

**DFT Investigation the Mechanisms of Csp<sup>3</sup>-H functionalization of  
Glycine Derivatives Induced by Radical Cation Salt**

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**1.The Cartesian coordinates (Angstrom) for the optimized transition states  
obtained at the M06-2X-D3/6-311+G(d,p) level of theory in the solvent of CH<sub>3</sub>CN.**

**TS0(1)**

N	-0.02744200	-0.01456300	0.60092900
C	0.55414100	1.29543500	0.32776400
C	1.67634700	1.66975800	1.07098700
C	0.03315900	2.12700800	-0.66290700
C	2.27903500	2.89320100	0.82961100
H	2.09048300	1.00673100	1.82591800
C	0.64040400	3.35069500	-0.90885900
H	-0.81801200	1.81813400	-1.26054800
C	1.75455000	3.72581300	-0.15972500
H	3.14642700	3.19221300	1.40675500
H	0.25250400	3.99662500	-1.68875200
C	-1.42485700	-0.17499600	0.26141000
C	-1.86863800	-1.24596700	-0.51869900
C	-2.33005200	0.77561000	0.76417000
C	-3.21810700	-1.35795900	-0.80885900
H	-1.17121800	-1.97014500	-0.92424500
C	-3.67826400	0.65914100	0.47638300
H	-1.98039500	1.60409200	1.37345800
C	-4.11378400	-0.40836100	-0.30900200
H	-3.56774900	-2.17190800	-1.43412900
H	-4.37968900	1.38748800	0.86639700
C	0.85808400	-1.13747000	0.30549400
C	0.67683700	-2.33450700	1.00234000
C	1.86519500	-1.00514100	-0.65014600
C	1.51697200	-3.40771500	0.74774800
H	-0.11715600	-2.43945900	1.73643600
C	2.69958800	-2.08194700	-0.91202300
H	1.99212700	-0.08059100	-1.20352900
C	2.52500600	-3.27110800	-0.20674700
H	1.38776100	-4.33572700	1.29357900
H	3.47503900	-1.99143000	-1.66405000
Br	2.58156400	5.38693100	-0.50226100
Br	-5.94388200	-0.57064300	-0.71881500
Br	3.67899100	-4.72455100	-0.55152900
H	-0.10289100	-0.03127700	1.96173400
O	-0.25236600	-0.06310500	3.11480000
O	-1.46918000	-0.37721400	3.34170100

**TS0(2)**

N	0.01953100	-0.00441700	0.59069800
C	0.24928600	1.41205800	0.32535700
C	1.21880300	2.07107800	1.08425300
C	-0.46173900	2.07748500	-0.67278100
C	1.47512000	3.41191100	0.84710500
H	1.77610100	1.54333400	1.85308600
C	-0.20279300	3.41966500	-0.91130400
H	-1.19458600	1.55215000	-1.27590000
C	0.76045300	4.07914000	-0.14959300
H	2.22178600	3.93532900	1.43236700
H	-0.73842700	3.94446000	-1.69324100
C	-1.30256700	-0.49578000	0.26001600
C	-1.48992000	-1.60454900	-0.56996200
C	-2.40197400	0.18529000	0.80932400
C	-2.77741300	-2.02918400	-0.85363000
H	-0.64557300	-2.11475500	-1.01885800
C	-3.68600200	-0.24127900	0.52571800
H	-2.24826800	1.04397200	1.45645100
C	-3.86847800	-1.35095600	-0.30283900
H	-2.93592300	-2.87523500	-1.51197800
H	-4.53857600	0.27599100	0.94917500
C	1.14233400	-0.88556700	0.28899600
C	1.17804500	-2.13644300	0.91314200
C	2.15423900	-0.48804500	-0.58441700
C	2.23253700	-2.99730000	0.65958800
H	0.38343700	-2.44312700	1.58714400
C	3.20836000	-1.35363900	-0.84133000
H	2.11851800	0.47724300	-1.07706800
C	3.24344500	-2.59991300	-0.21720700
H	2.27225300	-3.96694900	1.14130700
H	3.99270300	-1.06161300	-1.53011700
Br	1.11162400	5.89964700	-0.47611200
Br	-5.60812100	-1.93729000	-0.69055500
Br	4.67415400	-3.77251100	-0.56476700
H	-0.03538800	-0.06009800	1.94011000
O	-0.18064900	-0.21103900	3.08690400
O	-1.17100000	-1.00248800	3.23187100

**TS0(3)**

N	0.00301000	0.00257700	0.61167900
C	0.64584300	1.28194600	0.33597600
C	1.76807300	1.62386400	1.09607500
C	0.17960900	2.12531400	-0.67269200
C	2.42466600	2.81833600	0.84944500
H	2.13135400	0.95635400	1.87391400
C	0.84207100	3.31884300	-0.92326400
H	-0.68079500	1.84589200	-1.27271400
C	1.96034500	3.66551200	-0.16158100
H	3.29074300	3.09856100	1.43788900
H	0.49942900	3.97614000	-1.71475700
C	-1.40372800	-0.08517500	0.27721400
C	-1.90105300	-1.09500400	-0.55139600
C	-2.26592400	0.88270600	0.81871800
C	-3.25477500	-1.13053000	-0.84439800
H	-1.23452600	-1.83219600	-0.98597900
C	-3.61703200	0.84308400	0.52810600
H	-1.87363700	1.66085600	1.46812000
C	-4.11288400	-0.16570900	-0.30488600
H	-3.64905400	-1.89585000	-1.50344200
H	-4.28987700	1.58197700	0.94800700
C	0.81656600	-1.17111200	0.31577000
C	0.53377600	-2.36088800	0.99465600
C	1.84797400	-1.10901300	-0.62175900
C	1.28722900	-3.49368200	0.73319200
H	-0.27548800	-2.40472200	1.71886000
C	2.59456600	-2.24735100	-0.89012600
H	2.05887300	-0.18489800	-1.15042400
C	2.31634100	-3.43623100	-0.21190700
H	1.08444200	-4.41889800	1.26082500
H	3.38803700	-2.21643700	-1.62848600
Br	2.85282600	5.27550000	-0.50173600
Br	-5.93475400	-0.22354800	-0.71201200
Br	3.32649700	-4.96943200	-0.57563300
H	-0.06353300	-0.00591200	1.97058600
O	-0.22618100	-0.04688300	3.11393300
O	-1.39093800	-0.53518600	3.30123200

