

**Note: All the Cartesian coordinates are at the M06-2X/6-311++G(d,p) level of theory**

**Cartesian Coordinates of all the species involved in the reaction of different conformers of**  
**HFE-365mcf3 with OH.**

**A1**

0 1

C	-0.15575800	0.75172600	-0.04419200
C	1.08147400	0.74420200	0.84436000
H	1.64471200	1.65436400	0.59685700
H	0.73764900	0.80572500	1.87755200
C	2.61846800	-0.50591800	-0.46282100
H	1.98971400	-0.72302000	-1.32943400
H	3.17413100	0.42148100	-0.64065800
H	3.31898800	-1.32439900	-0.31095200
O	1.85288900	-0.40871600	0.72818900
F	0.16787700	0.95218100	-1.34487100
F	-0.95121600	1.77676000	0.33698200
C	-0.99902100	-0.53534700	0.01458900
F	-2.17029900	-0.35077000	-0.58677200
F	-1.22432600	-0.87179400	1.28368600
F	-0.37306700	-1.53886600	-0.59241400

**OH**

0 2

O	0.00000000	0.00000000	0.10800200
H	0.00000000	0.00000000	-0.86401400

**CR1a**

0 2

C	0.12592300	-0.54503300	0.26362200
C	-0.73994900	0.33811000	1.15113400
H	-1.69106500	-0.19416300	1.28757600
H	-0.23084800	0.41885300	2.11274700
C	-1.81955400	1.73911300	-0.43095800
H	-1.38232900	1.35836000	-1.35764700
H	-2.74675800	1.19693200	-0.21801500
H	-2.03277000	2.80008000	-0.54438300
O	-0.91152300	1.62775000	0.65637100
F	-0.53256800	-0.91425400	-0.87242400
F	0.42262000	-1.67959500	0.93366600
C	1.45251600	0.09001100	-0.19200800
F	2.23558600	-0.82826400	-0.75198400
F	2.09033300	0.60592200	0.85653000
F	1.23606100	1.05118000	-1.08303800

O	-3.14917800	-1.31885600	-0.27333300
H	-2.61252900	-1.89932500	-0.84007500

### TS1a

0 2

C	0.10507300	-0.58477300	0.00055300
C	-0.95129900	0.04268700	0.89947400
H	-1.92976400	-0.56559800	0.66125000
H	-0.69629400	-0.16529400	1.93934400
C	-1.72346900	1.81461900	-0.48438200
H	-1.00324000	1.74499600	-1.30175100
H	-2.60532400	1.20840800	-0.70929200
H	-2.01094500	2.85304500	-0.33922300
O	-1.14787000	1.39105500	0.74996600
F	-0.31937200	-0.65225000	-1.28863000
F	0.32154500	-1.84967000	0.41686800
C	1.46345100	0.14053200	-0.00930500
F	2.37080700	-0.58075300	-0.65732900
F	1.88088700	0.32762900	1.24051200
F	1.35882700	1.32245400	-0.60952500
O	-2.99107400	-1.27089500	0.01883400
H	-2.51965500	-1.62190600	-0.75583300

### PC1a

0 2

C	0.13617000	-0.50885900	0.17246700
C	-0.71291100	0.28736000	1.10582200
H	-3.06685200	-1.35408400	0.67510800
H	-0.51860900	0.12937500	2.15900200
C	-1.69704800	1.77052000	-0.49527700
H	-0.89124500	1.77911400	-1.22927100
H	-2.44923000	1.02419500	-0.75186600
H	-2.14261300	2.75911900	-0.42614400
O	-1.18319400	1.49852400	0.81778700
F	-0.44709300	-0.69522100	-1.04610600
F	0.33296600	-1.73003100	0.72080200
C	1.53752600	0.07301000	-0.11567100
F	2.23391300	-0.71824000	-0.92287400
F	2.20946800	0.21561700	1.02377400
F	1.42191100	1.27001100	-0.69280000
O	-3.28113900	-1.19254900	-0.24759900
H	-2.55969200	-1.59691900	-0.73755200

### P1a

0 2

C	-0.09239500	0.72450700	-0.06683200
C	1.07018700	0.71670300	0.86781700

H	0.88230400	1.09439100	1.86367400
C	2.57384000	-0.56948600	-0.47311500
H	1.85343800	-1.17776900	-1.01955100
H	2.83300200	0.31631400	-1.05443700
H	3.46398500	-1.15426600	-0.25726900
O	2.05471200	-0.18231600	0.80308300
F	0.28713000	0.78206700	-1.37134300
F	-0.84274900	1.81573200	0.19979800
C	-1.03900800	-0.49130900	0.04675700
F	-2.06288500	-0.38943200	-0.79197800
F	-1.51311600	-0.58316500	1.28673600
F	-0.37351100	-1.61438300	-0.23486100

### CR1b

0 2

C	0.59400100	-0.83287200	0.13055500
C	-0.85017700	-0.89046000	0.58704000
H	-1.05534200	-1.94828300	0.79946100
H	-0.95550400	-0.30748300	1.51060800
C	-3.04254600	-0.65547400	-0.17725100
H	-3.23159400	-1.73424300	-0.15983600
H	-3.35043400	-0.20648700	0.77207300
H	-3.60453300	-0.19788400	-0.98809000
O	-1.67088500	-0.40034300	-0.43122100
F	0.76940000	-1.53541000	-1.00458600
F	1.36034100	-1.39684300	1.09427900
C	1.16872100	0.57527200	-0.10849000
F	2.45340900	0.50025300	-0.43304400
F	1.05042000	1.30875700	0.99519100
F	0.52594600	1.19870200	-1.09944100
O	-1.96023300	1.96115600	0.41655100
H	-1.40928200	2.04994200	-0.37957800

### TS1b

0 2

C	-0.46532100	0.28793600	0.73673400
C	1.04373700	0.20230900	0.67422000
H	1.45387900	0.53511300	1.63833900
H	1.34375500	-0.92415300	0.59498700
C	2.92570400	0.91646700	-0.49032200
H	3.35806300	1.39353200	0.39530900
H	3.30015100	-0.10754000	-0.57835500
H	3.18321900	1.48902500	-1.37767600
O	1.50860100	0.90939800	-0.40536800
F	-0.86596500	1.53301400	1.06747600

F	-0.89894800	-0.55628600	1.69750600
C	-1.19704300	-0.09068700	-0.56816200
F	-2.49421900	-0.24980700	-0.33392200
F	-0.71374900	-1.25272700	-1.03445400
F	-1.04623000	0.83334500	-1.50105800
O	1.81471000	-2.23371700	0.22446700
H	1.10399700	-2.45541400	-0.40016000

### PC1b

0 2

C	0.60469200	-0.85135500	0.21047900
C	-0.83708700	-0.88880100	0.55296400
H	-1.15348300	-0.62799500	1.55598700
H	-1.32646700	2.69822000	0.70997000
C	-3.05708200	-0.76219200	-0.12828500
H	-3.31375000	-1.72287600	0.32288000
H	-3.26625700	0.06261900	0.55499600
H	-3.60744800	-0.62847100	-1.05585300
O	-1.67199100	-0.75287900	-0.47822300
F	0.88381100	-1.65316800	-0.84184900
F	1.32504300	-1.26870000	1.27799500
C	1.16541500	0.54097600	-0.15840800
F	2.45106600	0.48269500	-0.47663100
F	1.02345100	1.38165200	0.86899100
F	0.49759700	1.05002400	-1.20089800
O	-1.91706300	2.03793300	0.33966500
H	-1.50450100	1.77377500	-0.48848200

### P1b

0 2

C	-0.21881700	0.73101200	0.00120200
C	1.17868000	0.53627700	0.45819300
H	1.40744000	0.60813600	1.51537000
C	3.26588400	-0.43765600	0.12585200
H	3.80437500	0.50067200	0.27558000
H	3.21420700	-0.99526300	1.06457500
H	3.76328600	-1.03553400	-0.63271900
O	1.95510400	-0.17480100	-0.36015600
F	-0.26517100	1.20219400	-1.26560800
F	-0.82167500	1.62644500	0.81770800
C	-1.10102400	-0.53768100	0.02280700
F	-2.34792400	-0.26041900	-0.34320300
F	-1.12814900	-1.04415400	1.25813400

F	-0.61246700	-1.46087900	-0.79924100
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### CR1c

0 2

C	-0.57635000	0.73197500	-0.19361500
C	0.85427400	0.74071500	0.32619600
H	1.37944200	1.55490300	-0.18939700
H	0.81188500	0.96111000	1.39343400
C	1.92232000	-0.79176900	-1.15499900
H	2.56975500	-1.66337600	-1.08252300
H	1.06667500	-1.02346700	-1.79087700
H	2.48481300	0.04787000	-1.57774200
O	1.51028100	-0.48727200	0.17713400
F	-0.61239400	0.74202700	-1.54736300
F	-1.19140100	1.85449900	0.23803000
C	-1.42072100	-0.47002700	0.27048500
F	-2.70387900	-0.27068400	-0.00806300
F	-1.29198800	-0.63082800	1.58672300
F	-1.02840200	-1.58440900	-0.33951300
O	4.13470600	0.24692300	0.75010100
H	3.30297900	-0.21504800	0.97249500

### TS1c

0 2

C	0.43424200	-0.72092700	-0.03785200
C	-0.78813700	-0.43581200	0.82349200
H	-1.55471600	-1.17626400	0.56597600
H	-0.48968900	-0.56164300	1.86415500
C	-2.01290500	1.11896500	-0.46683100
H	-2.37325700	2.14418300	-0.42197900
H	-1.46600000	0.92269800	-1.39304900
H	-2.92793400	0.40376800	-0.48969000
O	-1.26759900	0.87505600	0.68767600
F	0.10140700	-0.87809900	-1.34172600
F	0.99015500	-1.87854800	0.38175900
C	1.52568000	0.36508800	0.01478100
F	2.64702900	-0.07577000	-0.54514500
F	1.78334800	0.68843900	1.28116600
F	1.13527200	1.45688000	-0.63708300
O	-3.94295400	-0.56421000	-0.06028900
H	-4.37214400	0.00050100	0.60321400

### PC1c

0 2

C	-0.42905900	0.63932300	-0.28011200
C	0.92453500	0.44676800	0.38274100
H	1.65630100	1.06991100	-0.13873500
H	0.85118600	0.77396800	1.41883300
C	1.90013700	-1.38886800	-0.72461100
H	1.98407000	-2.46519800	-0.73471000
H	1.82110400	-0.81336200	-1.63817000
H	3.83713600	-0.29724200	0.20230600
O	1.30624200	-0.90832100	0.39712900
F	-0.35560700	0.43536000	-1.61643900
F	-0.81883100	1.91787100	-0.08045600
C	-1.55220800	-0.27311600	0.24979300
F	-2.73288100	0.13917000	-0.20129800
F	-1.57288400	-0.23515100	1.58252500
F	-1.37124900	-1.52924800	-0.14051400
O	3.89624700	0.63289600	0.44748100
H	4.83292000	0.83866500	0.47235100

### P1c

0 2

C	-0.11554300	0.74440900	-0.02993400
C	1.13155000	0.68984300	0.84097000
H	1.71427600	1.59365400	0.63183700
H	0.81119800	0.69440800	1.88233700
C	2.71355900	-0.48048900	-0.44162800
H	3.18874000	-1.43433700	-0.60571500
H	2.52134000	0.21494200	-1.24775000
O	1.88013100	-0.47637300	0.63585400
F	0.19476000	0.98371100	-1.32479400
F	-0.88475200	1.76819800	0.40232200
C	-0.97974100	-0.53103900	-0.00135700
F	-2.15750800	-0.30174100	-0.57255100
F	-1.18767500	-0.90399600	1.26177900
F	-0.38433100	-1.52328500	-0.65073900

### A2

0 1

C	-0.26743800	0.75262700	0.02086800
C	1.16757700	0.66717900	-0.45441300
H	1.15838400	0.42305600	-1.52460300
H	1.60490400	1.66622400	-0.32031700
C	3.18215500	-0.43911600	-0.07402200
H	3.72538500	0.50069500	0.07798200

H	3.61061500	-1.21063200	0.56174600
H	3.27141000	-0.74162200	-1.12379800
O	1.82715600	-0.30244500	0.29715000
F	-0.92233500	1.62538200	-0.78128200
F	-0.33842300	1.21948900	1.28256200
C	-1.04876900	-0.57656200	-0.02406500
F	-2.35040900	-0.34578100	0.12707900
F	-0.65815800	-1.40630000	0.93033300
F	-0.86279700	-1.16422700	-1.20962800

