1.20565500
C	4.11221500	-1.25986000	-0.52502800
H	2.15857100	-2.21599700	-0.80974300
C	4.34115100	-0.01040300	-1.39563000
H	3.35613800	1.35790400	-0.02647400
H	3.02295200	1.73690100	-1.73143400
H	5.33218700	0.44204800	-1.23707200
H	4.26977400	-0.26787400	-2.46603900
H	4.51397700	-2.17348200	-0.98852600
H	4.63925600	-1.13907400	0.43502900
C	-2.87841900	0.66332000	-1.57524900
C	-4.74877800	-0.56858000	-0.40493200
H	-3.79300600	-0.28497300	1.51582600
H	-4.08251600	-1.98092700	1.11165500
C	-4.30901300	0.75207300	-1.04074900
H	-5.76616200	-0.47773300	0.01038100
H	-4.79931100	-1.34817200	-1.18693800
H	-2.83958600	-0.07157900	-2.40068200
H	-2.56629900	1.62875000	-2.00628800
H	-4.36376100	1.55551200	-0.28345700
H	-5.00020000	1.03979400	-1.85032900
H	-1.51715900	-1.11042200	2.24535200
H	0.01423200	-2.33714600	-0.11521900
H	0.96406000	-1.93749200	2.81824600
H	3.09386700	-1.38609800	1.90429200
H	-2.29845500	-1.88228100	-0.63404000
H	-1.89205500	1.00058300	0.30493700
C	0.70896300	1.28726600	0.83323300
H	1.64924900	1.10519400	1.37490500
H	-0.09209800	0.97160500	1.51996200
H	-0.40310600	-0.47228500	-1.96585900
C	0.57226400	2.79333000	0.56018100
H	1.36234700	3.10972200	-0.14191800
H	-0.38164800	2.97553100	0.03587700
C	0.64059500	3.63455500	1.83282300
H	0.53403800	4.70946800	1.61677700
H	-0.15900500	3.35378300	2.53871600
H	1.60200900	3.49170800	2.35396400

R2b Product_[4+2]

$G = -779.822927$ Hartree

C	-0.59992600	0.47197200	-1.06211100
C	-1.61926700	1.17649600	-0.55891800

C	0.50267200	-0.16310000	-0.24483300
C	1.74472500	-0.42427000	-1.14365700
C	2.85857200	-1.24819000	-0.44658700
C	2.47300300	0.82446500	-1.70850400
H	1.35359300	-1.01816700	-1.98486100
C	-2.49676400	-1.58374100	0.18007000
C	-1.34240200	-1.57560100	0.85655700
C	-3.86648000	-1.22143300	0.66602000
C	-0.02586100	-1.63222800	0.13693300
C	1.06362200	-2.41305400	0.83623900
C	2.36305000	-2.23065500	0.57423000
C	3.87325700	-0.19795400	0.04821200
H	3.37466700	-1.82608800	-1.23833300
C	3.89517300	0.84089300	-1.08504900
H	1.91118400	1.74145000	-1.49178500
H	2.53776500	0.76270500	-2.80510800
H	4.19330100	1.84061500	-0.73310800
H	4.63778200	0.54032000	-1.84163800
H	4.86487400	-0.63235200	0.25081500
H	3.52129500	0.25334800	0.98798900
C	-2.90656800	1.53516100	-1.23903500
C	-4.61568000	-0.26990700	-0.29324200
H	-3.81532000	-0.78414200	1.67802000
H	-4.48185700	-2.13679300	0.75350700
C	-4.15949800	1.19806100	-0.39753700
H	-5.67205500	-0.25638400	0.02419900
H	-4.61769900	-0.71777000	-1.30424900
H	-2.97044500	1.05303000	-2.22991100
H	-2.93047600	2.62586100	-1.42236600
H	-4.02457800	1.60884600	0.62023400
H	-5.00171600	1.76236600	-0.83224600
H	-1.33628300	-1.35178700	1.92999000
H	-0.22006600	-2.12385500	-0.83333000
H	0.75375400	-3.15747900	1.57666300
H	3.11621100	-2.82298700	1.10553300
H	-2.44344900	-1.80251300	-0.89482900
H	-1.57879700	1.47411800	0.49445300
C	0.77150100	0.59938000	1.07641100
H	1.49220700	0.02537600	1.67495300
H	-0.16036100	0.56886200	1.66296400
H	-0.65541700	0.14526300	-2.10925400
C	1.22597100	2.06191900	1.02167100
H	2.25423000	2.13450100	0.63956500
H	0.59694000	2.62780900	0.31650700

C	1.16842800	2.71891700	2.40120600
H	1.51916900	3.76273000	2.37003300
H	0.13958400	2.72326200	2.79904000
H	1.79679500	2.17706000	3.12810100

R2b TS_{CP}

$G = -779.797463$ Hartree

Imaginary frequency: -273.85 cm^{-1}

C	-0.51108700	0.60307600	-0.85927800
C	-1.79443900	0.80854800	-0.41597300
C	0.62121700	0.32843800	-0.04139100
C	1.94283500	0.12597000	-0.75889800
C	2.75514300	-1.24316000	-0.52335300
C	3.03985800	1.19206200	-0.57756600
H	1.70705300	0.11779300	-1.83544600
C	-2.28944700	-1.55554100	0.00991700
C	-1.22229700	-1.78785300	0.84155500
C	-3.72673200	-1.46581800	0.44062300
C	0.10911400	-1.82322200	0.36610900
C	1.24563400	-2.15700800	1.20384600
C	2.50508500	-1.89559800	0.79683700
C	4.23981100	-0.87468100	-0.77473700
H	2.39759900	-1.92457500	-1.31397100
C	4.24523200	0.57481800	-1.28530400
H	3.27376600	1.32016400	0.49150800
H	2.74408300	2.17439600	-0.97683700
H	5.19154800	1.09883200	-1.08011200
H	4.08695000	0.60167400	-2.37722500
H	4.73278600	-1.57234200	-1.46837800
H	4.79395100	-0.92705600	0.17687100
C	-2.96196800	1.13894200	-1.30357700
C	-4.62484200	-0.70642100	-0.54466400
H	-3.79273800	-1.01132900	1.44499500
H	-4.12986200	-2.49161000	0.54785800
C	-4.32848600	0.78836000	-0.69965800
H	-5.67370100	-0.82418100	-0.22480700
H	-4.55391300	-1.19178400	-1.53563200
H	-2.84266900	0.65197700	-2.28804700
H	-2.95116000	2.22807600	-1.50505600
H	-4.41628800	1.27859800	0.28759800
H	-5.11514200	1.23589600	-1.32988000
H	-1.38102600	-1.75434500	1.92712200
H	0.23098700	-2.01158700	-0.70315700

H	1.05794800	-2.53992300	2.21255800
H	3.35495500	-2.10353900	1.45389500
H	-2.13105500	-1.70409600	-1.06291300
H	-1.95339400	1.01962400	0.64304200
C	0.64682000	0.83772600	1.39248000
H	1.44402300	0.30536900	1.93149700
H	-0.29281300	0.55483500	1.89259800
H	-0.37883000	0.45169300	-1.93893000
C	0.86920800	2.35167300	1.61335800
H	0.97103300	2.49763900	2.70366100
H	1.83573000	2.65588700	1.18702000
C	-0.21402300	3.29644300	1.09466100
H	0.03211100	4.33997800	1.35009500
H	-0.32399900	3.23243800	0.00240400
H	-1.19773900	3.07097200	1.53774700

R2c reactant

$G = -779.809843$ Hartree

C	0.60528100	-1.13004300	-0.87614600
C	1.80549000	-1.37412700	-0.31770600
C	-0.72648700	-1.21356800	-0.24966500
C	-1.78931600	-0.93257500	-1.04529700
C	-2.71998600	1.86839300	-0.44558300
C	-3.27496400	-1.05795700	-0.83848600
H	-1.53331000	-0.63167800	-2.07058700
C	2.57230600	1.70678400	-0.08759800
C	1.57736100	2.00660100	0.77164400
C	4.02741000	1.60305000	0.24630400
C	0.19031100	2.01331100	0.37738900
C	-0.86742500	2.26858300	1.18573600
C	-2.26018600	2.09400300	0.80197000
C	-4.10093600	1.40072900	-0.77679000
H	-2.02744000	1.95044900	-1.29053700
C	-4.09330900	0.05045800	-1.52493900
H	-3.54394600	-1.11174200	0.22258400
H	-3.58955200	-2.02422700	-1.27890300
H	-5.13616300	-0.28578900	-1.64880000
H	-3.70032300	0.20336100	-2.54656700
H	-4.62505300	2.13904200	-1.41232100
H	-4.68982900	1.30589100	0.15141100
C	3.11037700	-1.44457100	-1.06283800
C	4.78466400	0.52543700	-0.54242100
H	4.15255100	1.44054900	1.33117800

H	4.51731000	2.57290700	0.02921400
C	4.37089300	-0.93882500	-0.32519600
H	5.85376300	0.61838100	-0.28684000
H	4.71688100	0.75720800	-1.62141100
H	3.01822300	-0.94992900	-2.04565600
H	3.28378600	-2.51379100	-1.29204900
H	4.26789200	-1.13891200	0.75696600
H	5.21777300	-1.56021000	-0.65941100
H	1.80917900	2.19947500	1.82683300
H	-0.00153300	1.71825100	-0.65813900
H	-0.67297800	2.53392300	2.23100100
H	-2.98214500	2.05433700	1.62667100
H	2.30333700	1.52821100	-1.13547700
H	1.86660200	-1.63970100	0.74306100
H	0.59241200	-0.86264700	-1.94074100
C	-0.76009300	-1.71794600	1.19053200
H	0.15348300	-1.32014600	1.66048300
C	-0.65866600	-3.25388600	1.21175200
H	0.20887700	-3.61175000	0.63859800
H	-0.56766600	-3.62723200	2.24516300
H	-1.56278600	-3.70232100	0.76842500
C	-1.91296500	-1.24724500	2.08446200
H	-2.84243500	-1.80602100	1.89929900
H	-1.64747500	-1.41784200	3.14021600
H	-2.11799100	-0.17768000	1.95358800

R2c TS_{AM}

$G = -779.780830$ Hartree

Imaginary frequency: -437.60 cm^{-1}

C	-0.57385000	0.82697400	-0.83466000
C	-1.86950300	0.94790200	-0.37142700
C	0.63039700	0.82412000	-0.08343900
C	1.84717600	0.60776100	-0.79931600
C	2.64556500	-1.30940400	-0.73312100
C	3.18299000	1.28703300	-0.56986300
H	1.64796700	0.54833800	-1.87728400
C	-2.43668900	-1.38963100	-0.03586100
C	-1.38437400	-1.84231400	0.73680000
C	-3.85139500	-1.25944100	0.45813000
C	-0.09044400	-1.96973800	0.21541400
C	1.06998700	-2.27325200	0.93632400
C	2.34862700	-1.97276300	0.48561700
C	4.09237900	-0.95326900	-1.03126800