**TS1a**

N	-0.48171500	0.28224900	0.01129600
C	-1.85338300	-0.19318400	-0.26592700
C	-2.79227700	-0.03433400	0.74778200
C	-2.20848100	-0.72425500	-1.50139700
C	-4.10360400	-0.44552800	0.54187000
H	-2.50779300	0.41382200	1.69589700
C	-3.52191400	-1.13172500	-1.71269300
H	-1.47915300	-0.82387500	-2.29910100
C	-4.45484000	-0.99843800	-0.68694900
H	-4.83572000	-0.33556900	1.33465700
H	-3.80823300	-1.54626300	-2.67338600
C	0.59181400	-0.40416400	-0.71791200
C	1.70280800	0.29573900	-1.18036700
C	0.55007700	-1.79836300	-0.78712100
C	2.76741400	-0.40053700	-1.74322200
H	1.76333200	1.37491300	-1.09824900
C	1.61359800	-2.49500200	-1.34492200
H	-0.29803600	-2.34938600	-0.39036200
C	2.71528400	-1.78821600	-1.82235700
H	3.63579600	0.14369200	-2.09843300
H	1.58278700	-3.57806700	-1.39268700
C	-0.44957700	1.75532400	-0.06261800
C	-0.26824200	2.50268900	1.09247300
C	-0.64155500	2.36781000	-1.29857500
C	-0.25709000	3.89336900	1.01169000
H	-0.14433700	2.01886800	2.05562400
C	-0.62704500	3.75281300	-1.38393400
H	-0.78815600	1.76985900	-2.19399800
C	-0.42970600	4.50370700	-0.22571900
H	-0.11670800	4.48573100	1.90915200
H	-0.76863200	4.23829600	-2.34292000
Br	-6.23655000	-1.57426000	-0.96770700
Br	4.17560000	-2.73109300	-2.56895100
Br	-0.40181700	6.39380000	-0.34145900
C	4.93986400	-1.06749000	1.28389200
C	3.69646600	-1.62528800	1.53007100
C	2.62523600	-0.80352600	1.93023500
C	2.82842100	0.58260800	2.06902500
C	4.07877200	1.11706100	1.81311100
C	5.16093500	0.31113600	1.41979500
H	5.75952800	-1.70983300	0.97095000
H	3.53169600	-2.69375800	1.40938800
H	2.00841000	1.23273000	2.35711200
H	4.22584700	2.18964000	1.91382900

C	6.50819200	0.90698400	1.17750400
H	6.43445400	1.88779700	0.69899400
H	7.04440400	1.05900600	2.12245300
H	7.13072000	0.26055300	0.55390300
N	1.39168800	-1.38175100	2.13217100
H	1.31873700	-2.37112900	1.90778000
C	0.21481100	-0.73312400	2.48189300
H	0.34872500	0.14224700	3.11510400
H	-0.25012500	-0.07005600	1.18904500
C	-0.91615800	-1.58568100	2.86393300
O	-1.82943900	-1.22727700	3.59384200
O	-0.85893800	-2.78922600	2.25796500
C	-1.99063400	-3.67312000	2.47394200
H	-1.99230000	-3.97607200	3.52596200
H	-2.90699400	-3.10489300	2.28273000
C	-1.83580600	-4.83753000	1.53954700
H	-0.90383200	-5.37949500	1.72663200
H	-2.66585900	-5.53403600	1.68235400
H	-1.84477800	-4.51025900	0.49465600

**TS1b**

C	2.51992600	-1.13552100	-0.91213300
C	1.59980800	-0.42876700	-0.11175900
C	2.08313300	0.52769100	0.79909400
C	3.45067500	0.74967400	0.90522000
C	4.37776500	0.04744100	0.12404200
C	3.87779900	-0.89608200	-0.78968500
H	2.14712300	-1.86959000	-1.62243500
H	1.39484500	1.10577900	1.40834200
H	3.81025700	1.49637600	1.60983400
H	4.57246500	-1.45191100	-1.41590100
N	0.25846400	-0.70589400	-0.23923500
C	-0.77730200	-0.09327600	0.46834900
H	-0.55849800	0.06979500	1.52669300
C	-2.08046600	-0.75053200	0.20976600
O	-2.27124000	-1.57673700	-0.67010200
O	-3.02159800	-0.28248100	1.04298600
C	-4.36638800	-0.80549400	0.86230000
H	-4.82711000	-0.68542900	1.84429500
H	-4.29599200	-1.87139800	0.63143300
C	-5.11426300	-0.04749700	-0.20164100
H	-4.65026800	-0.16955700	-1.18416700
H	-6.13842900	-0.42661100	-0.26423800
H	-5.16717600	1.01936800	0.03556800
H	-0.96498300	1.10049600	0.06750200
O	-1.26355300	2.30241800	-0.35901300
O	-2.34740600	2.05811700	-1.24089100
H	-3.12386200	2.20536200	-0.67250200
C	5.84861800	0.28276100	0.25656300
H	6.35018500	-0.57700600	0.71689300
H	6.32174000	0.43170400	-0.71977600
H	6.06131300	1.15799400	0.87564700
H	-0.02630600	-1.30703500	-1.00708600