## CR2a

0 2

C	-0.59574600	-0.83281100	0.13041400
C	0.84823800	-0.89170200	0.58749500
H	0.95313000	-0.30724800	1.51011300
H	1.05251200	-1.94933500	0.80162200
C	3.04110400	-0.66014100	-0.17672700
H	3.22866600	-1.73913800	-0.15755400
H	3.60375100	-0.20481100	-0.98842900
H	3.34972500	-0.21004400	0.77180700
O	1.66975200	-0.40345100	-0.43106400
F	-1.36308200	-1.39568900	1.09395600
F	-0.77187900	-1.53486400	-1.00477700
C	-1.16817200	0.57639400	-0.10837500
F	-2.45314400	0.50373600	-0.43265500
F	-0.52447900	1.19901900	-1.09915300
F	-1.04824100	1.30951600	0.99545500
O	1.96744900	1.96402200	0.41459000
H	1.40948800	2.04009200	-0.37804300

## TS2a

0 2

C	-0.46528000	-0.28790400	0.73673100
C	1.04377200	-0.20218100	0.67418200
H	1.34376000	0.92430700	0.59485500
H	1.45394200	-0.53488400	1.63832500
C	2.92572100	-0.91658100	-0.49030200
H	3.35801300	-1.39382200	0.39526800
H	3.18318000	-1.48904600	-1.37773200
H	3.30030200	0.10738700	-0.57819000
O	1.50861800	-0.90936900	-0.40536200
F	-0.89894900	0.55626200	1.69753000
F	-0.86581300	-1.53302300	1.06745800
C	-1.19708300	0.09066400	-0.56813700
F	-2.49425400	0.24974200	-0.33382400
F	-1.04628800	-0.83340600	-1.50100300
F	-0.71386800	1.25269400	-1.03451000

O	1.81466700	2.23390100	0.22441700
H	1.10429900	2.45538800	-0.40067400

### PC2a

0 2

C	-0.60500900	-0.85130900	0.21032100
C	0.83676200	-0.88922400	0.55270500
H	1.33110000	2.70165400	0.70693500
H	1.15310700	-0.62946200	1.55600700
C	3.05689200	-0.76276500	-0.12822300
H	3.31314000	-1.72421600	0.32152800
H	3.60737700	-0.62783400	-1.05554800
H	3.26636300	0.06098900	0.55629200
O	1.67178200	-0.75242300	-0.47825400
F	-1.32532200	-1.26893000	1.27766500
F	-0.88441400	-1.65269100	-0.84237400
C	-1.16543000	0.54130100	-0.15817900
F	-2.45109000	0.48333100	-0.47655200
F	-0.49744100	1.05056500	-1.20034800
F	-1.02352800	1.38162100	0.86953500
O	1.91831100	2.03666200	0.33970300
H	1.50503900	1.77188000	-0.48789200

### P2a

0 2

C	0.21881300	0.73101600	0.00120900
C	-1.17868300	0.53628500	0.45820200
H	-1.40742300	0.60806300	1.51538800
C	-3.26586800	-0.43768500	0.12586400
H	-3.80439700	0.50061800	0.27562100
H	-3.76326100	-1.03556400	-0.63271300
H	-3.21413100	-0.99531600	1.06456700
O	-1.95511200	-0.17476100	-0.36017500
F	0.82167300	1.62644300	0.81771600
F	0.26516000	1.20220500	-1.26559800
C	1.10101600	-0.53768300	0.02280500
F	2.34792000	-0.26040900	-0.34319000
F	0.61248500	-1.46087500	-0.79927100
F	1.12814500	-1.04417600	1.25812800

### CR2b

0 2

C	-0.41928400	-0.55798400	0.41979200
C	0.81353500	0.14200500	0.94959100
H	0.49683800	0.87573100	1.70132800
H	1.43811500	-0.62498200	1.42637600



C	2.63724100	1.43438000	0.26887900
H	3.33441700	0.75246300	0.76581800
H	3.09684900	1.82205300	-0.63719500
H	2.38396900	2.26373700	0.93800000
O	1.46505700	0.74271000	-0.12881500
F	-1.06131000	-1.13889700	1.45523300
F	-0.07902300	-1.53460100	-0.45678400
C	-1.43721700	0.35245300	-0.29730800
F	-2.58320500	-0.29737300	-0.47782700
F	-0.98817700	0.74552800	-1.47992600
F	-1.67837600	1.43042700	0.45241300
O	2.92475500	-1.33524000	-0.68652900
H	2.07649200	-1.41963800	-1.15528400

## TS2b

0 2

C	-0.26662800	-0.60108500	0.08976100
C	0.99689100	0.08176000	0.56258500
H	0.91467600	0.34872800	1.62442000
H	1.82963000	-0.73778000	0.49579900
C	2.50861000	1.78191700	0.08392400
H	3.33863100	1.07415800	0.00009600
H	2.64152100	2.59985600	-0.61954100
H	2.45971400	2.17718000	1.10395300
O	1.28970000	1.14105100	-0.25938400
F	-0.58344500	-1.57097900	0.97228700
F	-0.06810400	-1.18535200	-1.11459700
C	-1.49818900	0.31840600	-0.04382500
F	-2.59700400	-0.41166100	-0.20685500
F	-1.38131400	1.13942700	-1.07546400
F	-1.63293500	1.04062700	1.07102100
O	2.76916500	-1.66190300	-0.07792200
H	2.26601700	-1.88987600	-0.87846400

## PC2b

0 2

C	-0.34869500	-0.50687900	0.34349200
C	0.79830700	0.31421200	0.78296600
H	1.37567000	-0.01463100	1.63881700
H	3.34970000	-2.25045000	-0.44374100
C	2.60012600	1.66407000	0.18635000
H	3.33156000	0.87972500	0.38607400
H	2.90779900	2.25582900	-0.67135400
H	2.46307000	2.31036800	1.05619300

O	1.35441800	1.06293000	-0.16795700
F	-0.78300300	-1.25422400	1.37787200
F	-0.00399900	-1.37988000	-0.66772200
C	-1.56165600	0.27923200	-0.19680000
F	-2.55393000	-0.55455300	-0.49721200
F	-1.23841600	0.96089700	-1.28958200
F	-1.99760600	1.13331800	0.72698200
O	2.98342800	-1.36420100	-0.41369200
H	2.13353200	-1.42450200	-0.86189500

## P2b

0 2

C	0.22997400	0.73787200	-0.00632900
C	-1.17833700	0.57524500	0.41746000
H	-1.65764000	1.37196900	0.97491700
C	-3.26444500	-0.40632600	0.10254900
H	-3.75577800	0.56550800	0.00793200
H	-3.72317300	-1.12040500	-0.57565900
H	-3.33788000	-0.76561300	1.13123300
O	-1.89837700	-0.30310900	-0.28065800
F	0.82476400	1.63157800	0.81540500
F	0.34580900	1.21604200	-1.27837100
C	1.07456500	-0.55368000	0.03858300
F	2.34349200	-0.28369000	-0.25289600
F	0.62244500	-1.44835700	-0.83277700
F	1.02915000	-1.08726800	1.25900100

## CR2c

0 2

C	0.51990000	-0.59602400	0.41280700
C	-0.93627600	-0.27012100	0.16286100
H	-1.17481200	-0.51695700	-0.87875600
H	-1.53034100	-0.91994600	0.81848200
C	-2.47578600	1.47914200	0.25205000
H	-2.78663100	1.32297400	-0.78851400
H	-3.14372700	0.91995100	0.91865900
H	-2.53212700	2.53953100	0.49013000
O	-1.13579300	1.08382600	0.43908700
F	0.73198100	-1.88289700	0.04763500
F	0.83194300	-0.48311700	1.71971500
C	1.52733100	0.26686200	-0.37439000
F	2.74076700	-0.27746200	-0.31366700
F	1.59989400	1.49838600	0.10684100

F	1.16073300	0.32694800	-1.65780500
O	-3.80275400	-1.13061300	-0.63510100
H	-4.72286200	-0.88712800	-0.83632500

## TS2c

0 2

C	0.51889900	0.71654500	-0.01252600
C	-0.84917200	0.28015900	0.46587900
H	-0.77504500	0.02343700	1.52963700
H	-1.53457700	1.12632200	0.34070500
C	-2.48760900	-1.32509000	0.08343400
H	-2.52070000	-1.59013200	1.14651600
H	-3.29331400	-0.50956300	-0.09678200
H	-2.73046000	-2.17180200	-0.55499500
O	-1.25421800	-0.82068000	-0.30115300
F	0.94354700	1.71227500	0.80032600
F	0.46976000	1.19784700	-1.26846400
C	1.60072800	-0.38285700	0.01808200
F	2.80653000	0.15630800	-0.13390900
F	1.41669200	-1.27551900	-0.94266000
F	1.56728400	-1.00955200	1.19849500
O	-3.99648500	0.79259300	-0.09272500
H	-4.67165900	0.58166800	0.57262000

## PC2c

0 2

C	0.33843000	-0.56328600	-0.32246500
C	-0.81235200	0.23261500	-0.89974600
H	-0.44967900	0.80680000	-1.75819400
H	-1.57807800	-0.48646200	-1.20717200
C	-2.46297200	1.71031400	-0.18090300
H	-2.76848800	1.76820700	-1.21908200
H	-3.43370500	-0.47036600	0.64625400
H	-2.73890200	2.46683900	0.53764300
O	-1.29790100	1.08431500	0.11039900
F	0.83318400	-1.34993300	-1.30142000
F	-0.08362700	-1.36389300	0.68275000
C	1.51274100	0.27227300	0.22719000
F	2.55975500	-0.51093800	0.46370000
F	1.18453900	0.88729600	1.35393200
F	1.86663300	1.18957900	-0.67621300
O	-3.11897600	-1.35352400	0.42831800
H	-2.39557900	-1.51183300	1.04162300

**P2c**

0 2

C	0.23245000	0.75410700	-0.03176900
C	-1.20197600	0.70049500	0.45087500
H	-1.20089600	0.44533500	1.51628300
H	-1.62930900	1.69961400	0.31222700
C	-3.17859800	-0.45370400	0.06923200
H	-3.43878300	-0.26520300	1.10528700
H	-3.68597600	-1.20525400	-0.51464300
O	-1.88903000	-0.25999100	-0.30432900
F	0.89807900	1.62923900	0.75685800
F	0.30360000	1.19953700	-1.29989500
C	0.99506100	-0.58515200	0.03321800
F	2.29623500	-0.37827200	-0.14146500
F	0.57504000	-1.42966300	-0.89582500
F	0.81433300	-1.14184500	1.23434300

**A3**

0 1

C	0.06221900	0.22877100	0.12366600
C	0.99050500	-0.93760100	-0.20903200
H	0.57438700	-1.84071600	0.24087600
H	0.99713300	-1.04896800	-1.30127700
C	3.04190700	0.24699800	-0.29443500
H	2.99920700	0.16953000	-1.38674500
H	2.70244500	1.24030700	0.00901500
H	4.06642200	0.09740900	0.04003300
O	2.26895400	-0.77558700	0.31292700
F	0.32335300	1.30142300	-0.66745800
F	0.21696800	0.62235000	1.40142900
C	-1.42182200	-0.11669900	-0.07944100
F	-1.61662500	-0.54906000	-1.32807200
F	-2.19417400	0.93956300	0.12958900
F	-1.78819700	-1.08557400	0.75897200

**CR3a**

0 2

C	-0.33455000	-0.12740900	-0.43426600
C	0.79025400	-0.57517400	0.47610700
H	0.87688500	0.13678000	1.30723100
H	0.53928600	-1.56949600	0.86711300
C	3.07838100	-1.03864300	0.44086500
H	3.24895000	-0.39035700	1.30636300
H	2.94043400	-2.07384500	0.77149500

H	3.93478500	-0.97950000	-0.22685000
O	1.95183700	-0.59789400	-0.29769800
F	-0.53807200	-1.01381400	-1.42726400
F	-0.03947900	1.06614300	-1.00698800
C	-1.67117000	0.04843000	0.30581100
F	-2.01741900	-1.09894600	0.89256600
F	-2.63334300	0.40528600	-0.53164700
F	-1.55601300	0.98264300	1.24892300
O	2.58784100	1.86573400	0.20401600
H	2.02369200	1.81866200	-0.58729900

### TS3a

0 2

C	0.26317800	-0.45320000	0.34986000
C	-0.98662300	-0.13195200	-0.44270300
H	-1.14738500	1.02699800	-0.36646000
H	-0.84888200	-0.35100000	-1.51050100
C	-3.27565800	-0.52041900	-0.51994000
H	-3.50205200	0.54782800	-0.45485800
H	-3.23480600	-0.82770000	-1.57044700
H	-4.03664100	-1.09699800	-0.00007100
O	-2.04274700	-0.79595900	0.12649800
F	0.43784800	-1.78202600	0.46850800
F	0.16720100	0.06573300	1.59747300
C	1.54159600	0.12235100	-0.28350700
F	1.71903600	-0.39583700	-1.49973200
F	2.60146900	-0.16357300	0.45868000
F	1.44160000	1.44429400	-0.39981400
O	-1.53169200	2.28877000	0.19356700
H	-1.19406100	2.14038400	1.09351600