H	2.04107300	-1.60108800	-1.59722100
C	4.20983200	0.53329900	-1.41594700
H	3.47739000	1.25843700	0.48768300
H	3.12989800	2.35122100	-0.86177800
H	5.23466800	0.91091300	-1.27387300
H	3.96491000	0.66849400	-2.48414300
H	4.50907300	-1.59761400	-1.82367800
H	4.69236800	-1.13638000	-0.12454300
C	-3.03245400	1.27694500	-1.27303000
C	-4.76926900	-0.47478500	-0.48409000
H	-3.85873800	-0.80437400	1.46476600
H	-4.27437800	-2.27464300	0.58907700
C	-4.41149700	1.00257300	-0.66187600
H	-5.80557300	-0.54775300	-0.11391300
H	-4.76425500	-0.96735700	-1.47386500
H	-2.92963400	0.74508200	-2.23661800
H	-2.98171700	2.35382300	-1.52605900
H	-4.47235700	1.51136200	0.31794400
H	-5.17963500	1.47551100	-1.29638400
H	-1.52605900	-1.95501200	1.81926700
H	0.01566000	-1.77691100	-0.85424400
H	0.95624600	-2.62873600	1.96644800
H	3.17152400	-2.09276900	1.19908000
H	-2.31571800	-1.44702200	-1.12112800
H	-2.03253800	1.17276800	0.68555300
H	-0.45967700	0.66888700	-1.91534900
C	0.54524600	1.27063100	1.37761800
H	-0.38317000	0.83102900	1.77553000
C	0.39347600	2.80355500	1.43711200
H	-0.46644500	3.15122000	0.84716500
H	0.26110500	3.14181100	2.47829200
H	1.29539500	3.29504700	1.03722900
C	1.65969500	0.82680200	2.33346700
H	2.57954000	1.41557200	2.20395600
H	1.32773800	0.98420300	3.37229000
H	1.90997200	-0.23203900	2.21630400

R2c Product_[6+4]

$G = -779.828404$ Hartree

C	0.53000800	-0.55269400	-0.74231300
C	1.93799300	-0.49525400	-0.22566300
C	-0.62714900	-0.76129800	-0.07821200
C	-1.90872300	-0.40943200	-0.81697800
C	-2.45274000	1.09990400	-0.69707700

C	-3.16556800	-1.28051200	-0.66038800
H	-1.64795100	-0.48688600	-1.88434500
C	2.42251400	1.01245200	-0.15316700
C	1.44321200	1.79793500	0.66957800
C	3.86806200	1.08448300	0.35252300
C	0.25329900	2.15729600	0.15722100
C	-0.96587200	2.41173300	0.91299400
C	-2.15913600	1.89833500	0.55176500
C	-3.97990100	0.96076500	-0.94924800
H	-1.98953600	1.63731300	-1.53987200
C	-4.22370800	-0.47951200	-1.42214900
H	-3.46363700	-1.37887200	0.39457700
H	-3.01672500	-2.29627100	-1.05741500
H	-5.25368600	-0.82093300	-1.23597600
H	-4.04199700	-0.56667800	-2.50729200
H	-4.35756600	1.71539500	-1.65593900
H	-4.51695100	1.12191300	0.00031900
C	2.91572500	-1.31624300	-1.08398700
C	4.82236500	0.23990900	-0.49495700
H	3.89496900	0.73081600	1.40004300
H	4.19717900	2.13663500	0.37193300
C	4.35688700	-1.21606200	-0.57832500
H	5.84537000	0.29463600	-0.08721700
H	4.86995800	0.66368400	-1.51474500
H	2.86412400	-0.95296700	-2.12716100
H	2.58673800	-2.36810000	-1.10584000
H	4.41975800	-1.67465300	0.42551700
H	5.02978900	-1.79879900	-1.22916400
H	1.60319600	1.82565600	1.75547100
H	0.12337800	2.04977300	-0.92396200
H	-0.88022900	2.91648300	1.88196200
H	-2.99995300	2.04259900	1.23903700
H	2.39650100	1.39072000	-1.19220800
H	1.98576900	-0.88553400	0.80364200
C	-0.63714600	-1.35904300	1.32679200
H	0.39032300	-1.27520700	1.70972600
H	0.44397900	-0.21979100	-1.78613200
C	-0.93527700	-2.87101900	1.25635800
H	-0.78500800	-3.33632500	2.24447300
H	-1.97153500	-3.07462200	0.95008200
H	-0.26821900	-3.36902200	0.53650500
C	-1.52735300	-0.67343200	2.37171800
H	-1.19298900	0.35030500	2.57425200
H	-2.58188600	-0.62030500	2.06485200

H	-1.48810900	-1.24082100	3.31596300
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R2c Product_[4+2]

$G = -779.812308$ Hartree

C	0.55189500	-1.00820800	-0.58929100
C	1.71310500	-1.28741500	0.01308900
C	-0.55863800	-0.17380100	0.01105700
C	-1.82897200	-0.27679000	-0.89440500
C	-2.85858300	0.91832500	-0.77016500
C	-2.70733700	-1.54504000	-0.78192400
H	-1.44309300	-0.24278200	-1.92537500
C	2.33236500	1.50878500	-0.57120400
C	1.30123100	1.66597100	0.26686200
C	3.79289800	1.48878800	-0.24147100
C	-0.10517500	1.37352100	-0.16395600
C	-1.17039900	2.26608000	0.42132800
C	-2.45869100	2.02413400	0.16087000
C	-4.22639300	0.26594600	-0.49609000
H	-2.92208200	1.36897400	-1.77900400
C	-4.11253900	-1.09154900	-1.19404800
H	-2.76544200	-1.88870600	0.25828300
H	-2.31373600	-2.38265500	-1.37791000
H	-4.89905000	-1.80553800	-0.90394600
H	-4.17477300	-0.95729100	-2.28842900
H	-5.06743900	0.88213800	-0.85049900
H	-4.36288300	0.11581200	0.58932900
C	2.95051400	-1.86192600	-0.60932000
C	4.52724400	0.26188200	-0.82516200
H	3.94200700	1.53799800	0.85104200
H	4.28044300	2.38770000	-0.66371700
C	4.24709000	-1.12257600	-0.21140900
H	5.60919400	0.45090900	-0.72231200
H	4.33695100	0.21866200	-1.91358500
H	2.85023000	-1.89501900	-1.70819200
H	3.06774400	-2.91142600	-0.27875200
H	4.28727000	-1.04422300	0.89095100
H	5.09114900	-1.77551500	-0.49056500
H	1.49269500	1.88251000	1.32199900
H	-0.11920700	1.50850900	-1.26010300
H	-0.86976200	3.09915900	1.06344700
H	-3.24867400	2.65602000	0.58058700
H	2.10091200	1.28138100	-1.62033700
H	1.82910200	-1.02741100	1.06921900

C	-0.91102500	-0.54898100	1.50214100
H	-1.97496200	-0.28834400	1.61631900
H	0.45795300	-1.23090000	-1.66026900
C	-0.77856200	-2.05362700	1.81124200
H	0.26111700	-2.32452500	2.04360800
H	-1.39045700	-2.30827200	2.69211000
H	-1.08895400	-2.69788800	0.98037300
C	-0.18873500	0.22268200	2.61541800
H	-0.36826600	1.30367200	2.56348000
H	-0.56340200	-0.12221500	3.59293600
H	0.89765800	0.05204900	2.60795200

R2c TS_{CP}

$G = -779.788261$ Hartree

Imaginary frequency: -303.92 cm^{-1}

C	-0.61508800	0.80218500	-0.89649800
C	-1.90406600	0.96537600	-0.43803000
C	0.53156200	0.53399500	-0.09725500
C	1.85387800	0.44100200	-0.85370400
C	2.53401400	-0.99242600	-1.03011200
C	3.03324900	1.37552600	-0.42893500
H	1.60962000	0.71866300	-1.88921500
C	-2.35161200	-1.33989800	0.03956500
C	-1.21819500	-1.64867300	0.76055900
C	-3.74580300	-1.23151500	0.59421300
C	0.04705800	-1.67358600	0.13841800
C	1.27938400	-2.14353300	0.74696200
C	2.47200500	-1.84665500	0.19256800
C	3.96034900	-0.62739500	-1.45720000
H	1.99209400	-1.50030700	-1.84618000
C	4.32419600	0.53785000	-0.53125200
H	2.91578100	1.78505700	0.57782900
H	3.06847400	2.24092200	-1.10893900
H	4.59299100	0.14248300	0.46286900
H	5.18706900	1.12177500	-0.88640300
H	3.96052100	-0.28988900	-2.50741800
H	4.65539700	-1.47839200	-1.38473300
C	-3.09431500	1.25224400	-1.31483800
C	-4.72414100	-0.53170400	-0.35862600
H	-3.72843600	-0.71727400	1.57156200
H	-4.13217200	-2.24884800	0.79751600
C	-4.43830900	0.94761100	-0.63860500
H	-5.74371000	-0.62009300	0.05233100

H	-4.73456100	-1.08275200	-1.31706400
H	-3.01056600	0.69923000	-2.26771100
H	-3.08688800	2.32447900	-1.59009200
H	-4.48883700	1.51058300	0.31174000
H	-5.25047800	1.34629200	-1.26924100
H	-1.26842500	-1.68164700	1.85630800
H	0.02535800	-1.73173100	-0.95214600
H	1.22523300	-2.69078000	1.69391200
H	3.40310700	-2.16789700	0.66946900
H	-2.29591000	-1.47966500	-1.04402800
H	-2.06001800	1.20009900	0.61687200
C	0.45370200	1.02932100	1.35872600
H	-0.53613100	0.71715500	1.72388300
H	-0.49054700	0.67928200	-1.98054600
C	0.44545100	2.57451700	1.40667400
H	0.22205700	2.92033300	2.42931600
H	1.41485200	3.00517400	1.11756600
H	-0.31461200	2.98873200	0.72974900
C	1.45025100	0.46353000	2.38153400
H	1.21122000	-0.57083100	2.65213600
H	2.49149000	0.46698500	2.03273600
H	1.40460800	1.06623200	3.30292800

R2d reactant

$G = -819.092553$ Hartree

C	0.57349100	-0.91500300	-0.99537700
C	1.80568500	-1.31063300	-0.62467200
C	-0.76430000	-1.13847500	-0.39775800
C	-1.78812500	-0.65947200	-1.15766200
C	-2.66950200	2.09979400	-0.29234000
C	-3.29392000	-0.74208800	-1.11040800
H	-1.45803500	-0.16126300	-2.07879600
C	2.59807000	1.77956300	0.08213100
C	1.60618200	1.97699000	0.97367100
C	4.04719700	1.57265300	0.39703200
C	0.22338400	2.07278200	0.57632900
C	-0.84153000	2.19656200	1.40497900
C	-2.22888600	2.07487100	0.98131500
C	-4.03828000	1.70520900	-0.74388000
H	-1.96316700	2.35441600	-1.09087500
C	-4.00106700	0.49178200	-1.69626400
H	-3.68514900	-0.92600700	-0.10634300
H	-3.59376100	-1.61923600	-1.71642300