TS2(I)c

C	2.66914800	-0.84046500	-1.83563400
C	1.45733900	-1.05614300	-2.55886000
C	1.51839600	-1.78499100	-3.78541500
C	2.72052500	-2.26392800	-4.24713600
C	3.91893700	-2.05735600	-3.52837800
C	3.85835900	-1.33306300	-2.31682700
H	2.64142300	-0.28868300	-0.89898700
H	0.60031700	-1.95179800	-4.34348000
H	2.75603700	-2.81701200	-5.18205200
H	4.77429900	-1.16500600	-1.75673400
N	0.29155000	-0.58651000	-2.07283500
C	-0.92177100	-0.83261600	-2.69117000
C	-1.71161700	-2.01255300	-2.39301300
O	-2.82444200	-2.22203300	-2.86259100
O	-1.05762700	-2.85402100	-1.56000500
C	-1.74792500	-4.07734200	-1.19379000
H	-0.93930100	-4.76756700	-0.94408900
H	-2.27685500	-4.45461400	-2.07280200
C	-2.67425800	-3.85801000	-0.02863300
H	-3.48820300	-3.17435800	-0.28676000
H	-3.11789000	-4.81269400	0.26827000
H	-2.13525300	-3.45385700	0.83412900
H	-1.34031800	-0.08432600	-3.36012500
N	-0.06451400	0.59570600	0.23892000
C	-1.51789200	0.37363300	0.36535700
C	-2.06673000	-0.36669200	1.40473900
C	-2.32806100	0.91656100	-0.63343900
C	-3.44074800	-0.59041400	1.43152600
H	-1.44736100	-0.77628700	2.19541300
C	-3.69725900	0.68882700	-0.61161800
H	-1.89291600	1.52208000	-1.42391400
C	-4.24113000	-0.07564800	0.41791300
H	-3.87361300	-1.17075600	2.23921600
H	-4.32629500	1.09765000	-1.39483400
C	0.27929000	2.02489100	0.16190700
C	1.25863400	2.43398900	-0.73604800
C	-0.36161400	2.94080900	0.99113400
C	1.60217900	3.77987300	-0.80969100
H	1.76125100	1.72185600	-1.38233900
C	-0.01849900	4.28574000	0.92307700
H	-1.12279900	2.61070500	1.69229900
C	0.96000900	4.69332800	0.01962700
H	2.36010400	4.10628600	-1.51291500
H	-0.50998700	5.00336200	1.57097400



C	0.76055800	-0.17381300	1.18682400
C	1.45952500	0.44461500	2.21530400
C	0.83633600	-1.55371500	0.99449600
C	2.24783600	-0.32675300	3.06573200
H	1.40632700	1.51754800	2.36620500
C	1.62222100	-2.32427700	1.84100500
H	0.28112300	-2.02979200	0.18854200
C	2.32436900	-1.70099300	2.87056300
H	2.79435300	0.15024200	3.87174300
H	1.68585200	-3.39693700	1.69168600
Br	3.40692100	-2.74410100	4.02437100
Br	-6.10255800	-0.42886100	0.43238600
Br	1.42315400	6.52733100	-0.08842400
H	0.19371200	0.09011600	-0.85864700
C	5.20649600	-2.61614400	-4.01645500
H	5.38799900	-3.59939500	-3.56305600
H	5.20160600	-2.76067700	-5.09935700
H	6.05359600	-1.98340200	-3.73915100

**TS2(I)d**

C	-2.07389000	0.95351700	-0.61118500
C	-1.15831200	-0.12983600	-0.51673100
C	-1.60699100	-1.35096600	0.05487000
C	-2.91465200	-1.47905800	0.47360000
C	-3.82889700	-0.40871600	0.37999000
C	-3.37289400	0.80552000	-0.17173400
H	-1.73959900	1.88900500	-1.05160400
H	-0.90851900	-2.17837400	0.14529500
H	-3.25124300	-2.42447200	0.89261700
H	-4.06493400	1.63998300	-0.25539400
N	0.11077200	0.02893800	-0.98329700
C	0.99790800	-1.00108900	-1.13714400
C	2.35481700	-0.96365900	-0.67244600
O	3.19122200	-1.83584700	-0.91938700
O	2.61128700	0.14008300	0.07337300
C	3.95267400	0.27571900	0.58702100
H	4.08298900	1.35334700	0.71382200
H	4.66005200	-0.07914100	-0.16794600
C	4.11675700	-0.45938100	1.89228100
H	3.97456600	-1.53565500	1.76121500
H	5.12405700	-0.29569300	2.28678100
H	3.39944200	-0.10153200	2.63662400
H	0.67625700	-1.87136400	-1.70318400
H	0.51044500	1.17608300	-0.91531900
C	-5.22463700	-0.55006200	0.88154100
H	-5.61429600	-1.55811400	0.71098200
H	-5.26593900	-0.37792700	1.96518900
H	-5.89766600	0.17431400	0.41508600
O	0.50547200	2.64385200	0.59522000
H	-0.37683900	3.06180000	0.58927300
O	0.75008400	2.39856600	-0.76179800

TS3(I)e

C	0.31960800	3.21908000	-0.03207100
C	0.12258600	1.84888100	-0.36485300
C	1.28387700	1.07170400	-0.62166400
C	2.55675100	1.63189100	-0.50952500
C	2.73657300	2.96944500	-0.15920400
C	1.58331000	3.75502300	0.06845600
H	-0.56173300	3.82522000	0.16339000
H	1.19108200	0.05675600	-0.99194600
H	3.43004600	1.01464300	-0.71479100
H	1.70493600	4.80306500	0.33644000
N	-1.15299000	1.37976300	-0.34536500
C	-1.32554700	0.03732200	-0.44931400
H	-0.67902500	-0.54822900	-1.12167700
C	-2.75107100	-0.39279000	-0.67326300
O	-3.06359200	-1.25585000	-1.47403300
O	-3.61434700	0.24367300	0.12300300
C	-5.00507500	-0.13754000	-0.03511500
H	-5.08931100	-1.21449100	0.14105100
H	-5.29887900	0.05376100	-1.07181800
C	-5.80936900	0.66670000	0.94355000
H	-6.86698000	0.40571800	0.85281800
H	-5.49881400	0.46651800	1.97272200
H	-5.70739800	1.73859200	0.75409300
C	2.67621600	-1.97767000	1.02256400
C	1.29789600	-1.91917700	0.71548900
C	0.77462500	-2.87829800	-0.18191400
C	1.59777200	-3.84888000	-0.73671400
C	2.95468300	-3.89579600	-0.41182500
C	3.48993800	-2.95530500	0.47225600
H	3.08993200	-1.23379100	1.70063200
H	-0.28151300	-2.85873200	-0.44219900
H	1.18035800	-4.57639500	-1.42720500
H	3.59272500	-4.66019700	-0.84636400
H	4.54594100	-2.98624500	0.72559500
C	0.49525700	-0.87890500	1.29239000
H	1.01843100	-0.15664700	1.91607700
C	-0.90023000	-0.74437400	1.11822100
H	-1.43460400	-1.68715300	0.98369300
H	-1.39996000	-0.09220100	1.83131100
C	4.09855000	3.57217600	-0.04236100
H	4.23664600	4.39254900	-0.75589900
H	4.26093500	4.00145800	0.95270100
H	4.88352200	2.83395000	-0.22343700