### PC3a

0 2

C	-0.34044000	-0.26927000	-0.43968500
C	0.80558300	-0.55321700	0.44201700
H	2.27345000	2.92819400	0.09045400
H	0.89198800	-0.06403900	1.40441800
C	3.08651200	-1.00496500	0.58447600
H	3.33453000	0.00570700	0.91165500
H	2.94353600	-1.67309400	1.43680400
H	3.86642600	-1.39408400	-0.06434100
O	1.89526600	-0.96441800	-0.20151900
F	-0.62973700	-1.30378700	-1.25716600
F	-0.09826900	0.80283500	-1.27989800
C	-1.61332300	0.08623700	0.34534700
F	-1.98680400	-0.93359500	1.11427500
F	-2.60778200	0.38056900	-0.48090300
F	-1.38726600	1.14225900	1.13126500

O	2.32179300	1.97527500	-0.01037700
H	1.71232600	1.76322600	-0.72490600

### P3a

0 2

C	-0.06763900	0.46884900	0.03101700
C	1.12754700	-0.39968000	0.06574700
H	1.10490400	-1.34810000	0.58973300
C	3.44819000	-0.56655200	0.01712700
H	3.49534600	-0.98531600	1.02563400
H	3.44362500	-1.36952400	-0.72322800
H	4.29797100	0.08919800	-0.15099300
O	2.28251500	0.23591900	-0.12622700
F	-0.05268500	1.29399900	-1.03855400
F	-0.16300300	1.27378500	1.13231500
C	-1.36969100	-0.34926500	-0.02696300
F	-1.42329700	-1.06346200	-1.14915600
F	-2.42876500	0.44585000	0.01984000
F	-1.42473900	-1.19391900	1.00745400

### CR3b

0 2

C	0.18114500	-0.49847700	-0.26123500
C	-0.82196900	-0.63586300	0.87556700
H	-0.38038400	-1.30612400	1.61638100
H	-0.97842800	0.35256500	1.32385800
C	-3.00189300	-0.28042400	0.00688600
H	-3.21393800	0.44019100	0.80272100
H	-2.70147400	0.25945100	-0.89441700
H	-3.89472900	-0.86601100	-0.20341900
O	-2.00869500	-1.20805400	0.42189100
F	-0.31218300	0.29237500	-1.25578700
F	0.46047200	-1.69586800	-0.80579100
C	1.51372800	0.13520800	0.16975200
F	1.30710900	1.39780900	0.56134100
F	2.38607300	0.14664200	-0.82822400
F	2.03900700	-0.53828600	1.19116300
O	-1.52519800	2.44002400	-0.00045000
H	-0.71027300	2.51743800	-0.52679200

### TS3b

0 2

C	0.10555300	-0.43464600	-0.17625700
C	-0.90454700	0.05539400	0.85942300
H	-0.45979000	0.03536400	1.85559400

H	-1.11198200	1.17966100	0.59968300
C	-2.83428500	-0.65727200	-0.31143400
H	-2.95073300	0.36622700	-0.67904700
H	-2.35780500	-1.27623800	-1.07536700
H	-3.80400400	-1.07651300	-0.05495100
O	-2.07291100	-0.65808300	0.89307400
F	-0.21467600	0.00949300	-1.42171500
F	0.13808400	-1.77916100	-0.22405600
C	1.53263600	0.06243600	0.10451800
F	1.53766000	1.39772700	0.13527200
F	2.37141300	-0.34426200	-0.83677000
F	1.95856800	-0.38814300	1.28177200
O	-1.43154200	2.42724700	-0.03595500
H	-0.79564700	2.40182600	-0.77089600

### PC3b

0 2

C	0.18755700	-0.41412600	-0.19355500
C	-0.70756500	-0.37277200	0.98277600
H	-0.26756200	-0.29345100	1.96689500
H	-1.87120300	2.32116700	0.80295800
C	-2.63607900	-0.99878600	-0.27095600
H	-2.82444900	0.00257800	-0.65799800
H	-2.06912800	-1.59618900	-0.98654400
H	-3.56961300	-1.49914100	-0.02956000
O	-1.92759400	-0.89904200	0.97235400
F	-0.29587500	0.29402700	-1.26272700
F	0.39326700	-1.67745600	-0.67061800
C	1.56895200	0.18373100	0.12617300
F	1.43916500	1.46719900	0.47272600
F	2.36433800	0.11080300	-0.93020700
F	2.14015700	-0.46643800	1.13814400
O	-2.18063200	2.26586400	-0.10469600
H	-1.37888900	2.18896000	-0.62950900

### P3b

0 2

C	0.10433400	-0.21146900	-0.05745100
C	0.95114800	0.99122700	0.08157900
H	0.51383100	1.97054700	-0.04357200
C	2.96551400	-0.27630700	0.14329000
H	2.84589700	-0.58443700	1.18271300
H	2.59748900	-1.05754600	-0.52308700
H	4.00968800	-0.06683300	-0.07113400

O	2.27302800	0.95384300	-0.08523500
F	0.36379000	-1.15470800	0.89476300
F	0.28309600	-0.85382100	-1.25361800
C	-1.39261200	0.12928000	0.04648200
F	-1.66089400	0.68810100	1.22520100
F	-2.12694900	-0.96679400	-0.08132900
F	-1.73920100	0.98845900	-0.91240000

### CR3c

0 2

C	-0.25134900	0.13465900	-0.06115500
C	0.48330500	-0.98254000	0.66590200
H	0.13561700	-0.99680100	1.70088900
H	0.23728500	-1.93732500	0.18870100
C	2.58524600	-1.30793300	-0.41246400
H	3.63382400	-1.07718500	-0.23145200
H	2.44708500	-2.39326300	-0.42408000
H	2.27910100	-0.87859700	-1.36814000
O	1.85894900	-0.73322500	0.67273000
F	0.08846300	0.16592500	-1.36962100
F	0.08323400	1.32924700	0.47338500
C	-1.78081000	0.00624100	0.01218500
F	-2.15975400	-1.15885700	-0.51753700
F	-2.37733200	0.98782400	-0.64543000
F	-2.17993100	0.03587000	1.28404700
O	3.31167200	1.57700900	-0.00349600
H	2.59165300	1.19026600	0.52981600

### TS3c

0 2

C	0.20078700	-0.02750700	0.10821700
C	-0.37089000	1.37631400	-0.05575300
H	0.22911400	2.06034700	0.54613800
H	-0.28355100	1.64991000	-1.11425300
C	-2.66124800	0.85425200	-0.37605600
H	-3.62352700	1.29519100	-0.12264500
H	-2.44967600	0.92193800	-1.44763600
H	-2.77920500	-0.27590000	-0.11392400
O	-1.68275100	1.47440800	0.40474700
F	-0.32549400	-0.87128600	-0.82439200
F	-0.09025000	-0.53571000	1.31613000
C	1.72710900	-0.07536100	-0.06939700
F	2.05809200	0.44142800	-1.25463700
F	2.17558900	-1.31974000	-0.00606300



F	2.31977200	0.64390800	0.88182200
O	-3.01428800	-1.68075800	0.06767900
H	-2.13076800	-1.99427800	-0.18488800

### PC3c

0 2

C	0.20202600	0.54281900	0.24909200
C	-0.82343800	0.61441900	-0.87196900
H	-0.40179500	1.22093100	-1.67474100
H	-1.03446300	-0.39954500	-1.22366700
C	-3.00431300	0.43995400	-0.02473300
H	-3.84783900	0.98752100	0.36747100
H	-3.12915300	-0.48812900	-0.57191600
H	-1.76003400	-1.86981300	0.83655000
O	-1.97765500	1.25522100	-0.39413100
F	-0.29803900	-0.10634500	1.32813500
F	0.55502700	1.77923800	0.65225700
C	1.49184400	-0.18799300	-0.15957200
F	1.22555600	-1.45775000	-0.47172500
F	2.38010400	-0.17417100	0.82406700
F	2.02746700	0.40091900	-1.22941600
O	-1.65634200	-2.36498700	0.01738700
H	-0.96246900	-3.00503500	0.19346200

### P3c

0 2

C	0.08076600	0.27773500	0.13917700
C	1.04338400	-0.90270800	0.09572200
H	0.70385400	-1.64770500	0.81575000
H	1.02450000	-1.33007500	-0.91302100
C	3.08081500	0.09986600	-0.48661400
H	4.08269900	0.32953500	-0.16006300
H	2.84837300	-0.11493400	-1.52344600
O	2.33458700	-0.51787200	0.47142600
F	0.38561200	1.19085900	-0.80879400
F	0.13287100	0.89213100	1.33551300
C	-1.37823900	-0.14851900	-0.09778800
F	-1.48500200	-0.76066300	-1.27957100
F	-2.19001300	0.89718300	-0.08536100
F	-1.76529900	-1.00307500	0.85003400

#### A4

0 1

C	0.11899500	-0.04332000	-0.92996500
C	-0.93279200	0.38489800	0.07356500
H	-0.66467300	-0.03274600	1.05347100
H	-0.92231300	1.48140400	0.13795400
C	-3.21837200	0.24204700	0.48934200
H	-3.32188900	1.32995000	0.57678200
H	-4.12703000	-0.17255100	0.05836400
H	-3.06171600	-0.18572900	1.48653100
O	-2.15855300	-0.09693900	-0.37827300
F	-0.14804400	0.45885700	-2.15233500
F	0.16731000	-1.38668100	-1.03368100
C	1.53083600	0.43168900	-0.54426600
F	2.42543500	0.03903500	-1.43855400
F	1.87249400	-0.06305000	0.64726800
F	1.56198400	1.76356900	-0.46516200

#### CR4a

0 2

C	0.13703600	-0.20585100	-0.42777000
C	-1.08638300	0.46712800	0.15934500
H	-0.85426600	0.79233700	1.18185600
H	-1.32675000	1.34087300	-0.45984800
C	-3.33108200	0.04699200	0.64584200
H	-3.69066400	0.85935500	0.00495600
H	-4.05080200	-0.76833500	0.64052100
H	-3.20274100	0.40968400	1.67074500
O	-2.11301400	-0.47857300	0.14684800
F	-0.06625500	-0.54690000	-1.71444700
F	0.43113000	-1.34120800	0.25357800
C	1.39135900	0.68275600	-0.38056700
F	2.42729500	0.06956900	-0.93314800
F	1.69508800	0.98384900	0.88134000
F	1.16497400	1.82043000	-1.04005800
O	-1.55419700	-1.41832400	2.50076600
H	-1.06172200	-1.90509700	1.81723200

#### TS4a

0 2

C	0.20620600	-0.06935000	-0.72498300
C	-0.99925000	0.47325300	0.01397800
H	-0.80154200	0.30054800	1.15675900

H	-1.09224700	1.55992600	-0.11867400
C	-3.28743800	0.17556700	0.28801900
H	-3.49561000	1.23337600	0.09508700
H	-4.09686200	-0.43357300	-0.10643900
H	-3.18025600	0.00917800	1.36390000
O	-2.10650500	-0.22959700	-0.38637500
F	0.00210000	-0.07548900	-2.05487700
F	0.45308700	-1.34357100	-0.33714000
C	1.48728700	0.74083400	-0.46165000
F	2.51555100	0.21552900	-1.11180800
F	1.76274700	0.75395800	0.84024800
F	1.32098400	1.99964800	-0.87032400
O	-0.71199400	-0.39025500	2.40886600
H	-0.29989800	-1.20676600	2.07812200

#### PC4a

0 2

C	0.13220800	-0.21369000	-0.53470900
C	-1.10447200	0.41134200	-0.03366700
H	-0.73538600	-1.02409500	3.46050700
H	-1.05967400	1.19721900	0.71018000
C	-3.33302300	0.10766100	0.57222800
H	-3.61439200	1.09215400	0.19160500
H	-4.12593300	-0.60756500	0.37131600
H	-3.11692000	0.14386500	1.64084800
O	-2.18011700	-0.36675300	-0.12362300
F	-0.01040600	-0.70800700	-1.78247800
F	0.52394100	-1.28980800	0.24154400
C	1.32230400	0.75928800	-0.54210600
F	2.42699500	0.14740100	-0.94658900
F	1.52856900	1.24044700	0.68666400
F	1.08130600	1.78389300	-1.35632000
O	-1.21256200	-0.92810200	2.63368800
H	-0.69513900	-1.41389300	1.98311500

#### P4a

0 2

C	0.15285600	-0.24183100	-0.50779500
C	-1.07538300	0.35701100	0.05506600
H	-1.01636300	1.09429800	0.84719400
C	-3.34080800	0.13014200	0.53626300
H	-3.59591300	1.10774800	0.12135200
H	-4.13861000	-0.57911700	0.33417000
H	-3.17851400	0.21009500	1.61419300