H	-5.03715300	0.22437700	-1.96270800
H	-3.50854700	0.78337800	-2.64173200
H	-4.53166300	2.54224400	-1.27216700
H	-4.66521200	1.46633000	0.13218500
C	3.05115900	-1.12990000	-1.45018400
C	4.78828100	0.66189900	-0.59193000
H	4.15636700	1.18874600	1.42653000
H	4.56202400	2.55375600	0.38725000
C	4.35216100	-0.80943500	-0.67470100
H	5.85836800	0.68314600	-0.32457800
H	4.72665100	1.10757800	-1.60197900
H	2.88196100	-0.38358300	-2.24558100
H	3.22113500	-2.08610200	-1.98139800
H	4.28493900	-1.23228400	0.34414900
H	5.17554800	-1.35465600	-1.16431200
H	1.83255500	1.99665200	2.04712100
H	0.03827700	1.94071600	-0.49360000
H	-0.65820600	2.28989700	2.48119100
H	-2.95643500	1.86081700	1.77410800
H	2.32975800	1.77391400	-0.98110200
H	1.95753800	-1.88711900	0.28984800
H	0.52730300	-0.34573200	-1.93258800
C	-0.87395400	-1.93008600	0.92469900
C	-0.39482600	-3.38122100	0.68040900
H	0.64327300	-3.43858800	0.33311600
H	-0.47589500	-3.96613400	1.61118900
H	-1.02587000	-3.86641800	-0.08094900
C	-2.30121200	-2.03488400	1.48962800
H	-2.97297000	-2.60215200	0.83102300
H	-2.26078500	-2.56928900	2.45191400
H	-2.73724300	-1.04420100	1.68061000
C	-0.04012500	-1.25484000	2.03919900
H	0.99662800	-1.05260600	1.75226400
H	-0.48999300	-0.29082400	2.31199000
H	-0.03154400	-1.89617600	2.93534300

R2d TS_{AM}

$G = -819.060529$ Hartree

Imaginary frequency: -427.14 cm^{-1}

C	-0.58977900	0.67059600	-0.91275600
C	-1.91491700	0.82973200	-0.53597500
C	0.65741700	0.78974800	-0.23891400
C	1.78718100	0.34630400	-1.00085600

C	2.54003600	-1.58985200	-0.52777900
C	3.16530600	0.96897000	-1.12117600
H	1.46814100	0.01760600	-1.99667800
C	-2.51132500	-1.38014300	0.11487200
C	-1.50083900	-1.75547600	0.98531700
C	-3.93969500	-1.15722900	0.53359500
C	-0.20068000	-1.98253500	0.52320900
C	0.95020200	-2.18351300	1.29041800
C	2.23473000	-1.99350100	0.79164900
C	3.98137300	-1.34673900	-0.92142600
H	1.90423200	-2.00061200	-1.31702500
C	4.08898900	-0.06746600	-1.76375300
H	3.57929000	1.28423100	-0.15438500
H	3.10484300	1.87717700	-1.74770000
H	5.12899400	0.28809200	-1.83714400
H	3.74669500	-0.26845300	-2.79456900
H	4.39615800	-2.21083100	-1.46919900
H	4.58581100	-1.23121900	-0.00578500
C	-3.00550700	0.99379300	-1.56920700
C	-4.81760900	-0.55894600	-0.56934300
H	-3.97252700	-0.52030900	1.43596900
H	-4.37511900	-2.12783800	0.84063100
C	-4.42637300	0.85303200	-1.01149500
H	-5.86630800	-0.54937200	-0.22812600
H	-4.78820400	-1.23148500	-1.44623400
H	-2.85112500	0.28816600	-2.40642400
H	-2.91359300	2.00209700	-2.01675100
H	-4.53959300	1.54466400	-0.15634600
H	-5.14488700	1.19544000	-1.77493200
H	-1.68069000	-1.71755400	2.06702300
H	-0.07429500	-1.93890600	-0.56080100
H	0.83187200	-2.35652200	2.36572500
H	3.05581600	-1.98875100	1.51672900
H	-2.35864000	-1.61377900	-0.94232000
H	-2.16880800	1.22240500	0.44364700
H	-0.48078800	0.31765500	-1.94780300
C	0.85400600	1.57239600	1.08580600
C	1.24549600	3.01883900	0.69504500
H	0.48004500	3.46043200	0.03867800
H	1.32776300	3.64645000	1.59827300
H	2.20846200	3.06234100	0.16895500
C	1.94642600	0.97023300	1.99504300
H	2.19740200	1.69798800	2.78334000
H	1.58350300	0.05855500	2.48383900

H	2.87225900	0.71220600	1.47258300
C	-0.40042700	1.66578600	1.97752100
H	-1.15473300	2.35054300	1.57016600
H	-0.85903500	0.68026800	2.13666800
H	-0.10701300	2.06514100	2.96122200

R2d Product_[6+4]

$G = -819.108720$ Hartree

C	0.54431900	-0.37262600	-0.77302600
C	1.97851600	-0.39098700	-0.31951700
C	-0.65215500	-0.68415800	-0.22092800
C	-1.84986200	-0.09480800	-0.97518200
C	-2.40882700	1.34339200	-0.49056200
C	-3.11464600	-0.92796300	-1.27089800
H	-1.45134500	0.13246300	-1.97337200
C	2.46099300	1.09446900	-0.05044700
C	1.51900700	1.73549700	0.92654000
C	3.93078500	1.10254400	0.38410300
C	0.31175000	2.16536900	0.51995800
C	-0.88925700	2.27602200	1.33510600
C	-2.09464500	1.86454100	0.89168500
C	-3.92950700	1.26040500	-0.75698500
H	-1.97003500	2.05923100	-1.20442000
C	-4.11883400	0.11923300	-1.76037600
H	-3.51879500	-1.41809400	-0.37483300
H	-2.91109100	-1.71873600	-2.00948400
H	-5.15407400	-0.25341100	-1.80084200
H	-3.85035000	0.45448700	-2.77754700
H	-4.34788900	2.22028800	-1.09737800
H	-4.44783500	1.00235300	0.18313400
C	2.90109200	-1.05166700	-1.35898800
C	4.83762200	0.41245800	-0.63781600
H	4.01598800	0.58884300	1.35974900
H	4.25839900	2.14208700	0.55076900
C	4.36989800	-1.01606500	-0.92855500
H	5.88164700	0.41089300	-0.28311400
H	4.82835000	0.99443500	-1.57749200
H	2.78462300	-0.52907700	-2.32659500
H	2.57506600	-2.09127400	-1.52761900
H	4.49286400	-1.62964400	-0.01733400
H	5.00472900	-1.47842500	-1.70265000
H	1.71828200	1.58696000	1.99588300
H	0.15172800	2.24075000	-0.55975000

H	-0.78341500	2.57626400	2.38364400
H	-2.93065500	1.88479700	1.59901100
H	2.38031900	1.62487400	-1.01780000
H	2.10660600	-0.92751000	0.62378000
C	-0.89184700	-1.58768900	1.01062200
H	0.46851800	0.16879200	-1.72653600
C	-1.23326000	-3.00184800	0.47491700
H	-1.36735000	-3.70157700	1.31666000
H	-2.15345200	-3.01821200	-0.12185300
H	-0.41484500	-3.37720100	-0.15800500
C	-2.03870600	-1.09380800	1.91957900
H	-1.73220400	-0.20628100	2.48625500
H	-2.95419200	-0.83724400	1.37573500
H	-2.29473500	-1.88604500	2.64128100
C	0.32520500	-1.75177800	1.94065800
H	1.13641700	-2.32451900	1.47208200
H	0.71866400	-0.78102400	2.27283700
H	0.01422200	-2.31245900	2.83648400

R2d Product_[4+2]

$G = -819.087843$ Hartree

C	0.65140200	-0.92013900	-0.71474100
C	1.83883500	-1.25750700	-0.19959200
C	-0.48148700	-0.18559100	-0.00817300
C	-1.68056600	-0.12408600	-1.01822300
C	-2.67883800	1.09634400	-0.88455600
C	-2.58299300	-1.36421100	-1.23100500
H	-1.17672800	0.03993800	-1.98141900
C	2.43240200	1.57240600	-0.34200900
C	1.39450400	1.62520700	0.50178000
C	3.89388900	1.52452800	-0.01898800
C	-0.00082100	1.37374300	0.01243100
C	-1.08311900	2.24004600	0.60424800
C	-2.34407500	2.09526500	0.18435800
C	-4.09129400	0.48447400	-0.86292100
H	-2.60024700	1.64284900	-1.84406000
C	-3.93253600	-0.79348300	-1.69670400
H	-2.73383500	-1.92686200	-0.30380600
H	-2.14120800	-2.06772300	-1.95329400
H	-4.76500900	-1.50367400	-1.57375600
H	-3.88479600	-0.52993700	-2.76792800
H	-4.85137100	1.17332000	-1.26356300
H	-4.39058300	0.23420100	0.16717000

C	3.06116100	-1.70525900	-0.94615600
C	4.64150500	0.42387500	-0.80239000
H	4.04668700	1.39415600	1.06632100
H	4.36620800	2.48870800	-0.28638400
C	4.36731400	-1.04889500	-0.44601800
H	5.72173400	0.59757300	-0.66136600
H	4.45659400	0.57197600	-1.88250200
H	2.93688700	-1.53787600	-2.03026600
H	3.18430200	-2.79725500	-0.81557300
H	4.42761100	-1.17235300	0.65129700
H	5.20470600	-1.63932400	-0.85450100
H	1.57360000	1.73379900	1.57482900
H	0.03540400	1.60602600	-1.06585400
H	-0.81968600	2.97340500	1.37210600
H	-3.15322700	2.70962600	0.59326900
H	2.20478600	1.46566200	-1.41073800
H	1.99710900	-1.16881500	0.87727900
C	-0.82012400	-0.80271600	1.43984300
H	0.54551400	-0.99027400	-1.80492700
C	-0.64756100	-2.34189900	1.42712600
H	0.40430100	-2.64579400	1.38370700
H	-1.08073500	-2.76531400	2.34751200
H	-1.15026500	-2.81167200	0.57154500
C	0.08698700	-0.24683300	2.55810900
H	-0.10505600	0.81998000	2.73974000
H	-0.13549900	-0.77999200	3.49622800
H	1.15740200	-0.37188000	2.35884200
C	-2.25871300	-0.53109000	1.94413300
H	-2.46822600	0.53670400	2.05243500
H	-3.03250500	-0.96991000	1.30690600
H	-2.36910500	-0.99432700	2.93743500

R2d TS_{CP}

$G = -819.065314$ Hartree

Imaginary frequency: -267.55 cm^{-1}

C	0.63878400	-0.68012200	-0.93514300
C	1.91532500	-0.94302200	-0.49740000
C	-0.55735500	-0.45372400	-0.18894400
C	-1.74831200	-0.07138100	-1.07625300
C	-2.51860400	1.32068600	-0.81489000
C	-2.89819700	-1.11135600	-1.30376400
H	-1.29663300	0.08250500	-2.06361300
C	2.42097700	1.40633200	0.02348800