**TS3(D)f-1**

C	0.05926400	3.99767200	-1.78646100
C	-0.02640200	3.25419500	-0.57938900
C	-1.30413600	3.08704200	0.01818900
C	-2.42848600	3.61278500	-0.58632600
C	-2.34025000	4.32809500	-1.79318700
C	-1.07108200	4.51560200	-2.37700100
H	1.04095400	4.12702800	-2.23277700
H	-1.40175600	2.56982600	0.96796900
H	-3.40254800	3.47788800	-0.12240400
H	-0.99375100	5.07347000	-3.30661100
N	1.14044500	2.72873600	-0.12202500
C	1.15750700	1.87322800	0.89362200
H	0.34153000	1.79754500	1.62674900
C	2.48334500	1.53508000	1.50280100
O	2.58363300	1.20438700	2.67026900
O	3.48165600	1.59359100	0.62127900
C	4.77129400	1.12479100	1.10168800
H	4.93191000	1.51304400	2.11064800
H	5.49091000	1.58664000	0.42397200
C	4.83315700	-0.37824300	1.05589800
H	5.83374700	-0.71757800	1.33748600
H	4.11674100	-0.82504500	1.75061600
H	4.61944300	-0.74795700	0.04834500
C	-2.93759800	-0.10777900	0.83697800
C	-1.54561300	-0.18052000	1.02721900
C	-1.05679500	-0.44368200	2.31806800
C	-1.93532000	-0.63471400	3.37831000
C	-3.31288000	-0.57083200	3.17371100
C	-3.81105500	-0.30244000	1.89815100
H	-3.32343500	0.10098900	-0.15960500
H	0.01450900	-0.49562400	2.50025300
H	-1.54090500	-0.83356700	4.37080900
H	-3.99582500	-0.72477700	4.00430800
H	-4.88297100	-0.24367200	1.73181300
C	-0.65379500	0.01479800	-0.13134000
H	-1.11090500	0.55500900	-0.96986300
C	0.75580800	0.14800800	-0.00392400
H	1.33600400	0.29692300	-0.91166500
H	1.26592200	-0.46146500	0.74446700
In	-0.66013000	-2.05590800	-1.18944800
Cl	-2.34351200	-2.06725200	-2.84975800
Cl	1.43637400	-2.59341400	-2.15030300
Cl	-1.19366500	-3.70229900	0.42627200
C	-3.55589600	4.88386500	-2.44679700

H	-3.45956800	5.96418000	-2.60012400
H	-3.69286300	4.44795700	-3.44291900
H	-4.45823300	4.69402300	-1.86253900

**TS3(I)f-2**

C	0.09338100	4.09519900	-1.70732200
C	0.18471800	3.30413300	-0.50948700
C	-1.05158000	2.85267000	0.09160500
C	-2.28937200	3.18256700	-0.51123100
C	-2.34499100	3.89241700	-1.68994100
C	-1.11778700	4.35480300	-2.27545300
H	1.01990000	4.43539800	-2.16231200
H	-1.04810900	2.63859200	1.15634900
H	-3.21250100	2.87681700	-0.02235500
H	-1.17014500	4.92425600	-3.20111800
N	1.38187000	2.93196700	-0.08538300
C	1.37250900	1.91916800	0.89286100
H	0.73672500	2.11405600	1.77076500
C	2.74643600	1.56854400	1.41896700
O	2.96903300	1.35680100	2.59845700
O	3.64407700	1.44254900	0.43845000
C	4.93614600	0.89164100	0.81508600
H	5.23804800	1.32715300	1.77070500
H	5.61290200	1.24186600	0.03387300
C	4.86100300	-0.61030200	0.87020900
H	5.84531200	-1.02486200	1.10457900
H	4.16053500	-0.94420500	1.64147400
H	4.54030400	-1.02135600	-0.09171400
C	-3.01399100	0.07515600	0.63081900
C	-1.64661200	0.18911600	0.97139200
C	-1.26833200	-0.07043400	2.30665500
C	-2.21821700	-0.43398700	3.25174000
C	-3.56266300	-0.56083300	2.89384300
C	-3.95542100	-0.30466000	1.57888600
H	-3.32545100	0.30148500	-0.38707000
H	-0.22391100	0.00896400	2.60025900
H	-1.90823300	-0.62974500	4.27456900
H	-4.29876500	-0.85773300	3.63548000
H	-4.99977900	-0.39346700	1.29286600
C	-0.67844900	0.63892300	-0.02719400
H	-1.02756000	0.72180800	-1.05776000
C	0.77790200	0.58631800	0.21191200
H	1.33625400	0.46247600	-0.71717300
H	1.04709100	-0.23787700	0.88462600
In	-0.93430800	-2.01825100	-0.89824800
Cl	-2.59250400	-1.58547600	-2.47361100
Cl	1.22146900	-2.26428800	-1.75674800
Cl	-1.41605300	-3.40236100	0.89883600

C	-3.63663900	4.22351000	-2.35597800
H	-3.75135900	5.30550400	-2.48502600
H	-3.67605000	3.78995100	-3.36224100
H	-4.49281200	3.84975300	-1.78996800