O	-2.17452600	-0.37993600	-0.09845100
F	-0.04756800	-0.70295500	-1.76151000
F	0.59962700	-1.30738000	0.22373200
C	1.31169600	0.76933200	-0.56043400
F	2.42254500	0.19155100	-0.99420400
F	1.53844900	1.26811600	0.65870800
F	1.01290000	1.78037000	-1.37339100

#### CR4c

0 2

C	0.27760200	-0.36902600	0.05037100
C	-0.94633400	0.24783200	0.69526600
H	-0.65280900	0.64589600	1.67502300
H	-1.30757500	1.06568900	0.05824000
C	-3.08677900	-0.31753900	1.43719300
H	-2.88354700	-0.00815500	2.46817700
H	-3.52676900	0.51447400	0.87809300
H	-3.77881500	-1.15651100	1.43721100
O	-1.89823100	-0.76678600	0.80910800
F	-0.04700100	-0.95407100	-1.12936600
F	0.81570700	-1.31880700	0.83890500
C	1.38079800	0.65999800	-0.24837000
F	2.44591900	0.07377700	-0.77408100
F	1.74291600	1.27522500	0.87907700
F	0.93327400	1.57991300	-1.10187700
O	-2.95407200	-0.31748500	-1.51764300
H	-2.23661600	-0.97028700	-1.59369500

#### TS4c

0 2

C	-0.22413700	-0.43052600	-0.27902200
C	-1.53597300	0.18134700	0.16508000
H	-1.35439500	0.82307600	1.03570600
H	-1.93988400	0.78090500	-0.65954700
C	-3.70947500	-0.47536600	0.66867300
H	-3.80476400	0.35361500	1.37958600
H	-4.13934600	-0.07589200	-0.33646400
H	-4.29785500	-1.33851400	0.97139200
O	-2.39366700	-0.88123600	0.48251900
F	-0.40524900	-1.19739800	-1.37492600
F	0.30103700	-1.20835700	0.68837700
C	0.83163000	0.63039300	-0.63483100
F	1.96220100	0.06133100	-1.02479800
F	1.08293900	1.39796400	0.42734500

F	0.38337800	1.41159900	-1.61773900
O	-4.17267200	0.25080100	-1.76061500
H	-3.88982200	-0.62054500	-2.08553200

# **PC4c**

0 2

C	0.22625900	-0.39064300	0.05221000
C	-0.96300300	0.21666500	0.76519900
H	-0.61820300	0.68985500	1.69059900
H	-1.43374100	0.94894000	0.10231900
C	-3.06258200	-0.46456400	1.50202300
H	-3.16496400	0.52754300	1.92661600
H	-3.51944600	-0.19021500	-0.97177900
H	-3.67402700	-1.28968400	1.83448300
O	-1.84674300	-0.84329300	1.04300400
F	-0.16434100	-1.01702200	-1.08230300
F	0.84503400	-1.30145200	0.82801800
C	1.27379500	0.66200800	-0.34900800
F	2.30551200	0.09362500	-0.95424400
F	1.71241700	1.29967300	0.73834600
F	0.73240600	1.55807500	-1.17086100
O	-2.90285400	0.14843800	-1.62889800
H	-2.31787200	-0.59203600	-1.81388600

# **P4c**

0 2

C	0.21506400	-0.39404800	0.02959200
C	-1.01840100	0.22573300	0.65416300
H	-0.72261200	0.74099800	1.57534100
H	-1.45109100	0.94584100	-0.04827700
C	-3.03247400	-0.44217800	1.58863000
H	-2.96286400	0.41279800	2.25280600
H	-3.70650000	-1.26008800	1.78927300
O	-1.91363000	-0.81873700	0.92155600
F	-0.09710700	-1.04578200	-1.10718800
F	0.78726300	-1.27640300	0.87263800
C	1.28188400	0.65717200	-0.32414800
F	2.34929600	0.08721300	-0.86032300
F	1.65417500	1.31752000	0.77424500
F	0.78481700	1.53968700	-1.19190900

**Cartesian Coordinates of all the species involved in the reaction of different conformers of**  
**HFE-365mcf3 with Cl.**

**CR5a**

0 2

C	0.29909300	-0.42557200	0.35620600
C	-0.16151000	0.75690400	1.19778700
H	-1.20973500	0.56140300	1.46349200
H	0.44235900	0.75811800	2.10626000
C	-0.92368700	2.28448900	-0.45061300
H	-0.73681500	1.69139000	-1.34931700
H	-1.94646900	2.10386500	-0.10260800
H	-0.80016400	3.33995900	-0.68390100
O	0.01252200	1.98951500	0.57562600
F	-0.55339000	-0.66374800	-0.67836900
F	0.30543000	-1.53155200	1.13018500
C	1.70278300	-0.27432400	-0.25913900
F	2.11566700	-1.43386600	-0.76118200
F	2.56638200	0.11227800	0.67811800
F	1.69549700	0.62490300	-1.23710900
Cl	-3.32445300	-0.72894100	-0.19348100

**TS5a**

0 2

C	0.31365600	-0.49798400	-0.10410300
C	-0.62073800	0.24579000	0.84080600
H	-1.78632300	-0.26687400	0.50885200
H	-0.48680400	-0.08180300	1.87114200
C	-0.99624300	2.19288000	-0.49100700
H	-0.12705500	2.15664600	-1.14710200
H	-1.84416900	1.68272900	-0.95343500
H	-1.25146500	3.22324100	-0.26124700
O	-0.70368900	1.58273500	0.77396300
F	-0.01595300	-0.31140500	-1.39724200
F	0.22619600	-1.81071000	0.17407300
C	1.79514500	-0.09349100	0.05161800
F	2.56983700	-0.85392500	-0.70700100
F	2.16777700	-0.22930300	1.32186300
F	1.96205400	1.17866700	-0.30730100
Cl	-3.17734100	-0.71875900	0.01451000

**PC5a**

0 2

C	0.45278200	-0.50440500	-0.00693600
C	-0.42057900	0.23963500	0.95426300
H	-2.49273000	-0.63019200	0.48141300

H	-0.36681100	-0.09070300	1.98461200
C	-0.98464000	2.08240200	-0.47499900
H	-0.07059300	2.11881900	-1.06643800
H	-1.74670800	1.49358900	-0.98671500
H	-1.34823400	3.08838700	-0.28626800
O	-0.72823500	1.52727700	0.82334600
F	0.02309100	-0.39700200	-1.28814900
F	0.43044900	-1.81056400	0.33700500
C	1.93693700	-0.07605900	-0.00651600
F	2.65022100	-0.80554500	-0.85312400
F	2.44694100	-0.21593400	1.21432700
F	2.03719500	1.20682800	-0.36216200
Cl	-3.66747800	-0.61456500	-0.05525300

### P5a

0 2

C	-0.09232400	0.72450900	-0.06676400
C	1.07040600	0.71675400	0.86770700
H	0.88279600	1.09516800	1.86333700
C	2.57373400	-0.56972300	-0.47319400
H	1.85291900	-1.17724800	-1.01986600
H	2.83352300	0.31621300	-1.05400800
H	3.46343000	-1.15512300	-0.25723700
O	2.05459800	-0.18256000	0.80314500
F	0.28720600	0.78214600	-1.37134400
F	-0.84248300	1.81578100	0.19984800
C	-1.03902900	-0.49125900	0.04676200
F	-2.06320100	-0.38897000	-0.79156600
F	-1.51273000	-0.58347300	1.28690300
F	-0.37392300	-1.61439800	-0.23544700

### CR5b

0 2

C	-1.00596700	0.75215200	0.18378700
C	0.38497700	1.12970600	0.65734500
H	0.34113500	2.20229000	0.88049100
H	0.61994000	0.57777900	1.57429700
C	2.46420200	1.69187900	-0.29866600
H	2.17626900	2.73485500	-0.46019300
H	2.96846800	1.58534700	0.66648300
H	3.12870500	1.36176900	-1.09337100
O	1.31279300	0.86015200	-0.35989900
F	-1.34917700	1.47756300	-0.89833800
F	-1.87108300	1.05331800	1.18073600
C	-1.22537200	-0.73152500	-0.16421600
F	-2.51156500	-0.94988300	-0.42317500
F	-0.86913400	-1.48915600	0.87266600

F	-0.51524300	-1.08614300	-1.22464100
Cl	2.38834800	-1.37928400	0.20451500

## TS5b

0 2

C	-0.72602500	0.11362300	0.76089400
C	0.70700000	0.58595500	0.64074900
H	1.13560100	0.82689900	1.62120400
H	1.40218800	-0.45366500	0.32074600
C	2.14093600	2.13022700	-0.35875500
H	2.36490400	2.59284600	0.60590100
H	2.89523600	1.37694500	-0.60101700
H	2.09457400	2.88508900	-1.13809400
O	0.85537000	1.51436300	-0.31709900
F	-1.47880100	1.06728800	1.35187100
F	-0.74454000	-0.97618000	1.55058000
C	-1.40651700	-0.25260800	-0.57505000
F	-2.55797600	-0.86933800	-0.33411500
F	-0.62056000	-1.06665600	-1.27170200
F	-1.65263600	0.83405700	-1.29448100
Cl	2.49781100	-1.51227900	-0.06460900

## PC5b

0 2

C	-1.05799100	0.44660200	0.59548200
C	0.30426200	1.02431500	0.60748600
H	0.68641700	1.44626500	1.53006300
H	1.75383800	-1.33625500	0.02701800
C	1.97317300	2.19254100	-0.53016100
H	1.78030600	3.13079200	-0.00488200
H	2.76522000	1.62987900	-0.03314900
H	2.24787800	2.39254400	-1.56196600
O	0.77869200	1.41387800	-0.57564700
F	-2.02846200	1.37798200	0.36406100
F	-1.31050900	-0.09516000	1.80755400
C	-1.28315500	-0.65981000	-0.45813600
F	-2.46279500	-1.23731700	-0.27797400
F	-0.33666700	-1.60556100	-0.33384100
F	-1.22777900	-0.17576900	-1.68962700
Cl	3.01264600	-1.23374800	0.26638300

## P5b

0 2



C	0.23096200	0.73871100	0.00631500
C	-1.17825100	0.57866400	-0.41549400
H	-1.65952100	1.38121700	-0.96292700
C	-3.26361300	-0.40488100	-0.10136200
H	-3.75437400	0.56625800	0.00287100
H	-3.34068400	-0.75577700	-1.13268600
H	-3.72026300	-1.12436200	0.57253100
O	-1.89624100	-0.30510700	0.27800000
F	0.34982800	1.21824100	1.27760900
F	0.82640600	1.63068600	-0.81701800
C	1.07274400	-0.55468600	-0.03848100
F	2.34336100	-0.28603600	0.24692700
F	1.02130000	-1.09169700	-1.25711800
F	0.62285300	-1.44600800	0.83741600

## HCl

0 1			
H	0.00000000	0.00000000	-1.21203700
Cl	0.00000000	0.00000000	0.06939500

## CR5c

0 2			
C	0.91401900	-0.43886700	0.62125300
C	-0.58029200	-0.19732500	0.78150300
H	-0.98007100	-1.02362800	1.38174200
H	-0.71187000	0.73975800	1.32263600
C	-1.44643400	-1.27564000	-1.17260100
H	-2.15929800	-1.04119600	-1.95945100
H	-0.50572900	-1.61353900	-1.61019800
H	-1.85882800	-2.04918000	-0.51830000
O	-1.25141900	-0.06480700	-0.44252200
F	1.16799500	-1.69659600	0.18830800
F	1.49409300	-0.30023000	1.83263300
C	1.62321300	0.52441900	-0.34930900
F	2.94116700	0.40353000	-0.24019900
F	1.28573600	1.78056000	-0.06628400
F	1.28081800	0.25882400	-1.60674300
Cl	-3.55083400	0.57740700	0.27466100

## TS5c

0 2			
C	0.82164800	-0.69048800	-0.10296800
C	-0.43222100	-0.39561700	0.70610800

H	-1.20017200	-1.12117600	0.41777100
H	-0.19531000	-0.51257400	1.76236900
C	-1.65556800	1.16729400	-0.56133500
H	-1.89235600	2.22326500	-0.64645900
H	-1.38575400	0.64100400	-1.47753500
H	-2.86582500	0.58329400	-0.29950800
O	-0.88153300	0.93031800	0.52709000
F	0.54828600	-0.73315000	-1.42792900
F	1.27937800	-1.90351000	0.26568900
C	1.96919700	0.32117000	0.08641500
F	3.08772300	-0.14446900	-0.45365900
F	2.17531500	0.52733100	1.38647600
F	1.67231500	1.48097100	-0.49041100
Cl	-4.02904800	-0.27735700	0.10210800