C	1.34524700	1.66442700	0.83971600
C	3.84960500	1.29119400	0.47659400
C	0.02891400	1.71165500	0.33151500
C	-1.15451600	2.06460100	1.09307800
C	-2.38186700	1.88878400	0.55943800
C	-3.96413600	1.04668900	-1.26484200
H	-2.04740700	2.04023000	-1.50557900
C	-4.21289100	-0.42255500	-0.91668000
H	-2.73917400	-2.06075500	-0.78061400
H	-2.92360200	-1.35955500	-2.37695300
H	-4.39770600	-0.51997300	0.16461400
H	-5.08611700	-0.84854300	-1.43524400
H	-4.04667700	1.18412600	-2.35617200
H	-4.68464000	1.73563700	-0.79709600
C	3.08032300	-1.19920400	-1.41516600
C	4.75884300	0.58006100	-0.53382500
H	3.89568800	0.78322000	1.45641100
H	4.25579800	2.30718600	0.64718300
C	4.44864500	-0.89888400	-0.78683500
H	5.80273300	0.66461400	-0.18819000
H	4.71267200	1.12525900	-1.49462400
H	2.95769100	-0.63171800	-2.35534200
H	3.07078900	-2.26706500	-1.70859200
H	4.53056700	-1.45413000	0.16595100
H	5.23372200	-1.30998100	-1.44333900
H	1.49152200	1.65652100	1.92462100
H	-0.04130300	1.88978000	-0.74289200
H	-1.03647500	2.41346800	2.12421600
H	-3.28300300	2.11555300	1.13723500
H	2.28213100	1.55451800	-1.05130300
H	2.08543600	-1.25173400	0.53416500
C	-0.76827300	-1.24261000	1.15697800
H	0.57308000	-0.41515300	-1.99874000
C	-0.48081600	-2.74149400	0.87891800
H	-0.74570600	-3.34204200	1.76472800
H	-1.07291900	-3.11185900	0.02911400
H	0.57566600	-2.92439500	0.64609800
C	-2.19894500	-1.16988900	1.73810400
H	-2.54486600	-0.13884900	1.85729200
H	-2.93184100	-1.72089700	1.14068500
H	-2.19301300	-1.63645300	2.73550400
C	0.14743900	-0.79122400	2.31596900
H	1.20358900	-0.71290900	2.04282500
H	-0.16958900	0.18207900	2.71107700

H	0.06845300	-1.52246800	3.13623300
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R3a reactant

$G = -776.434968$ Hartree

C	0.49571100	-1.38981100	-0.71259400
C	1.61621700	-1.38024900	0.03211900
C	-0.86665300	-1.24942400	-0.19526700
C	-1.95843500	-1.19822600	-0.99041000
C	-2.81262000	1.69982300	-0.25279900
C	-3.39225900	-1.22422600	-0.54772600
H	-1.78007900	-1.20074200	-2.07139600
C	2.53581000	1.64264000	-0.44923100
C	1.60372400	1.95685200	0.47196000
C	4.01022700	1.59157100	-0.21438400
C	0.18568300	1.88863200	0.21776000
C	-0.77749800	2.04316000	1.15593800
C	-2.19602400	1.80750100	0.94003600
C	-4.21685500	1.22192000	-0.43681500
H	-2.24364500	1.89606500	-1.16912600
C	-4.28350100	-0.13279900	-1.17168800
H	-3.44185700	-1.16550000	0.55069900
H	-3.81426600	-2.20723400	-0.83193000
H	-5.33265600	-0.47297000	-1.18052400
H	-3.99969500	0.00556600	-2.23047900
H	-4.81092700	1.95677600	-1.01103000
H	-4.70046700	1.12095000	0.54977600
C	2.98332700	-1.75625100	-0.46582500
C	4.66458400	0.26586700	-0.63607400
H	4.22415500	1.78936300	0.85028300
H	4.50340700	2.40249000	-0.78480000
C	4.20284900	-1.00106300	0.10619500
H	5.75268600	0.37537200	-0.49142600
H	4.52350900	0.11858900	-1.72251400
H	3.00545700	-1.72713800	-1.56941000
H	3.12113600	-2.82319900	-0.20233700
H	4.02486200	-0.76584800	1.17119700
H	5.04876500	-1.70740000	0.09782600
H	1.92115900	2.21567400	1.49017200
H	-0.10426300	1.60157000	-0.79749800
H	-0.46794300	2.27142500	2.18204100
H	-2.79347900	1.63714000	1.84345500
H	2.19541400	1.37144000	-1.45658000
H	1.51981800	-1.18306500	1.10540400

H	0.57167700	-1.55624900	-1.79322900
O	-1.00744100	-1.19788700	1.17582200
C	-1.06401300	-2.45490300	1.82172700
H	-1.11675800	-2.26256900	2.90297900
H	-1.95899000	-3.02718500	1.51566100
H	-0.16912100	-3.06630700	1.60867500

R3a TS_{AM}

$G = -776.405587$ Hartree

Imaginary frequency: -454.20 cm^{-1}

C	0.51580400	-1.02616700	-0.67309000
C	1.76274600	-1.07943200	-0.09899200
C	-0.71373000	-0.83175600	0.00346600
C	-1.96361800	-0.73186800	-0.66152500
C	-2.78159400	1.14381000	-0.61369700
C	-3.23225500	-1.38208600	-0.14581300
H	-1.85653600	-0.82908000	-1.74935100
C	2.38144900	1.39781900	-0.27123900
C	1.34829900	1.86989800	0.49820500
C	3.81702400	1.36903500	0.16700500
C	0.01252000	1.90648300	0.05632000
C	-1.07866300	2.14849100	0.89101700
C	-2.38672100	1.80033300	0.57956700
C	-4.24943500	0.76942200	-0.76944100
H	-2.26329500	1.44532500	-1.52923500
C	-4.39626900	-0.75906500	-0.91425400
H	-3.33151400	-1.18937200	0.93480300
H	-3.20227800	-2.47721500	-0.28730000
H	-5.37724700	-1.11220900	-0.55929000
H	-4.31799500	-1.05080900	-1.97607200
H	-4.70723300	1.29208900	-1.62491100
H	-4.79243400	1.09843300	0.13095100
C	2.97700800	-1.61024900	-0.81105100
C	4.68477000	0.32586700	-0.54446700
H	3.87018600	1.22304300	1.26046400
H	4.26090400	2.36680100	-0.02203400
C	4.32745300	-1.13508300	-0.26082400
H	5.73625400	0.49315300	-0.25646600
H	4.63776000	0.50252500	-1.63505300
H	2.90877800	-1.38417400	-1.89082600
H	2.95951600	-2.71625800	-0.74327600
H	4.35298100	-1.31148700	0.83048600
H	5.11812000	-1.77419300	-0.68846100

H	1.53842100	2.08407000	1.55757100
H	-0.16728400	1.68201200	-0.99717200
H	-0.86988700	2.49076700	1.91015300
H	-3.13070200	1.87708100	1.37936100
H	2.19955000	1.25440200	-1.34106700
H	1.82909400	-1.00487100	0.98992500
H	0.44472500	-1.11795200	-1.76310000
O	-0.73372500	-0.84621800	1.38149800
C	-0.68408900	-2.12416600	1.98838000
H	-0.68610600	-1.96403500	3.07609700
H	-1.55900000	-2.74146600	1.71764700
H	0.23084000	-2.67454800	1.70677600

R3a Product_[6+4]

$G = -776.456116$ Hartree

C	0.47497900	-0.76374400	-0.78970100
C	1.84978000	-0.56562200	-0.21922000
C	-0.66129300	-0.82636800	-0.07359100
C	-2.04181200	-0.67679100	-0.66705700
C	-2.56369600	0.80690300	-0.80086000
C	-3.18779500	-1.38516000	0.08185800
H	-1.99546700	-1.05790700	-1.70067800
C	2.21265900	0.97671800	-0.12704900
C	1.16313700	1.67920900	0.67979200
C	3.63307200	1.15431100	0.42616000
C	-0.01745800	2.01841300	0.13688000
C	-1.26917500	2.20804000	0.86342000
C	-2.41998200	1.64212300	0.45003800
C	-4.03323800	0.56231100	-1.18234800
H	-2.01709200	1.29325200	-1.62428900
C	-4.48624300	-0.63251100	-0.31137200
H	-3.01036600	-1.29548800	1.16253700
H	-3.22835600	-2.45894800	-0.15714300
H	-5.01355200	-0.28251900	0.58960500
H	-5.19420800	-1.27692100	-0.85413800
H	-4.08618600	0.29090000	-2.24891100
H	-4.65871200	1.45754000	-1.04494900
C	2.92425900	-1.31492100	-1.02361900
C	4.68042400	0.38318300	-0.37907900
H	3.64773900	0.80527400	1.47541900
H	3.88043100	2.22833100	0.45389500
C	4.33148000	-1.10446300	-0.46183700
H	5.68055100	0.52126800	0.06426800

H	4.73166600	0.80080100	-1.40127400
H	2.89128900	-0.96303900	-2.07161200
H	2.67642400	-2.38900600	-1.05089900
H	4.38690600	-1.54671900	0.54979000
H	5.07159900	-1.64172400	-1.07792000
H	1.27723900	1.66460900	1.77084100
H	-0.10302300	1.94233900	-0.95202300
H	-1.24049800	2.71864800	1.83218000
H	-3.30626200	1.73847900	1.08686500
H	2.18610900	1.36221900	-1.16308900
H	1.86840600	-0.93806500	0.81735300
H	0.37767500	-0.69669700	-1.87910900
O	-0.61463000	-0.86695400	1.30588300
C	-0.40111600	-2.14394300	1.87308000
H	-0.39047000	-2.01522200	2.96504600
H	-1.20528600	-2.85253000	1.60494700
H	0.56259600	-2.57937500	1.55325100

R3a Product_[4+2]

$G = -776.444505$ Hartree

C	0.50115700	-0.95407900	-0.71945800
C	1.57154900	-1.30295500	0.00182400
C	-0.58610100	-0.05509000	-0.16994900
C	-1.90132000	-0.18123800	-0.97889800
C	-2.99382000	0.81834700	-0.52316400
C	-2.59561500	-1.56920600	-0.94234200
H	-1.60824000	0.05580400	-2.01331600
C	2.38871800	1.52348900	-0.28418200
C	1.22646300	1.63186700	0.36825500
C	3.76083600	1.36525700	0.29554200
C	-0.08710600	1.44297200	-0.33248400
C	-1.17192400	2.40632700	0.09174300
C	-2.47391700	2.12375000	-0.00147600
C	-3.86193300	0.01482100	0.46343300
H	-3.62764200	1.03139600	-1.40624300
C	-3.93124100	-1.38375900	-0.17097700
H	-1.94833800	-2.32758000	-0.48245600
H	-2.79020800	-1.92322900	-1.96572900
H	-4.10481100	-2.17706500	0.57259300
H	-4.77694600	-1.42568400	-0.87603400
H	-4.85532500	0.46488900	0.61719300
H	-3.35733000	-0.01184600	1.44014500
C	2.85671200	-1.90704400	-0.47665800