**TS3(I)g**

C	4.99127000	0.46570800	-4.10746800
C	4.28151100	-0.72027700	-3.82796300
C	5.00711500	-1.84777500	-3.39376400
C	6.38351700	-1.76530600	-3.21677000
C	7.08774600	-0.58471800	-3.47209400
C	6.35871000	0.52902200	-3.93100900
H	4.45988200	1.34593500	-4.46644800
H	4.51557000	-2.80039800	-3.22943800
H	6.92544900	-2.64681500	-2.88173000
H	6.88203500	1.45699300	-4.14838200
N	2.90198400	-0.72041600	-3.97264000
C	2.16683900	-1.77030100	-3.56477800
H	2.56965100	-2.78087700	-3.58260900
C	0.73791500	-1.66772800	-3.94417400
O	0.22960700	-0.58228700	-4.31182100
O	0.07051300	-2.77214200	-3.85795900
C	-1.37189800	-2.73457800	-4.18618700
H	-1.45322600	-2.39573100	-5.22134100
H	-1.82730600	-1.99024600	-3.52876100
C	-1.90315000	-4.11611600	-3.97154900
H	-2.97185400	-4.11940600	-4.19816700
H	-1.41505200	-4.83916700	-4.62944500
H	-1.77539300	-4.43518800	-2.93416100
In	1.67890500	0.96571200	-4.43210400
Cl	1.13906800	2.42958200	-2.70521300
Cl	1.53938700	1.80589900	-6.59260800
C	4.75127500	-3.79493800	-0.13323400
C	5.13688500	-5.10365900	0.11685900
C	4.29594600	-6.15805300	-0.24785900
C	3.06575300	-5.89699800	-0.85964800
C	2.66997900	-4.59066000	-1.10174200
C	3.50827100	-3.51254200	-0.74020700
H	5.40251900	-2.96585200	0.13481000
H	6.09316700	-5.30757900	0.59011300
H	4.59756900	-7.18392200	-0.05585000
H	2.41663900	-6.72017800	-1.14384800
H	1.70858400	-4.40062400	-1.57245500
C	3.15349900	-2.14174400	-0.98120300
H	3.90675900	-1.39928500	-0.71794900
C	1.95382900	-1.69809000	-1.52070600
H	1.09160000	-2.36036700	-1.47373800
H	1.72889200	-0.63708600	-1.44661700
C	8.56466200	-0.49827200	-3.27864100



H	8.98148700	-1.44499800	-2.92821000
H	9.07119800	-0.22528300	-4.21068900
H	8.82111000	0.27826900	-2.54961100

**TS3(I)h-1**

C	-1.68777500	2.78862400	1.56661600
C	-1.45736600	2.07761300	0.38349000
C	-0.27144900	2.34962400	-0.38575100
C	0.42384900	3.56917400	-0.09983700
C	0.17855300	4.29887900	1.04404900
C	-0.87554900	3.86517400	1.88571600
H	-2.51824300	2.50699200	2.20706000
H	-0.27040700	1.98868500	-1.41437800
H	1.22553800	3.87148200	-0.76869800
H	-1.07934400	4.42201300	2.79817700
N	-2.25203200	1.03495800	-0.00505200
C	-3.52427300	1.12210800	-0.04089300
H	-4.06545700	2.05945000	0.13177500
C	-4.32540400	-0.09839500	-0.35199200
O	-3.85917000	-1.19262900	-0.60218400
O	-5.62472700	0.20739100	-0.29483100
C	-6.56177200	-0.87339700	-0.57380600
H	-7.47016400	-0.57172100	-0.04985500
H	-6.17279600	-1.78869200	-0.12007600
C	-6.78280800	-1.01987000	-2.05439600
H	-7.53173700	-1.79615500	-2.23257900
H	-7.15110300	-0.08787600	-2.49181100
H	-5.86390800	-1.31136300	-2.57021300
C	3.25319800	2.07997100	0.09822200
C	2.24011800	1.31551400	-0.49870200
C	2.43678300	0.80719200	-1.79017700
C	3.62768700	1.05198500	-2.46615300
C	4.63625500	1.80188000	-1.85912400
C	4.44812600	2.31368400	-0.57437300
H	3.09645500	2.48273800	1.09785200
H	1.65270100	0.22660000	-2.27034200
H	3.77032600	0.65690300	-3.46788100
H	5.56649900	1.99001300	-2.38815500
H	5.23190800	2.89498500	-0.09746200
C	1.00937900	1.02127800	0.27322700
H	1.05733600	1.39279500	1.29954900
C	0.41049600	-0.31308700	0.14579200
H	0.24476600	-0.64062600	-0.88489200
H	-0.50101400	-0.44933900	0.72813300
In	1.79071300	-1.74880700	0.95572300
Cl	2.77534600	-3.52793800	-0.20416100
Cl	2.72541300	-1.63360700	3.10614300
C	0.99333200	5.49640100	1.40728700

H	0.36027900	6.36891900	1.59633500
H	1.56111800	5.31379400	2.32634300
H	1.70406600	5.74778300	0.61687600

**TS3(I)h-2**

C	-0.23175600	4.11058500	-0.40897900
C	0.02111800	2.87127700	0.24455400
C	-1.09696300	2.10168300	0.84954700
C	-2.40999200	2.79448600	0.84386400
C	-2.61292600	3.98682100	0.23758500
C	-1.48971200	4.63557800	-0.40615100
H	0.59622500	4.61299000	-0.89833500
H	-0.84865500	1.80371700	1.88045400
H	-3.23078100	2.30121000	1.35780600
H	-1.66749900	5.58794000	-0.90150700
N	1.23484200	2.34111600	0.16955000
C	1.50331600	1.28208300	0.91464200
H	1.15615900	1.22021900	1.94865600
C	2.75503700	0.47888600	0.66226000
O	3.18474100	-0.28298000	1.50120400
O	3.27050700	0.68514400	-0.53593000
C	4.40914100	-0.13485000	-0.90546400
H	5.09442700	-0.18328900	-0.05652800
H	4.88004500	0.41517100	-1.72041800
C	3.94927100	-1.50776000	-1.34811500
H	4.81782100	-2.08979400	-1.66954500
H	3.46033600	-2.04495700	-0.53059700
H	3.25628000	-1.42791600	-2.19034200
C	-3.56621700	-0.00329300	-0.44660800
C	-2.46908300	-0.02413200	0.42503400
C	-2.56212600	-0.76106200	1.62395300
C	-3.72832700	-1.47661600	1.92617700
C	-4.80508200	-1.45454500	1.04527600
C	-4.72347000	-0.71107400	-0.13589700
H	-3.49676000	0.55605700	-1.37601900
H	-1.74487900	-0.74432500	2.34525400
H	-3.78236500	-2.04239400	2.85078800
H	-5.70604300	-2.01469500	1.27413700
H	-5.56166700	-0.69668600	-0.82579600
C	-1.18176500	0.69881000	0.04736800
H	-1.25717500	0.96215300	-1.01184100
C	0.03984400	-0.17902100	0.23241900
H	0.31088300	-0.54810100	1.22581900
H	0.73969100	-0.29493300	-0.59383600
In	-0.97004800	-2.19145700	-0.07445400
Cl	-2.03785100	-2.83766800	-2.05688100
Cl	-0.40827900	-4.06549300	1.20878300
C	-3.94552000	4.67972400	0.21957100