### PC5c

0 2

C	0.84011200	-0.64822900	-0.27273700
C	-0.52066000	-0.42175900	0.36777800
H	-1.24789300	-1.03991800	-0.16887300
H	-0.46896700	-0.74247000	1.40727400
C	-1.43360200	1.42617100	-0.77100000
H	-1.55630700	2.49899500	-0.75506600
H	-1.27136900	0.88781000	-1.69718500
H	-3.38844100	0.61093900	-0.21744100
O	-0.88410000	0.93768400	0.36752900
F	0.78754800	-0.45874100	-1.61147700
F	1.19862900	-1.93044200	-0.05107600
C	1.96937200	0.25195300	0.26572500
F	3.14868400	-0.18581500	-0.15940000
F	1.96298300	0.23066600	1.59842200
F	1.81241700	1.50487300	-0.14488200
Cl	-4.13634700	-0.34179500	0.25106900

### P5c

0 2

C	-0.11550200	0.74428300	-0.02962500
C	1.13143000	0.68876300	0.84131000
H	1.71440700	1.59254300	0.63279100
H	0.81104700	0.69237400	1.88267100
C	2.71558600	-0.47936300	-0.44068100
H	3.19182200	-1.43262600	-0.60527200
H	2.52352100	0.21593200	-1.24701500
O	1.87965900	-0.47758100	0.63492900

F	0.19515500	0.98387700	-1.32433700
F	-0.88442700	1.76817700	0.40288000
C	-0.98019500	-0.53092400	-0.00162100
F	-2.15789100	-0.30065500	-0.57254200
F	-1.18816600	-0.90438100	1.26134200
F	-0.38533700	-1.52303300	-0.65166500

### CR6a

0 2

C	0.74115100	0.20325900	0.79852100
C	-0.73476800	0.54971200	0.85337600
H	-1.32709600	-0.37132500	0.81562100
H	-0.88803600	1.04044100	1.82182700
C	-2.16278600	2.25260200	0.07045000
H	-1.92192200	2.92077500	0.90249500
H	-2.34769000	2.83204800	-0.83075300
H	-3.04911300	1.65731100	0.30979700
O	-1.05102600	1.41116300	-0.20786400
F	1.00808800	-0.60766100	1.84942200
F	1.49176800	1.31443800	0.92900600
C	1.21960000	-0.53324500	-0.46610800
F	2.48766800	-0.90672000	-0.31922000
F	1.12936900	0.24193000	-1.53636500
F	0.47734600	-1.62417300	-0.65331100
Cl	-2.07090500	-0.02607800	-2.04647300

### TS6a

0 2

C	0.71389100	-0.02205000	0.75713900
C	-0.68191000	0.55713000	0.67054600
H	-1.43355800	-0.38610800	0.21620600
H	-1.11777600	0.70844000	1.66566900
C	-1.98593900	2.30339700	-0.15964500
H	-2.20313900	2.66259500	0.84960600
H	-1.87134700	3.14041000	-0.84198900
H	-2.78155200	1.63693600	-0.50310900
O	-0.74465900	1.60147300	-0.17045300
F	0.64177500	-1.19758900	1.40858000
F	1.51161200	0.80092600	1.47253900
C	1.40282400	-0.26991500	-0.60162500
F	2.50187900	-0.99305700	-0.41833300
F	1.74309400	0.87617900	-1.17583200
F	0.58135100	-0.93338000	-1.40829300
Cl	-2.58008400	-1.32282900	-0.31552600

**PC6a**

0 2

C	0.78955800	0.22635300	0.90353600
C	-0.58372200	0.77677200	0.88261400
H	-1.73071900	-1.10156700	-0.90288000
H	-1.17404200	0.74925000	1.79142400
C	-2.07291800	2.36809600	0.04977700
H	-2.07498900	2.94933000	0.97481500
H	-2.13678000	3.03217800	-0.80754100
H	-2.90334300	1.66001200	0.03942400
O	-0.83610300	1.66832200	-0.07532200
F	0.83402400	-0.79569100	1.78654400
F	1.72242900	1.14022800	1.30087000
C	1.29133700	-0.31699900	-0.45209200
F	2.45255200	-0.93838700	-0.30047800
F	1.43892100	0.65487100	-1.33955200
F	0.40868600	-1.20449900	-0.94118400
Cl	-3.01623300	-1.06952500	-0.89803900

**P6**

0 2

C	0.21884800	0.73103600	0.00113800
C	-1.17875100	0.53661300	0.45784800
H	-1.40815200	0.61017200	1.51475800
C	-3.26587100	-0.43754700	0.12581400
H	-3.80439800	0.50091800	0.27461800
H	-3.76305200	-1.03608700	-0.63236900
H	-3.21449200	-0.99431000	1.06506800
O	-1.95497900	-0.17518700	-0.36003400
F	0.82168300	1.62641700	0.81768700
F	0.26558400	1.20216500	-1.26575700
C	1.10087900	-0.53776600	0.02290700
F	2.34793100	-0.26049000	-0.34266200
F	0.61263700	-1.46078500	-0.79946600
F	1.12764100	-1.04433200	1.25819200

**CR6b (Optimized at the MP2/6-311++G(d,p) level of theory)**

0 2

C	-0.65102300	0.13118700	-0.44634600
C	0.76628900	-0.16932200	-0.88952300
H	0.72990100	-1.02599000	-1.57476100
H	1.12775300	0.71521700	-1.43326400
C	2.85895100	-0.86932000	-0.14429800
H	3.36415800	-0.08484200	-0.72058000

H	3.40946600	-1.05661000	0.77650300
H	2.80620400	-1.78932700	-0.73882800
O	1.55325600	-0.45108900	0.23903800
F	-1.40788600	0.26131100	-1.57007200
F	-0.71585600	1.29535800	0.23734400
C	-1.31100800	-0.95623900	0.42461200
F	-2.62136100	-0.72578600	0.53017100
F	-0.78881800	-0.98665600	1.64553100
F	-1.13710800	-2.15437100	-0.15316100
Cl	2.09777300	1.65358100	1.86628300

**TS6b** (*Optimized at the MP2/6-311++G(d,p) level of theory*)

0 2

C	-0.29087200	0.72902800	0.00754400
C	1.13968300	0.56806400	-0.46810500
H	1.18292300	0.22341400	-1.51013100
H	1.54681500	1.70317100	-0.52385200
C	3.19243000	-0.44208800	-0.06721800
H	3.74537600	0.49206200	-0.20752700
H	3.67067200	-1.05109500	0.69726300
H	3.14091100	-0.99481600	-1.01171400
O	1.87457100	-0.16033100	0.41337900
F	-0.94142500	1.49737400	-0.90035300
F	-0.33281900	1.34402600	1.20581300
C	-1.07568500	-0.59427200	0.12860900
F	-2.36488300	-0.34479800	0.35014000
F	-0.60720800	-1.34229100	1.12249400
F	-0.96275700	-1.27978800	-1.01879600
Cl	2.29986200	3.15943300	-0.59483800

**PC6b** (*Optimized at the MP2/6-311++G(d,p) level of theory*)

0 2

C	-0.72870400	-0.10061100	-0.77890900
C	0.64293500	-0.55760300	-1.12869400
H	0.76651800	-1.49686000	-1.65919100
H	1.55972500	1.10268400	1.35630800
C	2.91296100	-0.64410600	-0.58122200
H	3.23813200	-0.27426700	-1.55637000
H	3.56546900	-0.26672900	0.20374300
H	2.90305500	-1.73766600	-0.56930600
O	1.60210100	-0.14128300	-0.28337100
F	-1.56415400	-0.41889900	-1.80005800
F	-0.75434200	1.24516000	-0.59135100
C	-1.32855600	-0.72763500	0.49855800
F	-2.58010900	-0.31806700	0.69308700
F	-0.59557100	-0.38787700	1.56290200
F	-1.32753600	-2.06223600	0.38801000
Cl	2.15793300	1.63467000	2.35528500

**P6b** (*Optimized at the MP2/6-311++G(d,p) level of theory*)

0 2

C	-0.72153800	-0.09643900	-0.77048300
C	0.65265100	-0.54707600	-1.11544500
H	0.77110100	-1.48465300	-1.65093100
C	2.91174000	-0.64614800	-0.58772700
H	3.23802800	-0.28433100	-1.56634100
H	3.57761000	-0.27640100	0.18941100
H	2.89533500	-1.74045500	-0.57576700
O	1.61410900	-0.12948300	-0.28008100
F	-1.55001100	-0.43123300	-1.79658000
F	-0.76921500	1.24852900	-0.59412700
C	-1.33099300	-0.72583100	0.50141400
F	-2.59042300	-0.32429000	0.67787900
F	-0.62125800	-0.38902900	1.57897200
F	-1.32493500	-2.06183700	0.38763400

**CR6c**

0 2

C	-0.73034100	-0.37040000	0.66118800
C	0.38128000	0.57511500	1.07127400
H	-0.08253100	1.48067300	1.47856800
H	0.96783700	0.07925600	1.85480100
C	2.05760300	1.95304400	0.17360500
H	2.72704800	1.72869700	1.00979900
H	2.64072800	2.07161800	-0.73631500
H	1.49342700	2.86793400	0.37904200
O	1.16203400	0.87384500	-0.05345000
F	-1.56236400	-0.50927800	1.71989500
F	-0.25591100	-1.58775700	0.34489100
C	-1.58118400	0.11958500	-0.52977600
F	-2.70504200	-0.58548100	-0.60908400
F	-0.92829600	-0.00010500	-1.67474700
F	-1.90332200	1.40465400	-0.34867200
Cl	2.84632200	-1.02242900	-0.39450500

**TS6c**

0 2

C	-0.88957300	-0.72788400	-0.00478700
C	0.46543500	-0.25379500	0.48085100
H	0.37994800	0.05050200	1.52861900
H	1.16840100	-1.08893800	0.39065700
C	1.94375700	1.51087600	0.12404000

H	3.03317200	0.67504500	0.00700000
H	2.18919300	2.34240500	-0.52908600
H	1.96504000	1.69807300	1.20051600
O	0.87441700	0.82346100	-0.33260000
F	-1.29053400	-1.72111800	0.81847900
F	-0.81315400	-1.21900600	-1.25331700
C	-1.99500400	0.34849600	0.00709900
F	-3.18459300	-0.21270400	-0.16391800
F	-1.80593800	1.24398900	-0.95120200
F	-1.98716400	0.97744900	1.18678300
Cl	4.05021500	-0.42049600	-0.01832600

### PC6c

0 2

C	0.74000800	-0.64292200	-0.20906500
C	-0.40091100	0.15930700	-0.80013700
H	-0.06325000	0.61534600	-1.73615600
H	-1.22300700	-0.53738800	-0.99552600
C	-1.74641800	1.98736900	-0.27285400
H	-3.34090700	0.56006500	0.19056500
H	-1.94809400	2.78018100	0.43249900
H	-1.87583200	2.13688000	-1.34028100
O	-0.77729800	1.14139100	0.13584800
F	1.13765200	-1.53466000	-1.14465400
F	0.34102300	-1.32460100	0.87862300
C	1.98181900	0.18243300	0.18729400
F	3.00938000	-0.62387600	0.42678600
F	1.75484700	0.91035500	1.27036600
F	2.31074300	0.99962800	-0.81777200
Cl	-3.86825400	-0.62617300	0.20062000

### P6c

0 2

C	-0.23226000	0.75393000	0.03202500
C	1.20202700	0.70006800	-0.45101600
H	1.20054700	0.44568400	-1.51661500
H	1.62982800	1.69887300	-0.31164000
C	3.17909900	-0.45316600	-0.06868000
H	3.68606700	-1.20590300	0.51402500
H	3.44096400	-0.26145200	-1.10371600
O	1.88879600	-0.26129100	0.30330800
F	-0.89781400	1.62960200	-0.75618700
F	-0.30309100	1.19892900	1.30028400
C	-0.99532600	-0.58502100	-0.03333600

F	-2.29643800	-0.37753900	0.14124600
F	-0.57559100	-1.42983000	0.89564400
F	-0.81473300	-1.14135600	-1.23459500

### CR7a

0 2

C	-0.09840900	0.65140700	0.36138000
C	0.81759500	0.07421800	-0.70089700
H	0.38954700	-0.85904700	-1.08636500
H	0.89313700	0.80614500	-1.51339600
C	3.10587300	-0.31775300	-1.05724500
H	2.88133800	-1.15205400	-1.72913900
H	3.23907700	0.60278800	-1.63365700
H	4.01035700	-0.53856300	-0.49559500
O	2.06661400	-0.14689600	-0.10419900
F	0.35629200	1.85392000	0.77197100
F	-0.16961400	-0.15482800	1.43499700
C	-1.53286100	0.85940500	-0.15524100
F	-1.51924000	1.66357600	-1.22163100
F	-2.29941300	1.40262400	0.77704500
F	-2.06273200	-0.30752000	-0.52148000
Cl	1.98023700	-2.50954900	0.86953100