C	4.52592800	0.15241100	-0.28194300
H	3.70888500	1.29432500	1.39564100
H	4.36456400	2.26389600	0.06853400
C	4.10878200	-1.26350100	0.15925800
H	5.58642200	0.27546100	-0.00431200
H	4.50178200	0.20912000	-1.38603000
H	2.91972100	-1.86653000	-1.57786300
H	2.87748600	-2.97956100	-0.20551900
H	3.99332400	-1.27865400	1.25877000
H	4.95960500	-1.93138500	-0.05683600
H	1.20139400	1.67629200	1.46236600
H	0.09629300	1.57823500	-1.41334600
H	-0.84731100	3.37829000	0.47589500
H	-3.21718300	2.86270900	0.31729900
H	2.34665600	1.44224600	-1.37931700
H	1.55218800	-1.06351900	1.07019300
H	0.47905200	-1.13827100	-1.79967000
O	-0.74699100	-0.19480100	1.24274700
C	-1.03192700	-1.44650600	1.82199900
H	-0.69859300	-1.39473500	2.87043600
H	-2.11088500	-1.67537300	1.82333900
H	-0.50009800	-2.27600000	1.32915800

R3a TS_{CP}

$G = -776.415867$ Hartree

Imaginary frequency: -279.74 cm^{-1}

C	0.51985100	-1.12959600	-0.39847600
C	1.77779800	-1.10927100	0.15605100
C	-0.70265700	-0.56763700	0.06864500
C	-1.92456300	-0.64009300	-0.81203200
C	-2.81194600	0.69198200	-0.91291900
C	-2.93050900	-1.74593600	-0.35757900
H	-1.56907300	-0.86642100	-1.82565000
C	2.28893000	1.21615000	-0.49882400
C	1.20190400	1.76181300	0.13697800
C	3.71570000	1.34157600	-0.04433800
C	-0.12731300	1.60581500	-0.32292600
C	-1.26857600	2.15561600	0.37879900
C	-2.52321100	1.72850200	0.13103200
C	-4.26201300	0.17728800	-0.84889400
H	-2.59495900	1.13200700	-1.90155800
C	-4.18143500	-1.00422400	0.11977900
H	-2.49997800	-2.39913700	0.41306900

H	-3.18347300	-2.37782700	-1.22444400
H	-4.02138300	-0.63129900	1.14514800
H	-5.08505200	-1.63396700	0.12617500
H	-4.58574700	-0.17984100	-1.84136300
H	-4.96902600	0.96144000	-0.53673400
C	2.97097500	-1.77493800	-0.47526200
C	4.63023200	0.22520600	-0.56495300
H	3.75742500	1.38264600	1.05910300
H	4.12633600	2.30876800	-0.39489400
C	4.32219400	-1.18399300	-0.04918900
H	5.67250300	0.47332000	-0.30291300
H	4.58915100	0.21936000	-1.66989800
H	2.87557200	-1.75639100	-1.57585800
H	2.96725400	-2.84635300	-0.19491100
H	4.37890000	-1.18595500	1.05529500
H	5.12156100	-1.86184500	-0.39250800
H	1.34454000	2.18736300	1.13963700
H	-0.25459600	1.39176600	-1.38712200
H	-1.08106300	2.84806400	1.20713000
H	-3.35915400	2.10775400	0.72637900
H	2.15216500	0.87631000	-1.53059100
H	1.91532200	-0.83871100	1.20214000
H	0.47874000	-1.41160900	-1.45729500
O	-1.11779300	-0.53130000	1.36685600
C	-0.22903900	-0.46660100	2.45309300
H	0.35521000	-1.39599000	2.55891700
H	0.46050200	0.38833900	2.36253200
H	-0.84726200	-0.33135700	3.35145800

R3b reactant

$G = -717.277885$ Hartree

C	0.43162500	-1.62368800	-0.22261300
C	1.56913400	-1.42782500	0.46897800
C	-0.93760700	-1.41319300	0.26840000
C	-1.99095100	-1.52945700	-0.58667400
C	-2.87654100	1.40732000	-0.32745300
C	-3.45376300	-1.57329500	-0.24323300
H	-1.74658800	-1.69549000	-1.64043800
C	2.44039900	1.42205200	-0.71468500
C	1.53642600	1.93971100	0.14059200
C	3.92285300	1.43594900	-0.53169500
C	0.11262400	1.79046800	-0.03228300
C	-0.82051600	2.12800800	0.88781400

C	-2.23498300	1.80125700	0.79011000
C	-4.27331300	0.87831800	-0.37936600
H	-2.33659100	1.42066600	-1.28091800
C	-4.34438900	-0.54425400	-0.96489800
H	-3.61311700	-1.48128100	0.84554700
H	-3.83237700	-2.57894100	-0.51005100
H	-5.39373700	-0.88434500	-0.93667900
H	-4.06127300	-0.51540900	-2.03241400
H	-4.91137700	1.53469600	-1.00091100
H	-4.71015300	0.88247200	0.63451400
C	2.93098800	-1.89205500	0.03080100
C	4.57753200	0.05011900	-0.65354100
H	4.17287100	1.88052700	0.44729000
H	4.38514700	2.09077900	-1.29574700
C	4.15113400	-1.01080600	0.37764500
H	5.66846500	0.19311300	-0.57382200
H	4.40444200	-0.34663100	-1.67063500
H	2.92207800	-2.11504100	-1.05058900
H	3.09628100	-2.86943600	0.52487900
H	3.99376800	-0.53256200	1.36151500
H	5.00745800	-1.69082700	0.51492800
H	1.88537300	2.43798400	1.05427100
H	-0.20439400	1.26425800	-0.93764900
H	-0.48515100	2.59521800	1.82074200
H	-2.80027700	1.82525200	1.72997500
H	2.06789800	0.91371200	-1.61294200
H	1.51347600	-0.97919500	1.46773300
H	0.49499800	-2.03164100	-1.23712300
N	-1.07172100	-1.09879900	1.61737700
H	-2.01987200	-1.06768500	1.96956900
H	-0.43920300	-1.59037600	2.23992600

R3b TS_{AM}

$G = -717.258035$ Hartree

Imaginary frequency: -402.20 cm^{-1}

C	0.45396200	-1.28451700	-0.19401100
C	1.68672900	-1.23978400	0.38414800
C	-0.80827900	-0.95456500	0.40378100
C	-2.00809300	-1.00055400	-0.36146100
C	-2.82205900	0.87456100	-0.56816400
C	-3.29584500	-1.61114500	0.15928500
H	-1.82298500	-1.26489800	-1.40926000
C	2.38563200	1.24845900	-0.55889600

C	1.37472000	1.87788300	0.10507100
C	3.83777600	1.31227600	-0.19149000
C	0.00646800	1.77424800	-0.25537600
C	-1.03443900	2.17790800	0.56997200
C	-2.36241300	1.75223600	0.44722700
C	-4.29437500	0.49369700	-0.58407000
H	-2.36178200	1.00119100	-1.55374900
C	-4.44092000	-1.03368200	-0.66975400
H	-3.43617600	-1.36709700	1.22505900
H	-3.25582900	-2.71246800	0.08874200
H	-5.43084100	-1.37456900	-0.32719400
H	-4.33148100	-1.36747500	-1.71677000
H	-4.82294500	0.99241700	-1.41347100
H	-4.76096100	0.84776500	0.35015500
C	2.91852800	-1.87830900	-0.19357100
C	4.63927300	0.05539800	-0.55170900
H	3.94323800	1.53189200	0.88592800
H	4.30677100	2.16836900	-0.71723200
C	4.25987300	-1.23222200	0.18781400
H	5.70594500	0.26179000	-0.36035900
H	4.55842700	-0.12169900	-1.64027400
H	2.82810000	-1.94426900	-1.29253500
H	2.94710500	-2.92820800	0.16072600
H	4.27528400	-1.04792300	1.27820900
H	5.05442500	-1.97360400	-0.00015600
H	1.60841700	2.39052000	1.04835100
H	-0.22208500	1.27032000	-1.19684600
H	-0.77148400	2.76039900	1.46140400
H	-3.06486800	2.02359700	1.24276900
H	2.14970100	0.76650400	-1.51376500
H	1.78313700	-0.90710000	1.42439800
H	0.38904400	-1.62218900	-1.23354500
N	-0.92961300	-0.70011100	1.75126900
H	-1.67386400	-0.03221100	1.96035900
H	-0.06623000	-0.44159600	2.21738700

R3b Product_[6+4]

$G = -717.299983$ Hartree

C	0.42309400	-1.04573700	-0.33528500
C	1.82146800	-0.70484500	0.08746100
C	-0.68407300	-0.89267300	0.43319600
C	-2.06541900	-0.93195800	-0.18558100
C	-2.56610300	0.42487700	-0.81442500

C	-3.24821700	-1.33277400	0.70937200
H	-2.01766300	-1.64533900	-1.02486700
C	2.19975500	0.80328700	-0.24868700
C	1.16067100	1.72482500	0.31288700
C	3.62881300	1.11058400	0.21604900
C	-0.02143800	1.87747500	-0.30927800
C	-1.27473100	2.28904100	0.31200900
C	-2.42628300	1.62135100	0.09770200
C	-4.03713600	0.09396800	-1.15129600
H	-1.99011600	0.60884200	-1.73394600
C	-4.50275700	-0.96569600	-0.11223400
H	-3.23441100	-0.73089000	1.63316400
H	-3.22002000	-2.39297700	1.00487000
H	-5.30861900	-0.58756700	0.53459200
H	-4.90456100	-1.85399800	-0.62339400
H	-4.09568900	-0.32515900	-2.16728500
H	-4.66623300	0.99652600	-1.14623700
C	2.87007100	-1.64365000	-0.53236400
C	4.65421000	0.14680000	-0.38526700
H	3.66501900	1.04591500	1.31992000
H	3.88310900	2.15227100	-0.04090200
C	4.29562400	-1.31086300	-0.08576900
H	5.66492400	0.37998700	-0.01066700
H	4.68605000	0.29369600	-1.48035500
H	2.80032100	-1.56791400	-1.63341700
H	2.61928000	-2.68636700	-0.27813500
H	4.38304700	-1.48865900	1.00203500
H	5.01576800	-1.99156100	-0.56995500
H	1.28193200	2.05878800	1.35148300
H	-0.10319200	1.46042400	-1.31780200
H	-1.25074400	3.08514800	1.06450500
H	-3.31694500	1.92349100	0.66022200
H	2.16866000	0.87323100	-1.35161000
H	1.91418800	-0.80123000	1.18681400
H	0.26998900	-1.26861000	-1.39576600
N	-0.63542400	-0.52870200	1.76938400
H	-1.42010600	-0.80110900	2.34581700
H	0.25868100	-0.62009800	2.23428600

R3b Product_[4+2]