H	-3.87306400	5.66340300	0.69488000
H	-4.28039800	4.83986300	-0.81063900
H	-4.70151400	4.09190400	0.74463200

**TS3(D)i**

C	-2.55537900	-0.75589300	0.01697800
C	-1.97770700	0.53988500	0.15611900
C	-2.86968000	1.64088600	0.27531200
C	-4.24954700	1.44226800	0.28838500
C	-4.80273100	0.16732100	0.17649200
C	-3.91995100	-0.93029600	0.03122500
H	-1.88311400	-1.60494400	-0.08127100
H	-2.49092700	2.65691800	0.25697700
H	-4.90973700	2.30387100	0.37196400
H	-4.33640300	-1.93118000	-0.06486600
N	-0.62591900	0.61712900	0.22536800
C	-0.09777400	1.81740600	0.58249100
H	-0.53674800	2.75292300	0.20158300
C	1.38390500	1.87534600	0.42848600
O	1.99877600	2.91348600	0.08255500
O	2.03123400	0.79365000	0.72769700
C	3.50099600	0.81559100	0.61562800
H	3.86146400	1.62864500	1.24989300
H	3.74180400	1.04663000	-0.42469700
C	3.99521100	-0.52919700	1.04762200
H	5.08487600	-0.54498100	0.97151400
H	3.72470600	-0.73918400	2.08493700
H	3.59964100	-1.32370300	0.41081200
In	1.64326500	4.84066200	-0.58508400
Cl	-0.43870100	4.95366400	-1.63621100
Cl	3.46642100	5.08103700	-2.02441100
Cl	1.92092700	6.05074600	1.39706400
C	-2.25675200	3.70692500	2.63541900
C	-3.56327300	3.91035500	3.13408300
C	-4.16662800	5.15748000	3.05686600
C	-3.49195400	6.22992000	2.46417500
C	-2.20346900	6.04437600	1.95531900
C	-1.59029300	4.80298300	2.04612100
H	-4.09239800	3.06857900	3.57688700
H	-5.16960100	5.29796200	3.45130100
H	-3.96946500	7.20352600	2.39692100
H	-1.67611600	6.87079300	1.48512800
H	-0.58486400	4.66941900	1.65244300
C	-1.66603100	2.40077000	2.69373000
H	-2.29618300	1.59856000	3.07373200
C	-0.32374800	2.10135100	2.35650800
H	0.37868100	2.92711200	2.50153500
H	0.05372900	1.16541800	2.76408500

C	-6.27933300	-0.05081300	0.19572700
H	-6.61368000	-0.59887100	-0.69202000
H	-6.57786000	-0.65510500	1.06038200
H	-6.82654700	0.89383800	0.24075500

**TS4(Dj)**

C	-1.76412000	-3.49178600	-0.34151300
C	-0.47078800	-3.16965600	-0.57973300
C	-0.07207300	-1.79612100	-0.77104500
C	-1.13205000	-0.72216100	-0.73360000
C	-2.51535400	-1.19823400	-0.46772100
C	-2.82464300	-2.49827500	-0.27933500
H	-2.03634300	-4.53384300	-0.18236600
H	0.30804500	-3.92720300	-0.61091100
C	-0.67964500	0.39468400	0.27094100
H	-3.29837300	-0.44200500	-0.42770100
C	0.77534200	0.66580300	0.05876800
C	1.44578600	-0.08173100	-1.06213500
H	1.17879800	1.63667700	0.35244200
N	1.18495100	-1.51124700	-0.93858300
C	2.92742500	0.23467200	-1.07123300
O	3.46499100	0.98526700	-1.86063400
O	3.54367100	-0.36530800	-0.04309400
C	4.93147300	-0.00078500	0.17433500
H	5.34852300	-0.84475400	0.72684500
H	5.43062100	0.07209000	-0.79541200
C	5.02059200	1.28450600	0.95227400
H	6.06710500	1.52180600	1.16227400
H	4.59086800	2.11729900	0.38813500
H	4.49412500	1.20321800	1.90854500
H	1.39278600	-0.19376200	1.42105900
H	-1.11412500	-0.22961500	-1.72374400
C	-1.54441700	1.63065800	0.17803000
C	-1.41096500	2.53378300	-0.88409500
C	-2.52316100	1.86788700	1.14779200
C	-2.24034400	3.64892100	-0.96994300
H	-0.65433800	2.35784800	-1.64793300
C	-3.35308100	2.98300900	1.06350500
H	-2.63288000	1.16484900	1.97206900
C	-3.21318400	3.87685100	0.00376100
H	-2.12630900	4.34283300	-1.79906100
H	-4.10885900	3.15283400	1.82591900
H	-3.85758100	4.74906900	-0.06377000
H	-0.83185900	-0.02883100	1.27833700
H	1.03933600	0.28794700	-2.02323700
O	1.63513400	-0.74995700	2.27960400
O	0.53564700	-1.33062400	2.69308700
C	-4.21745400	-2.96748400	-0.01050800
H	-4.27824500	-3.49908500	0.94625700