### TS7a

0 2

C	-0.01844300	0.50326800	0.65442700
C	0.90106900	-0.27484100	-0.26763700
H	0.60688200	-1.50360200	-0.12876400
H	0.69328200	-0.10752500	-1.33091500
C	3.14425900	-0.63833800	-0.79123500
H	3.02692000	-1.72396100	-0.84887400
H	3.02041400	-0.19217700	-1.78167100
H	4.11844700	-0.38498700	-0.38335300
O	2.17904300	-0.10460900	0.11054100
F	0.25787500	1.82245900	0.55835300
F	0.16138800	0.13113400	1.93048900
C	-1.50798300	0.32708800	0.30695000
F	-1.71399300	0.68468200	-0.96349500
F	-2.25753300	1.08665300	1.09059300
F	-1.87179500	-0.94015700	0.45275500
Cl	0.56540700	-3.10109500	-0.08547200

### PC7a

0 2

C	-0.03144800	0.81162000	0.35138500
C	0.92565000	0.38291500	-0.68503400
H	0.89492500	-1.95624900	0.88322800



H	0.75189100	0.56852100	-1.73706400
C	3.07397500	-0.34607700	-1.21299800
H	2.71336000	-1.26717000	-1.67484000
H	3.21388200	0.43362900	-1.96564100
H	4.00819700	-0.53192100	-0.69068200
O	2.14110500	0.09200500	-0.22720500
F	0.24031400	2.04718600	0.85725900
F	-0.00314100	-0.03758700	1.41866100
C	-1.47834600	0.84436600	-0.16966000
F	-1.55619600	1.63640000	-1.24196400
F	-2.30224300	1.30521900	0.75980400
F	-1.87145100	-0.37686900	-0.52151000
Cl	1.09592600	-3.00250400	0.16277800

### P7a

0 2

C	-0.03469700	0.79301300	0.35927300
C	0.90971100	0.31638500	-0.67262300
H	0.76305900	0.57410300	-1.71504800
C	3.07650900	-0.33562500	-1.21570200
H	2.74602100	-1.22864000	-1.75070600
H	3.21199300	0.49311100	-1.91533800
H	4.00936300	-0.53735900	-0.69659600
O	2.12531600	0.01557100	-0.21815300
F	0.26231600	2.05304200	0.80019800
F	-0.02142400	-0.00146200	1.45167100
C	-1.48028700	0.84312600	-0.16595900
F	-1.54219400	1.60834300	-1.26018100
F	-2.29726900	1.34591400	0.74827400
F	-1.90286700	-0.37728500	-0.48860000

### CR7b

0 2

C	-0.49844700	0.55705700	-0.28942100
C	0.29430800	1.15900600	0.86341900
H	-0.41865700	1.65292900	1.52711700
H	0.78564900	0.34226000	1.40787900
C	2.46746000	1.61947100	0.02279200
H	2.90385000	1.00523600	0.81793300
H	2.40605500	1.03076900	-0.89552700
H	3.09760500	2.49005100	-0.14804300
O	1.19858900	2.11920000	0.41733200
F	0.31679400	-0.14394800	-1.12686600
F	-1.08998900	1.51699600	-1.02113800
C	-1.59496500	-0.41648700	0.17224000

F	-1.04908300	-1.41832300	0.86389000
F	-2.25200400	-0.92261000	-0.86098800
F	-2.46255400	0.21529500	0.96336500
Cl	2.14459900	-2.01269500	-0.00156200

### TS7b

0 2

C	-0.52762000	0.53629100	-0.18778700
C	0.58808800	0.47502800	0.85983600
H	0.15850800	0.33151900	1.85263900
H	1.18377200	-0.46448500	0.61464100
C	2.08307100	1.89557200	-0.30576300
H	2.59275200	1.00622000	-0.69254800
H	1.39488300	2.28081500	-1.06128100
H	2.81095500	2.65940200	-0.04499200
O	1.39562300	1.57809300	0.89941700
F	-0.05385400	0.27894000	-1.42731400
F	-1.08172500	1.76436800	-0.20880400
C	-1.64745900	-0.47989000	0.09268500
F	-1.12892800	-1.70304500	0.18671800
F	-2.55216100	-0.46700100	-0.87386900
F	-2.24787900	-0.18714300	1.24607800
Cl	2.42932900	-1.77501700	-0.05428800

### PC7b

0 2

C	-0.57286800	0.53441300	-0.17861900
C	0.30768100	0.79324000	0.97799000
H	-0.00277700	0.47997800	1.96365600
H	1.41963200	-1.71887500	-0.41528000
C	1.81435900	2.13656500	-0.28208100
H	2.33265100	1.29009100	-0.73461200
H	1.04565600	2.51631100	-0.95699900
H	2.51905000	2.92721900	-0.04070100
O	1.24089000	1.74079000	0.96779000
F	0.11465600	0.10294500	-1.28553900
F	-1.25884000	1.63849600	-0.59733600
C	-1.60570800	-0.56444600	0.12642800
F	-0.97344600	-1.71978100	0.36190900
F	-2.42206000	-0.73581700	-0.90181300
F	-2.32672400	-0.25577900	1.20063200
Cl	2.64091800	-1.65236800	-0.02478600

### P7b

0 2

C	0.10433100	-0.21152000	-0.05751100
C	0.95109000	0.99115500	0.08177400
H	0.51376500	1.97058000	-0.04237600
C	2.96551000	-0.27622600	0.14314300
H	2.84554500	-0.58466700	1.18243000
H	2.59776400	-1.05731400	-0.52359000
H	4.00973600	-0.06655200	-0.07082400
O	2.27293100	0.95389200	-0.08531700
F	0.36368200	-1.15478300	0.89494100
F	0.28323400	-0.85396000	-1.25341600
C	-1.39261500	0.12929500	0.04641800
F	-1.66089000	0.68811800	1.22511800
F	-2.12698000	-0.96675000	-0.08146300
F	-1.73906400	0.98855200	-0.91251800

### CR7c

0 2

C	-0.78390700	0.44928400	0.09288700
C	0.55623300	-0.25793700	-0.08253300
H	0.53782100	-1.19160400	0.48109700
H	0.69042600	-0.47861100	-1.14765500
C	1.92701200	1.68964300	-0.29169100
H	1.17215400	2.45417500	-0.09959000
H	2.89525000	2.02261700	0.07438000
H	1.98739200	1.48184900	-1.36413000
O	1.61988000	0.49740200	0.42883400
F	-0.94205600	1.42808900	-0.83350000
F	-0.87538500	1.02163800	1.30686200
C	-1.97648500	-0.50913700	-0.06514200
F	-1.89864600	-1.12972500	-1.24421700
F	-3.12542400	0.14619900	-0.00236400
F	-1.95479300	-1.43034600	0.89609400
Cl	3.56397200	-0.98949700	-0.02363400

### TS7c

0 2

C	0.93574000	-0.53102300	0.01292700
C	-0.38516400	-0.12636600	0.64852500
H	-0.20850000	0.12972200	1.69274900
H	-0.80397700	0.73773300	0.12400700
C	-2.11224000	-1.28995400	-0.43913600
H	-1.69674500	-0.99540100	-1.40357400

H	-2.70387100	-2.19983600	-0.41156200
H	-3.03296200	-0.29422000	-0.26463300
O	-1.27557700	-1.22130000	0.62521800
F	0.74002300	-0.94345600	-1.26120300
F	1.49630100	-1.55005800	0.68932000
C	1.95300800	0.62169100	-0.02672300
F	1.46463600	1.63143500	-0.74589900
F	3.09595500	0.22613900	-0.56338100
F	2.18430200	1.05890300	1.21104600
Cl	-3.79578500	0.97292000	0.00698600

### PC7c

0 2

C	-0.95430800	0.52424600	0.11495500
C	0.47738200	0.09582800	0.39609800
H	0.50239100	-0.46439600	1.33077200
H	0.83508700	-0.54079200	-0.41853200
C	1.91731500	1.69669500	-0.54896100
H	1.52046700	1.42218800	-1.51961500
H	2.40790100	2.64601600	-0.39162500
H	3.46557700	0.15769300	-0.28851800
O	1.28577200	1.23609200	0.55747700
F	-1.00949700	1.27876300	-1.00648900
F	-1.43995500	1.26351100	1.12953800
C	-1.90321800	-0.66864500	-0.08715300
F	-1.49827100	-1.39947500	-1.12655400
F	-3.14197400	-0.25883700	-0.31059000
F	-1.89403600	-1.44213000	0.99861200
Cl	3.80076300	-1.05733400	0.02455400

### P7c

0 2

C	0.06736300	0.33923600	0.01836600
C	1.05313000	-0.65951200	0.60703400
H	0.75851400	-0.86249400	1.63724400
H	1.01577500	-1.58608600	0.02559300
C	3.11761000	-0.35819700	-0.46683900
H	2.62449100	-0.58290500	-1.40404600
H	4.06611000	0.15443800	-0.43404300
O	2.34274900	-0.11290500	0.62647300
F	0.41503000	0.66641200	-1.24691100
F	0.04753200	1.47387800	0.74322400
C	-1.37066900	-0.20319700	-0.03008100
F	-1.41774500	-1.30032600	-0.78807700

F	-2.20442000	0.69537900	-0.53026700
F	-1.77500500	-0.52753100	1.19898500

### CR8a

0 2

C	0.61616900	-0.10691300	-0.43053000
C	-0.41214000	-0.75172100	0.47912400
H	-0.02793700	-1.73396500	0.77775500
H	-0.55621700	-0.12770000	1.36939000
C	-2.51174500	-1.79521200	0.33560700
H	-2.75686000	-1.49566300	1.35941500
H	-3.41232100	-1.77406300	-0.27335400
H	-2.08169400	-2.80142100	0.33197300
O	-1.60145300	-0.87686900	-0.25230100
F	0.17477700	1.06906100	-0.91000100
F	0.88594900	-0.91084800	-1.48044000
C	1.94822900	0.16035300	0.29194300
F	2.83951200	0.68521300	-0.53383100
F	2.43708100	-0.98261100	0.78059500
F	1.75834400	0.99985600	1.30966100
Cl	-2.88573000	1.30368700	0.11191200

### TS8a

0 2

C	0.62047400	-0.64138800	-0.30425100
C	-0.73936900	-0.53666600	0.35982400
H	-0.68848200	-0.52363800	1.45480700
H	-1.18598400	0.62392500	0.09977500
C	-2.83173000	-1.55652100	0.49680700
H	-3.37431800	-0.61006200	0.42283300
H	-3.37859500	-2.34605800	-0.01030400
H	-2.67261700	-1.81924700	1.54611100
O	-1.58027400	-1.43860700	-0.17377300
F	0.51727900	-0.46656900	-1.63020200
F	1.13869500	-1.86911100	-0.08113800
C	1.63368100	0.38258900	0.23893800
F	2.81950500	0.20099400	-0.32102000
F	1.75431400	0.23119000	1.56063100
F	1.22094300	1.61897200	-0.00798500
Cl	-2.07134000	1.93274000	-0.15020700

### PC8a

0 2

C	0.70371800	-0.39865700	-0.44424700
C	-0.34924500	-0.95070900	0.42816200
H	-0.15443400	-1.22837100	1.45605500
H	-1.82306600	1.11632200	-0.76676300
C	-2.45471200	-1.93210600	0.60570600
H	-2.83857500	-1.13932500	1.25055300
H	-3.23634600	-2.27832900	-0.06457100
H	-2.07580800	-2.76533500	1.20248300
O	-1.41450700	-1.41427600	-0.22140200
F	0.17310800	0.46585000	-1.35665900
F	1.35189600	-1.34989800	-1.17264500
C	1.77366700	0.37117700	0.34831100
F	2.73854900	0.79470800	-0.45449400
F	2.30821100	-0.42413400	1.27823900
F	1.23194600	1.42253300	0.95759300
Cl	-2.75468600	1.58173400	-0.01190700

### P8a

0 2

C	0.06768300	0.46899600	-0.03101800
C	-1.12756300	-0.39932600	-0.06593000
H	-1.10488300	-1.34800500	-0.58941800
C	-3.44812800	-0.56662000	-0.01728700
H	-3.44242100	-1.37133600	0.72116400
H	-4.29795800	0.08841800	0.15333100
H	-3.49628600	-0.98306500	-1.02670300
O	-2.28259000	0.23596500	0.12656100
F	0.05280500	1.29417100	1.03847400
F	0.16337100	1.27391400	-1.13236900
C	1.36959100	-0.34935200	0.02704600
F	2.42881200	0.44556200	-0.01989500
F	1.42441500	-1.19413100	-1.00738400
F	1.42312600	-1.06350800	1.14920400