$G = -717.287171$ Hartree

C	0.49898300	-1.01227700	-0.53492000
C	1.50472300	-1.43892100	0.23350000

C	-0.62229700	-0.12123600	-0.03267900
C	-1.94690900	-0.42481300	-0.77302000
C	-3.07548000	0.58965000	-0.43382600
C	-2.54166400	-1.82082300	-0.42967400
H	-1.71807600	-0.36548000	-1.84867200
C	2.27718500	1.43179300	-0.39093000
C	1.12661300	1.69544200	0.23831500
C	3.65999600	1.37350400	0.18114900
C	-0.20247700	1.37013500	-0.38802400
C	-1.32052500	2.32722500	-0.05178600
C	-2.60648100	1.96606900	-0.06901800
C	-3.93750800	-0.12522800	0.62454500
H	-3.70533500	0.68668000	-1.33987400
C	-3.96619800	-1.56987500	0.11368000
H	-1.92168100	-2.32995300	0.32435800
H	-2.54838800	-2.48554300	-1.30620600
H	-4.26206100	-2.29856500	0.88442000
H	-4.69999500	-1.65339200	-0.70600700
H	-4.94040600	0.31876400	0.72987800
H	-3.42352000	-0.06621200	1.59512600
C	2.81848000	-2.00942700	-0.20708000
C	4.43659600	0.10281300	-0.23279600
H	3.62818800	1.46187000	1.28078500
H	4.24640100	2.23786200	-0.18347000
C	4.03722000	-1.25537500	0.37722700
H	5.49401200	0.27372000	0.03048200
H	4.41794900	0.02062100	-1.33527100
H	2.88093600	-2.03641000	-1.30858000
H	2.89670000	-3.05803000	0.13557800
H	3.89411300	-1.13700200	1.46728800
H	4.90964600	-1.92115000	0.26685000
H	1.13609500	1.99217100	1.29527600
H	-0.05345600	1.37767800	-1.48285000
H	-1.04001800	3.35375400	0.20459500
H	-3.38051400	2.69951900	0.18293700
H	2.21260700	1.13513900	-1.44633500
H	1.42642600	-1.26888800	1.31426600
H	0.56618600	-1.13062300	-1.62380000
N	-0.84291500	-0.19242200	1.41243700
H	-0.88786100	-1.16375100	1.71557500
H	-0.06908300	0.23222800	1.91863100

R3b TS_{CP} $G = -717.267722$ HartreeImaginary frequency: -219.89 cm^{-1}

C	0.48249700	-1.16375500	-0.18038400
C	1.71726300	-1.17196200	0.39993700
C	-0.68619500	-0.53004000	0.34332700
C	-1.97118900	-0.65188400	-0.43364600
C	-2.90473200	0.64797700	-0.55766900
C	-2.92660600	-1.74873300	0.09132200
H	-1.68487600	-0.92011300	-1.46071600
C	2.30244500	1.16098200	-0.55386500
C	1.22538000	1.76236100	0.03348100
C	3.73245200	1.29569600	-0.11740300
C	-0.12081800	1.58031800	-0.38120200
C	-1.20262100	2.24952200	0.30861900
C	-2.48886600	1.83207500	0.25613400
C	-4.33497100	0.14871700	-0.25680800
H	-2.84297900	0.92791400	-1.62450500
C	-4.29234500	-1.36638600	-0.47862500
H	-2.94938900	-1.71323000	1.19182600
H	-2.58640900	-2.75575900	-0.19465300
H	-5.13064400	-1.89933200	-0.00330400
H	-4.32926800	-1.59402600	-1.55874700
H	-5.09485800	0.66104200	-0.86672700
H	-4.57648300	0.35362700	0.80073300
C	2.92689500	-1.88008500	-0.14015000
C	4.60847700	0.08663800	-0.47408100
H	3.77942000	1.49176700	0.96873900
H	4.17973700	2.18641500	-0.60172000
C	4.26970000	-1.23156000	0.23055500
H	5.65806700	0.33925100	-0.24743400
H	4.56636200	-0.07190100	-1.56766700
H	2.84412600	-1.98620500	-1.23641300
H	2.93294300	-2.91302000	0.26005900
H	4.30150100	-1.07780700	1.32535400
H	5.07207300	-1.95433300	0.00639300
H	1.38430200	2.28700200	0.98616700
H	-0.29803200	1.24072900	-1.40459900
H	-0.93888900	3.06349600	0.99477600
H	-3.25752800	2.35404300	0.83481200
H	2.15012400	0.68840700	-1.53029600
H	1.82393100	-0.81345500	1.43002700
H	0.40020900	-1.52150300	-1.21227700

N	-0.84547100	-0.37703300	1.71694800
H	-1.52870100	0.34854600	1.94042400
H	0.02296600	-0.20161500	2.21385500

R3c reactant

$G = -754.194739$ Hartree

C	0.52009000	-1.55319700	-0.45532200
C	1.65965000	-1.46646300	0.25261000
C	-0.83733500	-1.37507500	0.07303500
C	-1.94949300	-1.48876600	-0.69944600
C	-2.89652700	1.43031800	-0.51305300
C	-3.38090000	-1.50379900	-0.25879900
H	-1.77976500	-1.66843000	-1.76825700
C	2.46528500	1.48970800	-0.62770200
C	1.50729200	1.91613700	0.21926700
C	3.93527800	1.50709600	-0.35957100
C	0.09637600	1.79530000	-0.05455900
C	-0.88798700	2.07968900	0.83155800
C	-2.29906600	1.78675900	0.64172000
C	-4.28763800	0.89050100	-0.60634000
H	-2.32065700	1.45372300	-1.44603200
C	-4.31141800	-0.58097900	-1.06973200
H	-3.45654600	-1.27749400	0.81646900
H	-3.74164900	-2.54259500	-0.38436500
H	-5.34601200	-0.95523400	-1.00211400
H	-4.03616500	-0.63833500	-2.13819700
H	-4.89662000	1.48376100	-1.31281100
H	-4.77554900	0.96696200	0.37978300
C	3.01718100	-1.85918800	-0.25496800
C	4.64664900	0.17413200	-0.64167900
H	4.11925100	1.81516100	0.68411200
H	4.41196800	2.27742500	-0.99657200
C	4.23319200	-1.03327900	0.21723300
H	5.72729800	0.34276600	-0.49940700
H	4.52557600	-0.08515400	-1.70955000
H	3.00698500	-1.92392600	-1.35700800
H	3.18115700	-2.89623600	0.09665900
H	4.07794700	-0.71264900	1.26315800
H	5.09462000	-1.71982500	0.24443800
H	1.79567400	2.31815200	1.19849300
H	-0.16757700	1.36291400	-1.02483100
H	-0.59963300	2.46133100	1.81663900
H	-2.90526500	1.78195600	1.55480100

H	2.15371800	1.07946600	-1.59678900
H	1.59892900	-1.19267800	1.31274500
H	0.56499000	-1.81799600	-1.51772000
C	-0.98452500	-1.12336300	1.48184000
N	-1.10132900	-0.91803500	2.61854200

R3c TS_{AM}

$G = -754.170455$ Hartree

Imaginary frequency: -428.72 cm^{-1}

C	0.53380100	-1.28181600	-0.38541500
C	1.77304700	-1.24833500	0.18016100
C	-0.69642400	-0.90447000	0.24844200
C	-1.95977100	-0.97987400	-0.40773500
C	-2.81806300	0.83258500	-0.83300600
C	-3.21816000	-1.50885000	0.24944900
H	-1.85563700	-1.33550600	-1.44165500
C	2.32560700	1.28681100	-0.51063200
C	1.28637200	1.84991200	0.17416900
C	3.76413800	1.34072300	-0.09498700
C	-0.05329400	1.74866200	-0.26743200
C	-1.16562900	2.18048500	0.45154900
C	-2.46231800	1.75397500	0.18165500
C	-4.27292900	0.39222800	-0.91975400
H	-2.27445100	0.91308000	-1.77961800
C	-4.38708700	-1.12549100	-0.65577500
H	-3.33060300	-1.07145500	1.25516800
H	-3.15162600	-2.60332500	0.37854000
H	-5.36287200	-1.39148800	-0.22119600
H	-4.29930300	-1.68282500	-1.60443700
H	-4.71320000	0.65532100	-1.89477200
H	-4.84925800	0.93558100	-0.15440700
C	3.00441500	-1.84843200	-0.43674700
C	4.62861900	0.18355600	-0.61119100
H	3.83561500	1.41244800	1.00417700
H	4.19591200	2.28396800	-0.48467600
C	4.33265100	-1.19927100	-0.02241500
H	5.68352700	0.42818700	-0.40358400
H	4.54187900	0.13411300	-1.71245000
H	2.91269600	-1.85754500	-1.53782400
H	3.04980200	-2.91334600	-0.13534400
H	4.37596500	-1.14293700	1.08070800
H	5.14944300	-1.87724200	-0.32093000
H	1.46850700	2.28224900	1.16516100

H	-0.20984600	1.28398600	-1.24297700
H	-0.99397800	2.75188500	1.36867600
H	-3.23172100	2.00979100	0.91757900
H	2.12729000	0.90551900	-1.51753300
H	1.85170100	-0.95431700	1.23233600
H	0.44088200	-1.60971800	-1.42771800
C	-0.68769000	-0.61578700	1.65025500
N	-0.70349000	-0.38515300	2.79046100

R3c Product_[6+4]

$G = -754.217377$ Hartree

C	0.48123100	-1.03374800	-0.51228600
C	1.85102600	-0.69433000	-0.01302400
C	-0.66839200	-0.91123400	0.18791000
C	-2.04394400	-0.94350000	-0.44444900
C	-2.58197200	0.45529900	-0.94098200
C	-3.18972200	-1.50339400	0.42935500
H	-1.95861000	-1.55724700	-1.35577100
C	2.20222800	0.82390000	-0.33653900
C	1.14957900	1.71488100	0.25429900
C	3.62124000	1.14442200	0.15178200
C	-0.03511100	1.88629800	-0.35604400
C	-1.29006700	2.25553000	0.29304000
C	-2.43638300	1.58895700	0.04863900
C	-4.05197900	0.10740600	-1.22708900
H	-2.04851900	0.71869200	-1.86831700
C	-4.48160100	-0.78960600	-0.04837300
H	-2.99856200	-1.28531600	1.49030900
H	-3.25134800	-2.59811400	0.33850200
H	-4.89676100	-0.17644700	0.76656000
H	-5.27220700	-1.49661900	-0.34063200
H	-4.11057600	-0.45723800	-2.17184300
H	-4.68283700	1.00182400	-1.34279800
C	2.92705300	-1.62413400	-0.59736100
C	4.67281500	0.19352700	-0.42243200
H	3.63431300	1.08489100	1.25539000
H	3.86186100	2.18878000	-0.10595500
C	4.33191200	-1.26504900	-0.11030700
H	5.67060000	0.44874700	-0.02951900
H	4.72475300	0.32820700	-1.51834200
H	2.89208900	-1.55762800	-1.70075700
H	2.68572300	-2.66841200	-0.34005700
H	4.38827300	-1.42680700	0.98126600

H	5.07358000	-1.94197500	-0.56513700
H	1.26875700	2.00255800	1.30589500
H	-0.12334900	1.51060200	-1.38131200
H	-1.26647800	3.00281900	1.09297400
H	-3.32067800	1.84589500	0.64155000
H	2.17680300	0.91865700	-1.43777700
H	1.86356900	-0.78410800	1.08628000
H	0.39293300	-1.26964700	-1.58004400
C	-0.59855500	-0.60260300	1.59003700
N	-0.55135600	-0.37826300	2.72892300

R3c Product_[4+2]