H	-4.92516300	-2.13524500	0.01668200
H	-4.55235800	-3.67566700	-0.77731900

**TS4(I)k**

C	-1.65300100	-3.50103200	0.17366300
C	-0.34599400	-3.21200700	-0.02167500
C	0.06853400	-1.90439900	-0.46709600
C	-0.99718400	-0.85811000	-0.72792300
C	-2.39938000	-1.29313400	-0.48242100
C	-2.71602000	-2.53623400	-0.06274400
H	-1.93800700	-4.49292800	0.51943600
H	0.43385900	-3.94496300	0.16533100
C	-0.57445800	0.45667800	-0.03197500
H	-3.18808000	-0.57375300	-0.68942100
C	0.86304300	0.72929000	-0.14643400
C	1.60071300	-0.28228300	-1.03570900
H	1.09499900	1.76993900	-0.39240700
N	1.32992900	-1.64041100	-0.61177800
C	3.07144600	0.06931600	-1.03821900
O	3.55655500	0.87493000	-1.81170400
O	3.73715500	-0.53505700	-0.04996100
C	5.10468700	-0.09324700	0.16086900
H	5.58835800	-0.93846600	0.65352800
H	5.57551400	0.07096900	-0.81177300
C	5.12160300	1.14638700	1.01449900
H	6.15323900	1.44864700	1.21472100
H	4.61640000	1.97686000	0.51271500
H	4.62739900	0.96799600	1.97444800
H	1.29137000	0.61377800	0.90959700
H	-0.90687500	-0.58779000	-1.80094900
C	-1.52436000	1.60210900	-0.08375900
C	-1.28695800	2.67060800	-0.96381800
C	-2.68201200	1.62396800	0.70984500
C	-2.19573500	3.71970700	-1.05889500
H	-0.40547900	2.66101200	-1.59973500
C	-3.57598500	2.68495000	0.62711900
H	-2.87030000	0.81050900	1.40699300
C	-3.33747500	3.73365900	-0.26071100
H	-2.00775500	4.52938400	-1.75833200
H	-4.45966800	2.69373600	1.25829300
H	-4.03943500	4.55995900	-0.32855100
H	-0.62499600	0.11132300	1.19957800
H	1.23391100	-0.12824300	-2.06535400
O	0.99271300	0.11341800	2.47275400
O	-0.28268700	-0.17257800	2.35390400
C	-4.12605500	-2.97501400	0.15976600
H	-4.27380500	-3.31343100	1.19168900

H	-4.83662300	-2.16975500	-0.04062800
H	-4.38101900	-3.82584400	-0.48242400

**TS5(Dj)**

C	0.53802400	-3.52731900	-0.90878500
C	-0.40572400	-3.14624800	-0.00246100
C	-0.53387700	-1.77212600	0.40814800
C	0.59150800	-0.87659700	0.04962100
C	1.43326600	-1.29229600	-1.05146700
C	1.44863000	-2.58907800	-1.50043400
H	0.58059300	-4.56404400	-1.23594200
H	-1.14230400	-3.84958600	0.37562300
C	0.40753700	0.55507300	0.38368800
H	2.12469400	-0.57134500	-1.48056100
C	-0.70519300	0.91680500	1.05785100
C	-1.80024300	-0.03906800	1.40311000
H	-0.84738000	1.95192100	1.36282600
N	-1.59207800	-1.43206700	1.09802200
C	-3.05803900	0.49273400	0.69343000
O	-3.80575000	1.31393300	1.18043200
O	-3.15062300	-0.00248000	-0.54469400
C	-4.19108500	0.57416500	-1.38028400
H	-4.37197500	-0.18548700	-2.14221400
H	-5.09441300	0.69746800	-0.77788100
C	-3.72608300	1.87498500	-1.97659400
H	-4.48917300	2.26843700	-2.65399400
H	-3.54513700	2.62236800	-1.19952200
H	-2.80366800	1.73575900	-2.54788600
H	1.34865800	-1.26172200	1.05382800
C	1.45404900	1.54961600	0.07772200
C	2.81746200	1.25596800	0.23828600
C	1.09399200	2.83990800	-0.33989200
C	3.78565900	2.22771200	0.00515000
H	3.12746700	0.26650200	0.56667200
C	2.06361300	3.80750000	-0.57993800
H	0.04226100	3.07451800	-0.48863100
C	3.41325300	3.50595300	-0.40581300
H	4.83480400	1.98389400	0.14811900
H	1.76358700	4.79875600	-0.90896000
H	4.17086700	4.26177500	-0.59218600
H	-2.03629600	0.04993400	2.47286300
O	1.01328200	-1.43428900	3.10086700
O	1.90324200	-1.58159700	2.19570800
C	2.36809400	-3.04100300	-2.58500600
H	1.81162900	-3.47954800	-3.42064800
H	2.97324200	-2.21730700	-2.97031700
H	3.04680800	-3.82247400	-2.22385100

**TS2(II)**

C	-0.62220700	-3.03951500	0.31744800
C	-0.30757500	-1.79699500	-0.26101700
C	-1.35169700	-1.00963100	-0.77167100
C	-2.66486500	-1.45922500	-0.69022400
C	-2.99237100	-2.69269800	-0.11606800
C	-1.93789800	-3.47073200	0.38361700
H	0.18101400	-3.65563400	0.71605400
H	-1.14820600	-0.04268600	-1.22236000
H	-3.45945500	-0.82660800	-1.08280100
H	-2.15572200	-4.43407100	0.84090700
N	1.02357700	-1.41074500	-0.32343900
C	1.48336300	-0.15039000	-0.62343000
H	0.86008700	0.45247800	-1.27401000
C	2.91498100	0.05516000	-0.76794600
O	3.41887700	1.05960100	-1.25578500
O	3.62749300	-0.95884100	-0.21414100
C	5.05622300	-0.74900100	-0.12567600
H	5.40170800	-0.29436800	-1.05797900
H	5.47442700	-1.75445100	-0.04664700
C	5.40179400	0.09997800	1.06928500
H	6.48729900	0.20414300	1.15275200
H	4.97203900	1.10134000	0.97624900
H	5.03290800	-0.35340100	1.99401900
C	-2.41658500	2.00550100	1.16145100
C	-1.06328800	2.05680300	0.76133900
C	-0.73037500	2.91534200	-0.31095700
C	-1.70243500	3.68260200	-0.93856800
C	-3.03510000	3.62064400	-0.52398200
C	-3.38484000	2.77541000	0.53086300
H	-2.69412000	1.33703800	1.97516600
H	0.29913100	2.96959900	-0.65898200
H	-1.42210400	4.33085700	-1.76519200
H	-3.79260000	4.21984300	-1.02165800
H	-4.41955900	2.71435700	0.85872800
C	-0.09388800	1.20751400	1.40947700
H	-0.49420400	0.49754400	2.13453100
C	1.25052700	1.13251700	1.08427200
H	1.73664800	1.96042300	0.57134500
H	1.90729300	0.55209400	1.72942100
C	-4.40769600	-3.17519700	-0.05552500
H	-4.60563200	-3.94181500	-0.81472200
H	-4.64043000	-3.62962300	0.91304100
H	-5.11718500	-2.36095600	-0.22633500