### CR8c

0 2

C	0.38319100	0.45829200	-0.87109500
C	0.19500400	-0.62936600	0.16727500
H	1.14236000	-0.78329800	0.69537200
H	-0.58272100	-0.33103700	0.87955600
C	-0.19824200	-2.92162700	0.23061600
H	0.69578000	-3.06135500	0.84662700
H	-1.09183400	-2.83068800	1.07382300
H	-0.47245300	-3.77988700	-0.37756100
O	-0.19620800	-1.79036100	-0.52544100

F	-0.75276900	0.66529200	-1.56101200
F	1.34791700	0.11219200	-1.74761400
C	0.79536200	1.80020600	-0.24030900
F	0.97389600	2.72345800	-1.17086400
F	1.93354500	1.64883200	0.44029200
F	-0.14613600	2.21484800	0.60545400
Cl	-2.14783900	-2.38039700	2.25503900

### TS8c

0 2

C	-0.73342200	1.22952000	-1.10097000
C	-0.94707200	0.15704100	-0.05159500
H	-0.00531300	-0.01134500	0.48086600
H	-1.72337100	0.47332000	0.65288400
C	-1.30174900	-2.14390600	-0.01341000
H	-0.42071000	-2.26273600	0.62226300
H	-2.27790300	-2.04932500	0.95294800
H	-1.60623000	-3.00302300	-0.60307100
O	-1.35819000	-1.00540900	-0.73638400
F	-1.85969400	1.44488000	-1.80349700
F	0.23367900	0.85720900	-1.96400100
C	-0.30622800	2.57198900	-0.48143200
F	-0.10211000	3.48065500	-1.42067700
F	0.82149700	2.40923800	0.21373600
F	-1.25024800	3.01140500	0.34859000
Cl	-3.24585800	-1.67329800	2.03206100

### PC8c

0 2

C	-0.79976400	0.39956800	-0.37998300
C	0.33869100	0.70140500	0.57316400
H	-0.05830300	1.22682400	1.44815200
H	0.80727400	-0.24026400	0.87700100
C	2.35835600	1.85816600	0.55807100
H	2.31316300	1.84705300	1.64254900
H	3.30702300	-0.08169700	0.06884400
H	2.98738800	2.56063000	0.03111800
O	1.24964200	1.51296300	-0.12920600
F	-0.34883700	-0.23107500	-1.47903200
F	-1.40935800	1.53734700	-0.77021800
C	-1.87272000	-0.49794700	0.26150000
F	-2.85846500	-0.73668900	-0.58838300
F	-2.37432900	0.09877800	1.34532600

F	-1.33474100	-1.65810300	0.63559300
Cl	3.26061900	-1.36916000	-0.08235800

**P8c**

0 2

C	-0.01376700	0.42062600	0.01672100
C	1.14079300	-0.55536600	-0.08421000
H	1.09026200	-1.24631300	0.76526800
H	1.05351200	-1.11574300	-1.02096300
C	3.45862900	-0.53961900	-0.03299900
H	3.41549500	-1.52262100	0.42398300
H	4.35640900	0.05761900	-0.00415100
O	2.32166100	0.19885800	-0.05553500
F	0.00454000	1.29486700	-1.00786000
F	0.05072100	1.12263800	1.16550700
C	-1.38031700	-0.28657500	-0.00946100
F	-2.36895300	0.58866700	0.08113300
F	-1.47064800	-1.14300500	1.00989800
F	-1.51799100	-0.97407800	-1.14425200



**Cartesian Coordinates of all the species involved in the reaction of product radical (P1a)**

**AIM1a**

0 1

C	0.36596500	-0.62732200	-0.08154000
C	-0.93090700	0.06659600	0.33773200
H	-0.90374000	0.24150600	1.41743100
C	-2.04931600	2.10766900	0.07486600
H	-3.04012300	1.66472000	-0.04548100
H	-1.87651700	2.35945300	1.12591800
H	-1.96556800	3.00158400	-0.53713000
O	-1.04689300	1.21159200	-0.38823200
F	0.31799300	-1.05223100	-1.35009200
F	0.56806300	-1.68884900	0.72213800
C	1.60408500	0.29030000	0.06097300
F	2.71177300	-0.44153200	0.02677200
F	1.55510100	0.92521700	1.23721600
F	1.66499000	1.18877600	-0.90764800
Cl	-2.30230300	-1.08034500	0.07279200

**AIM2a**

0 2

C	0.42613000	-0.61597000	-0.19136000
C	-0.93285800	-0.03557000	0.20018600
H	-1.03886500	-0.00326600	1.29067400
C	-2.24883800	1.88759800	-0.01012600
H	-3.15044500	1.37162000	-0.34609000
H	-2.27015400	2.00054300	1.07768400
H	-2.18136700	2.86240700	-0.48522000
O	-1.08154600	1.17081000	-0.40851000
F	0.47929600	-0.88139300	-1.50338400
F	0.60074400	-1.76600100	0.48770500
C	1.60794300	0.31429400	0.16142800
F	2.74589200	-0.36680200	0.11186800
F	1.44606600	0.78071800	1.40370800
F	1.69001800	1.33648600	-0.67337500
O	-1.91303200	-0.98756100	-0.27557900
O	-2.89686800	-1.11581200	0.56702500

### AIM3a

0 1

C	-0.95622900	-0.48827600	0.41007200
C	0.15743100	0.49525500	0.03217500
H	0.50527200	0.28008200	-0.98674000
C	0.54977200	2.79268600	-0.24515100
H	1.40011800	2.86695500	0.43522500
H	0.90642100	2.60232100	-1.26244700
H	-0.02577700	3.71407200	-0.22116200
O	-0.33634900	1.75830000	0.17158200
F	-1.22521300	-0.42777200	1.72221100
F	-0.55031500	-1.73377100	0.11081500
C	-2.27128000	-0.23535500	-0.36328100
F	-3.06068600	-1.29771800	-0.25862000
F	-1.99166400	-0.04187100	-1.65643700
F	-2.92147800	0.81852000	0.09925700
O	1.22434100	0.20921500	0.93749700
O	2.42920200	0.54579100	0.34330300
N	3.04584800	-0.65182200	-0.24128700
O	2.39685200	-1.63707000	-0.24712100
O	4.13083800	-0.39411500	-0.63448400

### AIM4a

0 2

C	0.33197900	0.69091600	0.07956000
C	-1.13141800	0.42441500	-0.33328300
H	-1.12853600	0.27836600	-1.43758800
C	-2.83567600	-1.16148100	-0.05206400
H	-3.59325800	-0.40214000	0.14985400
H	-2.84092200	-1.41783900	-1.11728300
H	-3.03939600	-2.05171300	0.53715600
O	-1.54801300	-0.70565300	0.33905200
F	0.39276800	1.12401200	1.34794100
F	0.82713900	1.64946900	-0.72265600
C	1.24983000	-0.54456600	-0.05476400
F	2.52227300	-0.16136100	-0.02748100
F	1.01562000	-1.14136200	-1.22790900
F	1.05387500	-1.41516100	0.91974200
O	-1.87589400	1.53530800	-0.16099800

### AIM4a-TS1

0 2

C	0.32179500	0.71147300	0.20191200
C	-1.29852500	0.44920200	-0.76381800
H	-0.79842400	0.57418700	-1.73879700
C	-2.45866400	-1.15850600	0.50646700
H	-2.07097600	-0.75464900	1.44457500
H	-3.44054800	-0.72672000	0.31142500
H	-2.51772700	-2.24210100	0.55833000
O	-1.56555600	-0.87087800	-0.57005700
F	0.04845900	0.79524200	1.48906600
F	0.82494300	1.84261100	-0.25017000
C	1.27215800	-0.46450800	-0.07645100
F	2.50421600	-0.14262000	0.31918000
F	1.30642600	-0.72660300	-1.37800700
F	0.88896400	-1.54368500	0.58571900
O	-1.97819200	1.35823000	-0.26447900

### AIM4a-PC1

0 2

C	0.68953700	0.79272100	0.34240000
C	-2.14870300	0.31306100	-0.85940300
H	-1.97963500	0.31047700	-1.94322900
C	-2.11464400	-1.04403900	1.04655300
H	-1.50392600	-0.33040600	1.60147800
H	-3.16456100	-0.87104300	1.28299400
H	-1.82511300	-2.06304700	1.28530900
O	-1.89911500	-0.89900200	-0.36201200
F	0.93769400	0.97351400	1.62077900
F	0.93769500	1.86747600	-0.36779300
C	1.30457200	-0.46974900	-0.22394900
F	2.64004000	-0.42172600	-0.18286800
F	0.93439800	-0.62131800	-1.48996900
F	0.90747700	-1.52142600	0.48437500
O	-2.49176700	1.26317600	-0.21809600

### AIM5a

0 2

C	0.86559000	0.00004700	-0.37381900
F	1.49803000	1.08935200	-0.00061400
F	1.49785600	-1.08935700	-0.00050700
C	-0.60689900	0.00006400	-0.02069600
F	-0.78845200	-0.00048600	1.30343600
F	-1.18991500	-1.08315200	-0.52010400
F	-1.18997900	1.08356900	-0.51920100

### AIM6a

0 1

C	0.82724000	0.43210700	-0.00002200
H	1.41679800	1.35690500	0.00000200
C	-1.35590700	-0.39797500	-0.00003000
H	-1.18861400	-1.00745000	-0.88813400
H	-1.18866400	-1.00750700	0.88807500
H	-2.36040500	0.01505800	0.00012900
O	-0.47223700	0.72796900	0.00001200
O	1.28384800	-0.67319300	0.00001800

### AIM4a-TS2

0 2

C	-0.34068300	0.68751000	-0.12536800
C	1.16719700	0.46354600	0.16647600
H	0.91601100	0.27956700	1.79913000
C	2.92396800	-1.05508400	-0.07428100
H	3.46342800	-0.41099800	-0.76770200
H	3.28048600	-0.87682800	0.94213600
H	3.03599200	-2.10081300	-0.34316400
O	1.51930400	-0.78670200	-0.14554500
F	-0.45644700	1.07207800	-1.41045800
F	-0.79054300	1.67721800	0.65569700
C	-1.26606100	-0.53323700	0.07632000
F	-2.53258400	-0.14085000	-0.01431000
F	-1.07498800	-1.06196700	1.28532200
F	-1.04859700	-1.46239100	-0.84145800
O	1.92144500	1.40868600	0.27524200

### AIM4a-PC2

0 2

C	-0.34071200	0.65346100	-0.26845500
C	1.10300300	0.42735800	0.23183400
H	1.03096000	-1.98960700	1.53964100
C	3.11423700	-0.65525200	-0.21958200
H	3.69463800	0.26580000	-0.17639900
H	3.12568100	-1.14059400	0.75696200
H	3.49224100	-1.31998300	-0.98972500
O	1.76142700	-0.35933000	-0.59829300
F	-0.37061100	0.77402300	-1.60606300
F	-0.82100800	1.77545600	0.27906500
C	-1.28770400	-0.49944200	0.12118500
F	-2.51837800	-0.23826500	-0.29719300
F	-1.30356500	-0.64431700	1.44296700
F	-0.88045700	-1.63926600	-0.42927600
O	1.50978500	0.90669900	1.24505800

### AIM7a

0 1

C	0.34048700	0.63314300	0.30403600
C	-1.12968500	0.48083800	-0.14540800
C	-3.03013500	-0.85432700	0.06009100
H	-3.65232400	-0.02155600	0.38581200
H	-3.12312700	-0.98218300	-1.01783100
H	-3.29450600	-1.76653100	0.58534200
O	-1.65859700	-0.59858900	0.40209000
F	0.41223300	0.66823000	1.64760300
F	0.82666600	1.77685400	-0.18489000
C	1.24705800	-0.51331300	-0.19255000
F	2.52102300	-0.20923600	0.01615800
F	1.05514300	-0.68967200	-1.50019600
F	0.97194800	-1.64744200	0.43615700
O	-1.66384200	1.24904200	-0.88256900

### AIM4a-TS3

0 2

C	-0.08150800	-0.67084900	-0.01546600
C	1.04533800	-0.54839700	-1.06433200
H	0.66574000	-0.31196100	-2.06671900

C	2.50973800	1.26043500	0.36747900
H	2.16676100	0.68743800	1.22984300
H	3.55362300	1.05033800	0.13296300
H	2.40683600	2.33270800	0.58364800
O	1.68852800	1.08391900	-0.75619400
F	0.41280000	-0.98623200	1.18994000
F	-0.87432000	-1.68423200	-0.43278500
C	-0.98623000	0.56829500	0.14681500
F	-2.13025200	0.22939700	0.72898500
F	-1.25749800	1.08793100	-1.05058100
F	-0.40255500	1.49873100	0.89763800
O	2.09037200	-1.18344200	-0.88984800