$G = -754.207519$ Hartree

C	0.53277400	-1.02689500	-0.60681900
C	1.54910200	-1.40764600	0.17166000
C	-0.58208700	-0.11113700	-0.14639700
C	-1.91651700	-0.40488200	-0.88224200
C	-3.03678900	0.62603500	-0.55811100
C	-2.51864500	-1.79473700	-0.53601400
H	-1.66793700	-0.34548900	-1.95306700
C	2.33105300	1.45202200	-0.45269200
C	1.17948300	1.67941200	0.18786000
C	3.70861000	1.36811600	0.12870100
C	-0.14561400	1.39259000	-0.45817900
C	-1.26512300	2.33095000	-0.07866200
C	-2.55318100	1.97249200	-0.10788600
C	-3.98154500	-0.11192600	0.41213000
H	-3.60797100	0.78128600	-1.49333600
C	-3.98804900	-1.53821200	-0.14679600
H	-1.97661200	-2.23294900	0.31585500
H	-2.41954200	-2.50562500	-1.36923800
H	-4.37242900	-2.28309100	0.56612100
H	-4.63238900	-1.57975600	-1.04168300
H	-4.98160200	0.34670200	0.45785200
H	-3.55840100	-0.09863200	1.42879500
C	2.85176700	-2.00412700	-0.26297400
C	4.47824000	0.09916100	-0.30391800
H	3.66708300	1.43390900	1.22919000
H	4.30309800	2.23552300	-0.21415100
C	4.08200900	-1.25928600	0.30640600
H	5.53854400	0.26579900	-0.05056800
H	4.44812800	0.02292400	-1.40667400
H	2.91036200	-2.05404300	-1.36388800

H	2.91025000	-3.04626900	0.10166200
H	3.95445700	-1.14411600	1.39827100
H	4.94793600	-1.93040800	0.18050100
H	1.17333300	1.88921000	1.26400800
H	-0.00172600	1.41925300	-1.55338200
H	-0.98258100	3.33867800	0.23946400
H	-3.32115100	2.69302400	0.19309000
H	2.27441600	1.21376700	-1.52366300
H	1.47713100	-1.19940100	1.24589000
H	0.57438600	-1.18416900	-1.69092000
C	-0.77133300	-0.22696100	1.30917600
N	-0.91167200	-0.32084900	2.45548600

R3c TS_{CP}

$G = -754.183290$ Hartree

Imaginary frequency: -272.77 cm^{-1}

C	0.52668500	-1.18727000	-0.32301800
C	1.78486600	-1.11691500	0.22936900
C	-0.62132000	-0.53807000	0.19981400
C	-1.96706900	-0.72228100	-0.46094800
C	-2.83982900	0.57697700	-0.79991400
C	-2.95629800	-1.63082500	0.29030100
H	-1.76119800	-1.19867300	-1.43256600
C	2.25722600	1.12231500	-0.56619200
C	1.18535400	1.75325100	0.02780900
C	3.68278000	1.27054900	-0.11277100
C	-0.13414900	1.60073300	-0.43466300
C	-1.27526500	2.24631600	0.19084900
C	-2.53103900	1.78495800	0.02742500
C	-4.31264600	0.10304100	-0.67501600
H	-2.60608900	0.81523800	-1.85183200
C	-4.26691800	-1.41938800	-0.46666600
H	-3.05457400	-1.28663500	1.33380100
H	-2.61811400	-2.67796800	0.31776000
H	-5.14927000	-1.80395900	0.06713000
H	-4.22077000	-1.94090600	-1.43836400
H	-4.92075200	0.39549300	-1.54412600
H	-4.76972300	0.57691800	0.20863300
C	2.98012500	-1.85497500	-0.30678200
C	4.61434000	0.13657000	-0.55680300
H	3.71612000	1.38506600	0.98462400
H	4.07525200	2.21960700	-0.52635000
C	4.32854500	-1.22983400	0.07072500

H	5.65142400	0.42414500	-0.31769300
H	4.57019000	0.04662300	-1.65797300
H	2.90127900	-1.95590200	-1.40406700
H	2.95740800	-2.88706000	0.09255700
H	4.38656400	-1.14303300	1.17106300
H	5.13122600	-1.92671800	-0.22191300
H	1.32878800	2.22271200	1.00825500
H	-0.26617000	1.23995400	-1.45781700
H	-1.08176900	3.05911400	0.89723800
H	-3.35323600	2.26241100	0.56847100
H	2.12228600	0.74886600	-1.58644600
H	1.86701300	-0.76542800	1.26257900
H	0.42238900	-1.61654900	-1.32662300
C	-0.62383400	-0.24219500	1.60548700
N	-0.61680100	-0.01586600	2.74566100

R3d reactant

$G = -866.439637$ Hartree

C	0.56660900	-1.31182000	-0.70504500
C	1.76537200	-1.39473100	-0.10131700
C	-0.78387500	-1.25869400	-0.13918100
C	-1.88350200	-1.16750100	-0.92881400
C	-2.78818300	1.63326600	-0.50980800
C	-3.35199600	-1.29940600	-0.66140100
H	-1.63901900	-1.09627400	-1.99586700
C	2.55853500	1.64958200	-0.34112700
C	1.56872700	1.91805100	0.53378900
C	4.01813400	1.58856200	-0.02390700
C	0.17305600	1.87907500	0.17440700
C	-0.86053600	2.04771200	1.03467100
C	-2.26080500	1.83338600	0.71561400
C	-4.18274900	1.14659200	-0.74465900
H	-2.15691600	1.75243900	-1.39841600
C	-4.20657700	-0.25015500	-1.39729400
H	-3.56854500	-1.29278200	0.41241000
H	-3.64406800	-2.29350800	-1.05211600
H	-5.24932000	-0.60453900	-1.44479700
H	-3.86238600	-0.17407600	-2.44491800
H	-4.74128100	1.84008800	-1.39998000
H	-4.72170200	1.10786700	0.21635300
C	3.05984900	-1.61127200	-0.83450000
C	4.75305700	0.40019700	-0.66190600
H	4.16285000	1.58048800	1.07019700

H	4.50620600	2.51302500	-0.39020000
C	4.33650800	-1.00807900	-0.21030400
H	5.82834500	0.52256400	-0.44873800
H	4.65934200	0.46564800	-1.76173300
H	2.96571600	-1.30360800	-1.89085300
H	3.20829100	-2.70801800	-0.86334600
H	4.25364800	-1.03694800	0.89110700
H	5.17092500	-1.68302200	-0.46067100
H	1.81457500	2.11409400	1.58483300
H	-0.04069700	1.62655300	-0.86895300
H	-0.62882200	2.26669300	2.08260100
H	-2.92854100	1.73707700	1.57774600
H	2.28250400	1.45302800	-1.38498500
H	1.81725700	-1.42479500	0.98818800
H	0.54972200	-1.28789600	-1.80085400
N	-0.95098300	-1.38915300	1.32394400
O	-1.92633400	-0.86903000	1.84803700
O	-0.10753500	-2.02079700	1.94197200

R3d TS_{AM}

$G = -866.426506$ Hartree

Imaginary frequency: -297.90 cm^{-1}

C	0.59953400	-1.28981000	-0.32105100
C	1.85334300	-1.28419900	0.19866700
C	-0.66613100	-0.88991000	0.24488200
C	-1.86774900	-0.99856800	-0.50212300
C	-2.73339200	0.87109100	-0.96387000
C	-3.19462200	-1.59470400	-0.07553200
H	-1.63206600	-1.30038200	-1.53115700
C	2.39949300	1.33448500	-0.62290200
C	1.37653900	1.90737800	0.06585600
C	3.84375500	1.34745800	-0.22972700
C	0.02885600	1.78989500	-0.37103100
C	-1.08200100	2.22622500	0.32579300
C	-2.38250500	1.77225700	0.05667300
C	-4.17495700	0.42068500	-1.09182300
H	-2.15113700	0.91528200	-1.88952200
C	-4.25259400	-1.11584500	-1.06811700
H	-3.44466500	-1.29469400	0.94820400
H	-3.10616700	-2.69594600	-0.09643000
H	-5.26199800	-1.46722500	-0.80374100
H	-4.02557100	-1.52080700	-2.07057300
H	-4.63755500	0.82383500	-2.00819300

H	-4.74478200	0.82289700	-0.23914300
C	3.04659900	-1.86898500	-0.50276300
C	4.66811000	0.16916400	-0.76784300
H	3.93627200	1.41689400	0.86774300
H	4.29338600	2.27883900	-0.62753400
C	4.39067400	-1.20922300	-0.15655600
H	5.73357200	0.40316800	-0.60714200
H	4.53574700	0.11259500	-1.86427400
H	2.89313700	-1.87617500	-1.59719400
H	3.12245700	-2.93377900	-0.20762100
H	4.48301300	-1.14483700	0.94286500
H	5.19564000	-1.88709400	-0.48618800
H	1.56458600	2.36081600	1.04533000
H	-0.12005300	1.27839200	-1.32469500
H	-0.92608000	2.80407300	1.24149500
H	-3.15436400	2.02935300	0.78705900
H	2.17225900	0.90636900	-1.60534000
H	1.99247000	-0.96490700	1.23010600
H	0.49373700	-1.65237000	-1.35090700
N	-0.76151600	-0.44648600	1.61182100
O	-1.87574500	-0.10095800	2.02287400
O	0.25087800	-0.37570000	2.30873800

R3d Product_[6+4]

$G = -866.464088$ Hartree

C	0.55813100	-1.01868700	-0.32043700
C	1.94567500	-0.67926400	0.10764600
C	-0.65468500	-0.73238200	0.19849000
C	-1.91616600	-0.80800900	-0.61673900
C	-2.69608100	0.57639400	-0.85678100
C	-2.99740700	-1.83180000	-0.19935300
H	-1.56651500	-1.11412300	-1.61275800
C	2.32653400	0.72565000	-0.55083800
C	1.32160800	1.76015700	-0.14632600
C	3.77070000	1.08653900	-0.17895400
C	0.11489100	1.84927200	-0.73380600
C	-1.06952800	2.41649100	-0.09564400
C	-2.28157200	1.82820000	-0.11398100
C	-4.17407500	0.21193600	-0.59846300
H	-2.57083900	0.78089000	-1.93433900
C	-4.27656000	-1.29361100	-0.84716500
H	-3.10763200	-1.84359900	0.89184100
H	-2.73175300	-2.84827400	-0.52871000

H	-5.19211500	-1.73960100	-0.42950200
H	-4.27386400	-1.50336900	-1.93171800
H	-4.86230900	0.81010500	-1.21564100
H	-4.40902500	0.42086100	0.45807000
C	2.96036800	-1.74922200	-0.32576800
C	4.77060700	-0.00268400	-0.57199400
H	3.81921000	1.25843900	0.91144700
H	4.03460400	2.04354300	-0.65807700
C	4.39299500	-1.35456600	0.03776300
H	5.78830100	0.28774300	-0.26385200
H	4.79211100	-0.09460800	-1.67330800
H	2.88495600	-1.89942000	-1.41909000
H	2.69821200	-2.71280900	0.14098400
H	4.48245300	-1.29637800	1.13736200
H	5.09561000	-2.13707200	-0.29242600
H	1.48999800	2.26615000	0.81136400
H	-0.05215700	1.28441600	-1.65807100
H	-0.92559400	3.28526600	0.55589700
H	-3.06561900	2.28360500	0.49945200
H	2.26996500	0.57555200	-1.64492200
H	1.99330900	-0.54421600	1.19376700
H	0.50364500	-1.42587100	-1.33768400
N	-0.80360800	-0.22294400	1.57391200
O	0.18212700	0.14593500	2.19569500
O	-1.93741600	-0.20632300	2.03638400