H 1.68425400 -2.02547900 0.13582600

**TS3(II)**

C	-0.58768700	-2.31591800	0.87788300
C	0.04094400	-1.42532200	-0.02264000
C	-0.76270100	-0.59498600	-0.85156700
C	-2.16967800	-0.69337700	-0.77825300
C	-2.78551500	-1.53952200	0.11930000
C	-1.95834600	-2.35713500	0.94201200
H	0.02666600	-2.93640300	1.52398000
H	-0.31742800	-0.12202300	-1.72090600
H	-2.77040500	-0.07271800	-1.43877900
H	-2.43337700	-3.02690700	1.65535100
N	1.39086000	-1.29340800	-0.05072100
C	1.95357700	-0.07445200	-0.53894300
H	1.69386600	0.06476200	-1.59589500
C	3.46731000	-0.03417700	-0.46781800
O	4.10008600	0.95546900	-0.77128300
O	3.98373000	-1.19255800	-0.05492500
C	5.43722600	-1.23658300	0.06556900
H	5.86479100	-0.71255600	-0.79255700
H	5.67323100	-2.29913300	-0.00909100
C	5.88337500	-0.64332100	1.37281500
H	6.96811400	-0.74095800	1.46688000
H	5.63255900	0.41881500	1.43119600
H	5.42185800	-1.16067500	2.21832500
C	-2.11375500	2.63969600	-0.23730900
C	-0.78050200	2.31410000	-0.56688200
C	-0.17375000	2.96000300	-1.66482300
C	-0.87777300	3.90399600	-2.39570100
C	-2.19253900	4.22496300	-2.04751900
C	-2.80905300	3.59109200	-0.96703600
H	-2.58611200	2.13199300	0.60088900
H	0.84922700	2.71746800	-1.94099100
H	-0.40322800	4.39874000	-3.23770800
H	-2.73618400	4.97158900	-2.61944000
H	-3.83087500	3.84146800	-0.69867900
C	-0.09588300	1.32560700	0.22234000
H	-0.63151200	0.99081100	1.10835100
C	1.37371800	1.16578600	0.23881400
H	1.86565400	2.03606200	-0.19998300
H	1.70844900	1.05966300	1.27474500
C	-4.27088300	-1.62818200	0.23988600
H	-4.59810600	-1.38368300	1.25656300
H	-4.77136200	-0.94610200	-0.45107800
H	-4.62740100	-2.64378800	0.03666800

H 1.91386900 -1.78068400 0.66802000



**TS2(III)**

C	-0.61948100	-3.18386600	0.16299600
C	-0.35623000	-1.90271100	-0.34955100
C	-1.41659000	-1.07436900	-0.74177100
C	-2.72304400	-1.52760800	-0.60149200
C	-3.00746000	-2.79633800	-0.08464300
C	-1.92689600	-3.61558200	0.29042500
H	0.21058000	-3.81851000	0.46292100
H	-1.23526100	-0.09746300	-1.17792300
H	-3.54217600	-0.88057900	-0.90613500
H	-2.12339800	-4.60577200	0.69404700
N	0.96965000	-1.48457400	-0.41934600
C	1.38108100	-0.22776200	-0.62514200
H	0.76088500	0.42390600	-1.23131600
C	2.84893100	0.01010500	-0.75237800
O	3.30269400	0.98484400	-1.31862200
O	3.54741700	-0.95380000	-0.15560100
C	4.99665400	-0.76651200	-0.09149600
H	5.33268200	-0.38121700	-1.05662600
H	5.38178400	-1.77744200	0.04514000
C	5.35023100	0.14396300	1.05088200
H	6.43727600	0.23712000	1.11763700
H	4.93423700	1.14550700	0.90883200
H	4.98530900	-0.25637700	2.00068100
C	-2.43424900	2.13018100	0.96972000
C	-1.05558800	2.08983700	0.67086300
C	-0.52345600	3.05594100	-0.21096500
C	-1.34642700	4.02591400	-0.76349800
C	-2.70860800	4.05823300	-0.44721300
C	-3.25092800	3.10839200	0.42168600
H	-2.84673700	1.37804300	1.63913900
H	0.53335400	3.03949800	-0.46609800
H	-0.93064400	4.76279300	-1.44458700
H	-3.34658400	4.82306000	-0.88129000
H	-4.30936100	3.13175700	0.66398800
C	-0.25831900	1.04978000	1.26372300
H	-0.80575400	0.32220100	1.86409300
C	1.10837600	0.88603000	1.13234600
H	1.71666500	1.72202300	0.79300400
H	1.60393800	0.18005700	1.79399100
C	-4.41279400	-3.27841300	0.06060600
H	-4.59208200	-4.16564000	-0.55686900
H	-4.62545000	-3.57233200	1.09420400
H	-5.13362600	-2.51123500	-0.23169800

H

1.65980800

-2.13430100

-0.04851000

**2. The number of imaginary frequencies and Electronic Energy + Zero-point Energy Correction for the optimized transition states obtained at the M06-2X-D3/6-31+G(d,p) level of theory in the process.**

Table 1. The number of imaginary frequencies and the relative electronic energy in the reaction of R1+R2 to P in path I.

Transition states	Imaginary frequency (cm <sup>-1</sup> )	Electronic Energy + Zero-point Energy Correction(a.u)
TS0(1)	-1132.56	-8620.58269
TS0(2)	-1109.12	-8620.55564
TS0(3)	-1007.70	-8620.49262
TS1a	-1472.56	-9102.94777
TS1b	-1455.61	-784.25539
TS2(I)c	-1175.23	-9102.31633
TS2(I)d	-1677.73	-783.61772
TS3(I)e	-166.34	-941.65696
TS3(I)f-1	-466.06	-2324.36164
TS3(I)f-2	-379.68	-2324.34315
TS3(I)g	-448.13	-1863.98385
TS3(I)h-1	-308.25	-1863.93082
TS3(I)h-2	-666.02	-1863.89867
TS3(I)i	-205.05	-2324.37532
TS4(I)j	-258.76	-1091.98441
TS4(I)k	-968.98	-1091.98284
TS5(I)j	-1674.42	-1090.82300

Table 2. The number of imaginary frequencies and the relative electronic energy in the reaction of R1+R2 to P in path II and III.

Transition states	Imaginary frequency (cm <sup>-1</sup> )	Electronic Energy + Zero-point Energy Correction(a.u)
TS2(II)	-549.37	-942.26042
TS3(II)	-191.44	-942.11771
TS2(III)	-442.69	-942.11394