### AIM4a-PC3

0 2

C	-0.86468400	0.68047400	0.04528400
C	0.42996000	1.35915400	0.54645500
H	0.62595400	1.22763100	1.62104200
C	3.05158100	-0.38283100	-0.36778900
H	2.54912700	0.16327000	-1.17419400
H	3.82555800	0.28824400	0.04686700
H	3.56557100	-1.27993400	-0.72916400
O	2.22009600	-0.65931300	0.68613000
F	-1.20793500	1.16286800	-1.15292800
F	-1.84346000	0.96882400	0.93349800
C	-0.78600100	-0.85151300	-0.06491100
F	-1.95497000	-1.34315100	-0.45715500
F	-0.47509000	-1.37872100	1.11366800
F	0.13906300	-1.19830800	-0.95833300
O	1.09617500	2.01749600	-0.18957300

### AIM8a

0 1

C	-0.41346000	0.49084800	0.00836000
C	-1.56754200	-0.34111300	-0.58929600
H	-1.58510900	-0.36774900	-1.69238400
F	-0.68817200	0.85332200	1.26314100
F	-0.25292400	1.59666200	-0.75027400
C	0.91902500	-0.27683800	0.00207500
F	1.90935800	0.48560600	0.43707100
F	1.19050400	-0.66947800	-1.24485200
F	0.82499600	-1.35281900	0.77388600

O	-2.36211200	-0.88615800	0.10685000
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**AIM9a**

0 2

C	2.51975100	1.40754700	0.43603900
H	2.41866900	0.47333800	1.00133100
H	3.53856300	1.41734000	0.00889000
H	2.43917900	2.28640600	1.08667000
O	1.67876600	1.46921800	-0.64127900

**O2**

0 3

O	0.00000000	0.00000000	0.59443000
O	0.00000000	0.00000000	-0.59443000

**NO**

0 2

N	1.43854100	2.05140700	-0.06351700
O	0.30016900	2.05140700	-0.06351700

**NO2**

0 2

O	0.25132700	2.45133500	1.30347100
N	1.24821800	3.06640400	1.45614100
O	1.51783700	4.21505800	1.51097800

**Cartesian Coordinates of all the species involved in the reaction of product radical AIM5a**

**SIM1**

0 2

C	-0.09832000	0.53038200	0.00000000
F	0.24847500	1.21556700	1.07994100
F	0.24847500	1.21556700	-1.07994100
C	0.59600400	-0.84810400	0.00000000
F	1.90882700	-0.66960700	0.00000000
F	0.24847500	-1.53013200	-1.08095800
F	0.24847500	-1.53013200	1.08095800
O	-1.48474500	0.28723700	0.00000000
O	-2.15408600	1.41213200	0.00000000

**SIM2**

0 1

C	0.48795800	-0.48599800	-0.15534800
F	-0.01785300	-0.17795000	-1.35037200
F	0.74607400	-1.79176000	-0.14228900
C	1.79228700	0.30911200	0.07921300
F	2.66842900	-0.02392600	-0.85808600
F	2.29552000	0.01752500	1.26927600
F	1.55090600	1.60833300	0.00863200
O	-0.37566400	-0.13396900	0.86330600
O	-1.60692200	-0.72672700	0.62228800
N	-2.52540900	0.28679400	0.04355200
O	-2.08730400	1.36528100	-0.12272500
O	-3.57902200	-0.20911500	-0.13693100

**SIM3**

0 2

C	-0.81051800	0.00000000	0.08548600
F	-1.27403100	1.08100600	-0.55933000
F	-1.27403100	-1.08100700	-0.55933000
C	0.75407800	0.00000000	-0.01478800
F	1.08821700	0.00000000	-1.29404000
F	1.24752400	-1.08073600	0.56786100
F	1.24752400	1.08073600	0.56786000
O	-1.12227400	0.00000000	1.38357700



### **SIM3-TS1**

0 2

C	-0.69181500	-0.33802400	0.25770200
F	-1.47798900	1.09632300	-0.61048800
F	-1.04124200	-1.33869200	-0.51619800
C	0.78124900	0.05554800	0.01069900
F	1.02979000	0.17222400	-1.28250800
F	1.54968800	-0.91327900	0.50903200
F	1.05993400	1.18748900	0.62412600
O	-1.32727800	-0.01771700	1.23423900

### **SIM4**

0 1

C	0.94607500	0.15640100	-0.00002000
F	1.49716900	-1.05001500	-0.00003500
C	-0.58823500	0.01759400	-0.00009900
F	-0.98047900	-0.65239700	1.08020300
F	-0.98040300	-0.65255200	-1.08002300
F	-1.15381600	1.20973500	-0.00014300
O	1.55134000	1.15788700	0.00008600

### **SIM3-TS2**

0 2

C	0.11525300	1.04502300	0.00000000
F	-0.62646700	1.32563700	-1.07329500
F	-0.62646700	1.32563700	1.07329500
C	0.03339100	-0.88086000	0.00000000
F	-0.62646700	-1.20538900	-1.07980600
F	-0.62646700	-1.20538900	1.07980600
F	1.22869900	-1.39678900	0.00000000
O	1.32533200	1.17770800	0.00000000

### **SIM5**

0 2

C	0.27553600	0.17610100	0.00000000
F	0.27553600	-0.56645200	1.08379200
F	0.27553600	-0.56645200	-1.08379200
F	-0.73476200	1.01550400	0.00000000

## CF<sub>2</sub>O

0 1

C	-0.00044400	0.14284200	0.00000000
F	-0.00044400	-0.62935500	1.05882100
F	-0.00044400	-0.62935500	-1.05882100
O	0.00133200	1.30891800	0.00000000

**Cartesian Coordinates of all the species involved in the reaction of product radical (P1b)**

**AIM1b**

0 1

C	-0.73519000	0.74572300	0.01586200
C	0.42450600	0.56455300	0.98431400
H	1.12034100	1.39400100	0.82118000
H	0.02388000	0.61928700	1.99552600
C	1.87747600	-0.87565600	-0.22873600
H	2.21809000	-1.90469800	-0.19196300
H	1.39325200	-0.64272900	-1.17505800
O	1.05512000	-0.68587800	0.86907300
F	-0.29595500	0.98335800	-1.24418400
F	-1.45014500	1.82134200	0.40739600
C	-1.70020600	-0.45263500	-0.06683200
F	-2.80392000	-0.11582800	-0.72263600
F	-2.03666300	-0.84873300	1.15875500
F	-1.12802600	-1.47074700	-0.70636200
Cl	3.35507900	0.16498300	-0.15686100

**AIM2b**

0 2

C	-0.79610700	0.74895200	-0.00032200
C	0.48141100	0.64543300	0.81844400
H	1.08732300	1.53040100	0.60028500
H	0.20521700	0.64951100	1.87203100
C	1.97343400	-0.58676400	-0.55063200
H	2.36057200	-1.59860400	-0.64235000
H	1.46208400	-0.24278000	-1.45121100
O	1.17791400	-0.55582400	0.58313700
F	-0.52593000	1.02144400	-1.30114200
F	-1.53248100	1.76948500	0.48560000
C	-1.67619700	-0.51656600	0.01555600
F	-2.87762900	-0.24966900	-0.48233600
F	-1.81985700	-0.95153800	1.26562500
F	-1.12459100	-1.48084400	-0.71626400
O	3.08643200	0.31755500	-0.41719400
O	3.97489900	-0.14482500	0.41650900

**AIM3b**

0 1

C	-1.60510900	-0.18091400	-0.66353400
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C	-0.13997400	0.21556000	-0.65357100
H	0.34137200	-0.25365100	-1.51641700
H	-0.06522000	1.29732900	-0.75962800
C	1.07490700	-1.39912200	0.57724900
H	1.29801000	-1.63045400	1.61713300
H	0.47229400	-2.17599400	0.10109600
O	0.47404600	-0.14828300	0.56283300
F	-1.73507700	-1.52995400	-0.61385800
F	-2.15465500	0.24670200	-1.81908900
C	-2.45135900	0.39314800	0.48977500
F	-3.74322600	0.19183200	0.25540500
F	-2.23779700	1.70516700	0.59158500
F	-2.13984800	-0.18231000	1.64470000
O	2.27318900	-1.41864500	-0.18772900
O	3.21768900	-0.65071900	0.48340500
N	3.30934400	0.66899700	-0.10658700
O	2.64388800	0.89306800	-1.06077800
O	4.09278300	1.32768300	0.48673500

#### AIM4b

0 2

C	-0.38399500	0.74407500	0.01752300
C	0.77923800	0.60902200	0.98813200
H	1.43499000	1.47138400	0.83088000
H	0.37609200	0.64197700	1.99980400
C	2.34501400	-0.70368700	-0.24294500
H	2.84399600	-1.67810800	-0.13559200
H	1.79333400	-0.72419500	-1.20479500
O	1.45971800	-0.60969900	0.85292000
F	0.05831600	0.97068700	-1.24554500
F	-1.13370900	1.80484900	0.38352600
C	-1.31236400	-0.48354100	-0.05416900
F	-2.42832300	-0.18496400	-0.70977600
F	-1.63538000	-0.88214600	1.17424700
F	-0.71314700	-1.48870400	-0.68944300
O	3.24708400	0.27422900	-0.34774800

#### AIM4b-TS1

0 2

C	-0.34494600	0.65427400	0.08178700
C	0.80900700	0.24730800	0.98276000
H	1.46278400	1.11617200	1.07619500
H	0.41731600	-0.04464600	1.95669400

C	2.68460500	-0.60303200	-0.18500500
H	3.69770600	-1.01769500	1.04359200
H	3.02311900	-1.52132200	-0.68368200
O	1.49101000	-0.85976500	0.42906000
F	0.09870200	0.97210500	-1.14870700
F	-0.93015100	1.74650900	0.62156100
C	-1.44897700	-0.40668400	-0.08862000
F	-2.48039600	0.10250800	-0.75132900
F	-1.87293400	-0.80804300	1.11219300
F	-0.99829800	-1.46350600	-0.75333800
O	3.11506900	0.50603200	-0.41177900

### AIM5b

0 1

C	-0.29813600	0.65616600	0.04770100
C	0.84173900	0.28952600	0.98219500
H	1.51039000	1.15002100	1.03168400
H	0.44095200	0.05639800	1.96748600
C	2.68249800	-0.66279400	-0.14906300
H	3.06609200	-1.63221800	-0.48442700
O	1.51342900	-0.86052700	0.49924800
F	0.16489500	0.89446300	-1.19443600
F	-0.87287200	1.78581400	0.51478800
C	-1.41446000	-0.39881300	-0.07363300
F	-2.43418200	0.08658400	-0.77074400
F	-1.85125300	-0.72939800	1.14371600
F	-0.97158800	-1.49497800	-0.67715500
O	3.21128500	0.39039200	-0.31218000

### AIM4b-TS2

0 2

C	-0.71996400	0.79509500	0.66850300
C	0.55333600	0.02444500	0.98041200
H	1.38596500	0.66027100	0.67045000
H	0.59844000	-0.15845500	2.05441000
C	1.33747400	-1.30301000	-0.84616200
H	2.38557300	-1.87897000	-0.46258500
H	0.93468200	-2.12748200	-1.45995100
O	0.55319800	-1.21323100	0.31243700
F	-0.83820100	1.01345100	-0.65527300
F	-0.65157700	1.99264300	1.29359900
C	-2.02326900	0.12112600	1.13770500
F	-3.05302100	0.94519800	0.97807000
F	-1.92728100	-0.18824500	2.43336000

F	-2.26314000	-0.99072600	0.45392700
O	1.82599400	-0.28677700	-1.39152000
O	3.82708200	-1.73521900	-0.06780900
O	4.14748600	-0.62965100	-0.40093700

## AIM6b

0 1

C	-0.72402100	0.89177400	0.27460400
C	0.55278900	0.11150400	0.53593000
H	1.38705800	0.73869700	0.21870100
H	0.62597400	-0.11801300	1.59788600
C	1.23634500	-1.17110000	-1.32461400
H	1.09824800	-2.16075600	-1.77281400
O	0.52684300	-1.11301000	-0.17603100
F	-0.87251300	1.13008000	-1.04264200
F	-0.62740600	2.07652100	0.91626600
C	-2.01881700	0.21860800	0.76812200
F	-3.04795800	1.04637800	0.63823500
F	-1.89183100	-0.10237900	2.05765100
F	-2.27401800	-0.88719100	0.07953400
O	1.90916800	-0.29423500	-1.76492700

## HOO

0 2

H	3.50440800	-2.11504000	-1.22230600
O	3.89320500	-1.71172600	-0.42654500
O	4.25700600	-0.50312900	-0.7672170