R3d Product_[4+2]

$G = -866.457996$ Hartree

C	-3.36857991	-1.19335346	0.00000000
C	-2.26991291	-1.37427246	0.74128900
C	-4.46171391	-0.19966646	0.30481500
C	-5.73383491	-0.47059646	-0.51984600
C	-6.85007591	0.61143554	-0.34242100
C	-6.43328691	-1.84650146	-0.34442000
H	-5.36131191	-0.40137646	-1.55270500
C	-1.55068391	1.26315254	-0.33122100
C	-2.61028991	1.61688654	0.40607200
C	-0.10928591	1.25079754	0.07613100
C	-4.00291591	1.28880254	-0.04537000
C	-5.09952791	2.21820354	0.42482500
C	-6.39066091	1.88398254	0.31169700
C	-8.02694191	-0.12360346	0.32773300
H	-7.18918491	0.88064754	-1.36112700

C	-7.94226291	-1.53316046	-0.27048800
H	-6.09899291	-2.33425546	0.57739200
H	-6.19629691	-2.52364146	-1.17869300
H	-8.49965191	-2.28236546	0.31178600
H	-8.37459291	-1.52561246	-1.28621100
H	-8.99138891	0.37047354	0.13036500
H	-7.87616991	-0.15826146	1.41546100
C	-1.02652391	-2.10614746	0.34285500
C	0.60063109	-0.08853346	-0.22513800
H	-0.01032391	1.50239654	1.14573300
H	0.43519209	2.03568054	-0.48152600
C	0.26470509	-1.31358146	0.64655600
H	1.68404709	0.09114754	-0.12471300
H	0.44193909	-0.34586646	-1.28884100
H	-1.06335391	-2.38891546	-0.72329200
H	-0.96735391	-3.05051346	0.91534100
H	0.25345809	-1.01024846	1.70930700
H	1.10500709	-2.02102946	0.54971100
H	-2.48029291	2.00032554	1.42113600
H	-3.98763791	1.28148254	-1.14839700
H	-4.80486291	3.16291454	0.88939000
H	-7.16642791	2.56440854	0.67786600
H	-1.74180091	0.85699754	-1.33390800
H	-2.22654591	-0.90069346	1.72633700
H	-3.43338991	-1.64083546	-0.99778400
N	-4.74185691	-0.22030646	1.82273000
O	-3.91497991	0.30604454	2.54793000
O	-5.74496891	-0.77214146	2.23220000

R3d TS_{CP}

$G = -866.439286$ Hartree

Imaginary frequency: -115.20 cm^{-1}

C	0.64187800	-1.18857700	-0.41468100
C	1.88731000	-1.17755200	0.15304600
C	-0.56830100	-0.60076300	0.05122000
C	-1.83738600	-0.75368100	-0.74061300
C	-2.67200200	0.57437000	-1.07589600
C	-2.89466100	-1.76773300	-0.18730800
H	-1.50331600	-1.12629000	-1.71868900
C	2.31025700	1.23410300	-0.53809400
C	1.22165500	1.78999800	0.08561800
C	3.72776500	1.32405000	-0.05633900
C	-0.08093300	1.64478500	-0.43429500

C	-1.26333800	2.21583600	0.15479000
C	-2.48747900	1.70647600	-0.11858600
C	-4.12025500	0.06626300	-1.16380500
H	-2.31474400	0.91532000	-2.06269900
C	-4.21238100	-0.99347800	-0.06202000
H	-2.58476500	-2.21326200	0.76554600
H	-3.00216700	-2.58843900	-0.91480200
H	-4.25374600	-0.50300100	0.92206000
H	-5.09970700	-1.63834600	-0.15750000
H	-4.29140900	-0.40091500	-2.14859300
H	-4.85505100	0.87922500	-1.05702000
C	3.08840900	-1.83581100	-0.46204700
C	4.65984200	0.23075100	-0.59753000
H	3.75060100	1.34280300	1.04664300
H	4.12887800	2.30378900	-0.38198400
C	4.42004000	-1.18490900	-0.06348700
H	5.69769200	0.51776700	-0.36142000
H	4.59311800	0.21961100	-1.70121900
H	2.99134400	-1.87139400	-1.56217000
H	3.11602700	-2.89112900	-0.12839300
H	4.49211300	-1.17171800	1.03913200
H	5.24243700	-1.83037600	-0.41391600
H	1.33276100	2.20040800	1.09461700
H	-0.15769400	1.29079300	-1.46485600
H	-1.14423600	2.96249300	0.94518900
H	-3.36319900	2.08752600	0.41368200
H	2.17971100	0.88996100	-1.56922700
H	1.97859700	-0.84836400	1.18668800
H	0.56617300	-1.57893300	-1.43653200
N	-0.73960600	-0.30614400	1.45277600
O	-1.89520900	-0.12175000	1.84696800
O	0.23962100	-0.19191200	2.19255600

R4 TS_[3,3]

$G = -866.457996$ Hartree

Imaginary frequency: -246.98 cm^{-1}

C	0.63425016	-1.34542662	-0.18337461
C	1.82722516	-1.31676362	0.46417839
C	-0.61803084	-0.75962662	0.20363339
C	-1.81687884	-0.79836162	-0.69229461
C	-2.62826884	0.57861638	-0.85287461
C	-2.90510084	-1.83189762	-0.31601461
H	-1.44636284	-1.06763262	-1.69371861

C	2.40208216	1.23352038	-0.90392661
C	1.43176016	1.92440238	-0.25573261
C	3.86328516	1.26751138	-0.58738661
C	0.05128316	1.75280838	-0.57450561
C	-1.00621384	2.26825938	0.15230239
C	-2.26073584	1.62972538	0.14997539
C	-4.11815084	0.17204038	-0.78339761
H	-2.38839184	0.96677138	-1.85671661
C	-4.15148284	-1.33685462	-1.04769161
H	-3.06853484	-1.80325762	0.77098339
H	-2.59960684	-2.85250162	-0.59190861
H	-5.08120584	-1.81228462	-0.69949261
H	-4.06284384	-1.54129662	-2.12941061
H	-4.74086284	0.75314638	-1.48055161
H	-4.49265584	0.36480038	0.23425939
C	3.06638116	-1.99804062	-0.03147361
C	4.62599716	-0.04502562	-0.82959361
H	4.01651716	1.61661238	0.44785439
H	4.32321416	2.03892338	-1.23666461
C	4.37201216	-1.20293262	0.14581539
H	5.70182416	0.19349338	-0.79349561
H	4.43216316	-0.38977962	-1.86224361
H	2.94860416	-2.30109262	-1.08748961
H	3.18289716	-2.93984862	0.53982439
H	4.42880816	-0.82745562	1.18358439
H	5.20929316	-1.91239662	0.03797739
H	1.68252316	2.51241438	0.63355439
H	-0.16292484	1.13934438	-1.45162061
H	-0.80399084	2.98934438	0.94917839
H	-3.07796984	2.10072338	0.69987339
H	2.11223016	0.64339538	-1.78070761
H	1.86859016	-0.83886862	1.44360539
H	0.59956216	-1.83367862	-1.16490061
N	-0.81046284	-0.18636262	1.42844739
O	-1.99334484	0.31580438	1.62456339
O	0.08448716	0.00585338	2.26911839

R4 Product_{H[4+2]}

$G = -866.435068$ Hartree

C	0.96676733	-0.57401812	0.00000000
C	2.12807833	-0.57792212	0.69026000
C	-0.30674667	-0.00130312	0.39590700
C	-1.41860767	0.18786688	-0.60490300

C	-2.09252067	1.61281488	-0.56291000
C	-2.59436967	-0.80927512	-0.46415200
H	-0.97206767	0.04446188	-1.59982600
C	2.96220533	2.29632588	-0.76028600
C	2.06324133	2.92604888	0.01878200
C	4.43730133	2.21676788	-0.53475700
C	0.63936733	2.74538688	-0.18423600
C	-0.32607467	3.01389088	0.71470400
C	-1.66583467	2.33818788	0.71159200
C	-3.61591867	1.34201088	-0.60786600
H	-1.78630267	2.19737088	-1.44229700
C	-3.75989867	-0.08793212	-1.14152800
H	-2.81640667	-0.95576112	0.60468600
H	-2.35764167	-1.79305812	-0.89648200
H	-4.74048367	-0.53600912	-0.91908100
H	-3.63007167	-0.10545812	-2.23797100
H	-4.15516467	2.09224288	-1.20566500
H	-4.02213767	1.38184888	0.41587100
C	3.42416433	-1.12319012	0.17267700
C	5.03153133	0.80250688	-0.67577700
H	4.69239333	2.63801488	0.45260800
H	4.94475033	2.85636688	-1.28290800
C	4.67858633	-0.24583312	0.39830600
H	6.12806533	0.91866288	-0.68074500
H	4.77481433	0.40106588	-1.67333800
H	3.33757133	-1.39094512	-0.89515200
H	3.60576533	-2.07576312	0.70699300
H	4.61095333	0.24072388	1.38769200
H	5.53782933	-0.93238212	0.46650400
H	2.39051333	3.45832388	0.91923500
H	0.37582133	2.20414788	-1.09752300
H	-0.06999167	3.52245188	1.65005600
H	-2.45786367	3.01383288	1.06804700
H	2.58538433	1.74583688	-1.63222900
H	2.12626033	-0.18518012	1.70857500
H	0.96642533	-0.97253412	-1.02099100
N	-0.47983067	0.50045288	1.60728900
O	-1.64741967	1.30928888	1.76872700
O	0.28088233	0.49977588	2.57474000

III. xTB_md.inp, Fetch distance data.py

xTB_md.inp

```
$md
    temp=300.00 # in K
    time= 0.15  # in ps
    dump= 1.0   # in fs
    step=  0.1  # in fs
    velo=false
    nvt =true
    hmass=4
    shake=0
    sccacc=2.0
$end
```

Fetch distance data.py

```
import pandas as pd
with open("xtb.trj") as f:
    lines = f.readlines()
frame_coords = []
for i in range(2, len(lines), 43):
    frame_coords.append([])
    for j in range(0, 41):
        coords_line = lines[i + j].split()
        frame_coords[-1].append([float(coords_line[1]),      float(coords_line[2]),
float(coords_line[3]))]
results = []
for i, coords in enumerate(frame_coords):
    results.append([i + 1,
                    ((coords[1][0] - coords[7][0])**2 + (coords[1][1] -
coords[7][1])**2 + (coords[1][2] - coords[7][2])**2)**0.5,
                    ((coords[10][0] - coords[2][0])**2 + (coords[10][1] -
coords[2][1])**2 + (coords[10][2] - coords[2][2])**2)**0.5,
                    ((coords[3][0] - coords[4][0])**2 + (coords[3][1] -
coords[4][1])**2 + (coords[3][2] - coords[4][2])**2)**0.5
                    ])
df = pd.DataFrame(results, columns=["Frame", "Dist(2-8)", "Dist(11-3)", "Dist(4-5)"])
df.to_excel("results.xlsx", index=False)
```