

Supporting Information

Manuscript Title:

The Pincer Ligand Supported Ruthenium Catalysts for Acetylene Hydrochlorination: Molecular Mechanisms from Theoretical Insights

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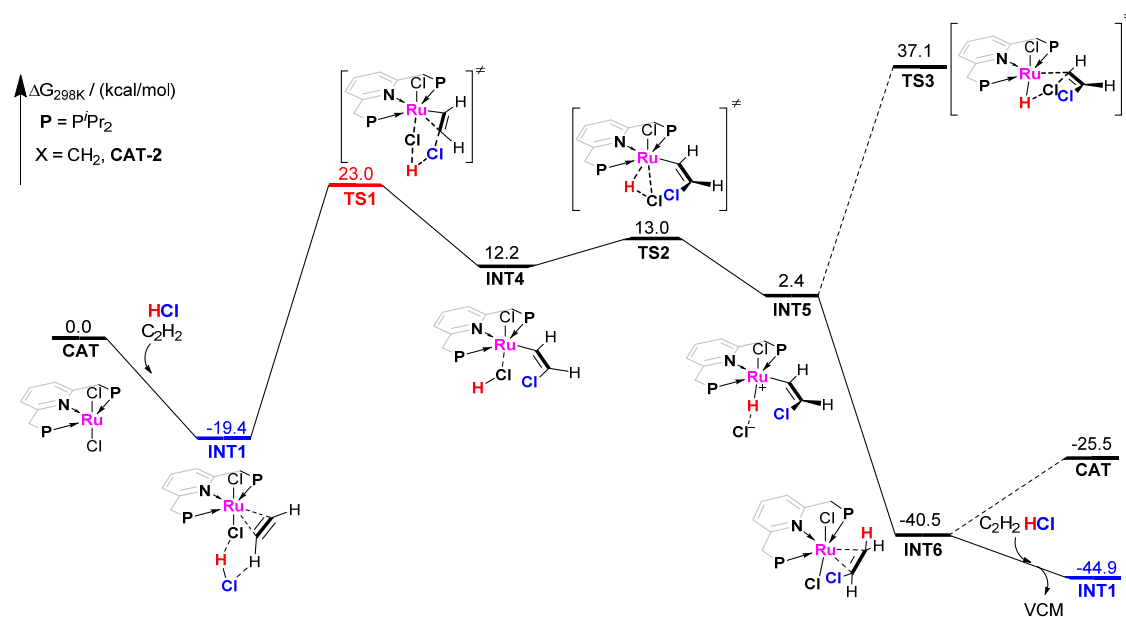


Figure S1. The Gibbs free energy profile for molecular complex **CAT-2** catalyzed acetylene hydrochlorination mechanism *pathway-1*.

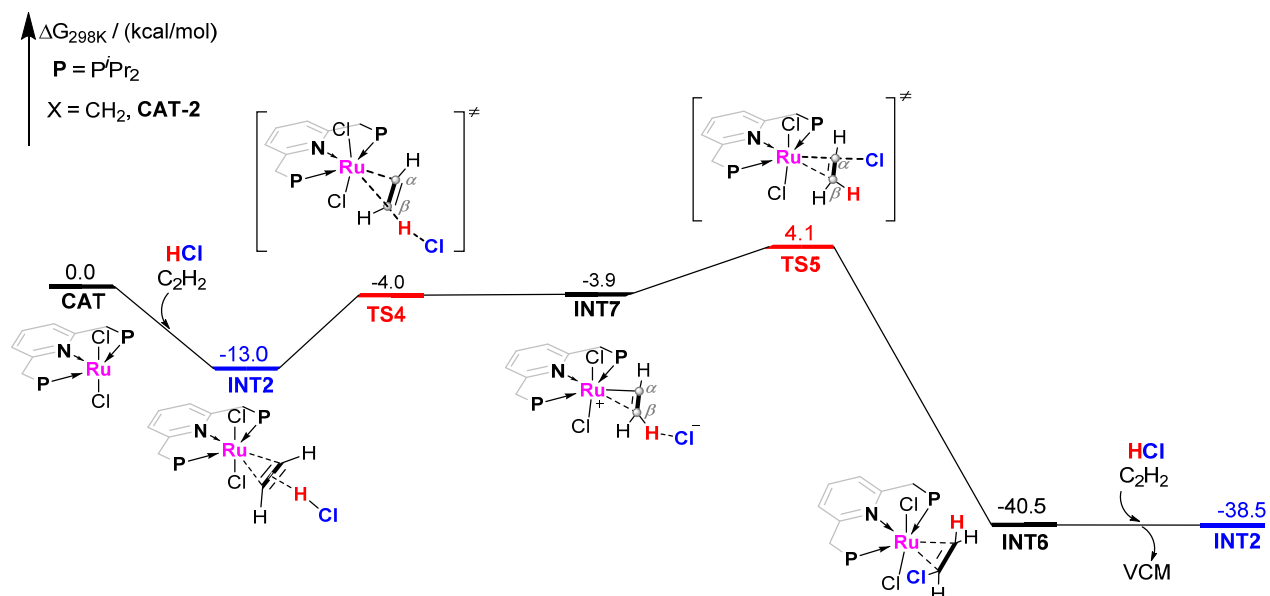


Figure 2. The Gibbs free energy profile for molecular complex **CAT-1** catalyzed acetylene hydrochlorination mechanism *pathway-2*.

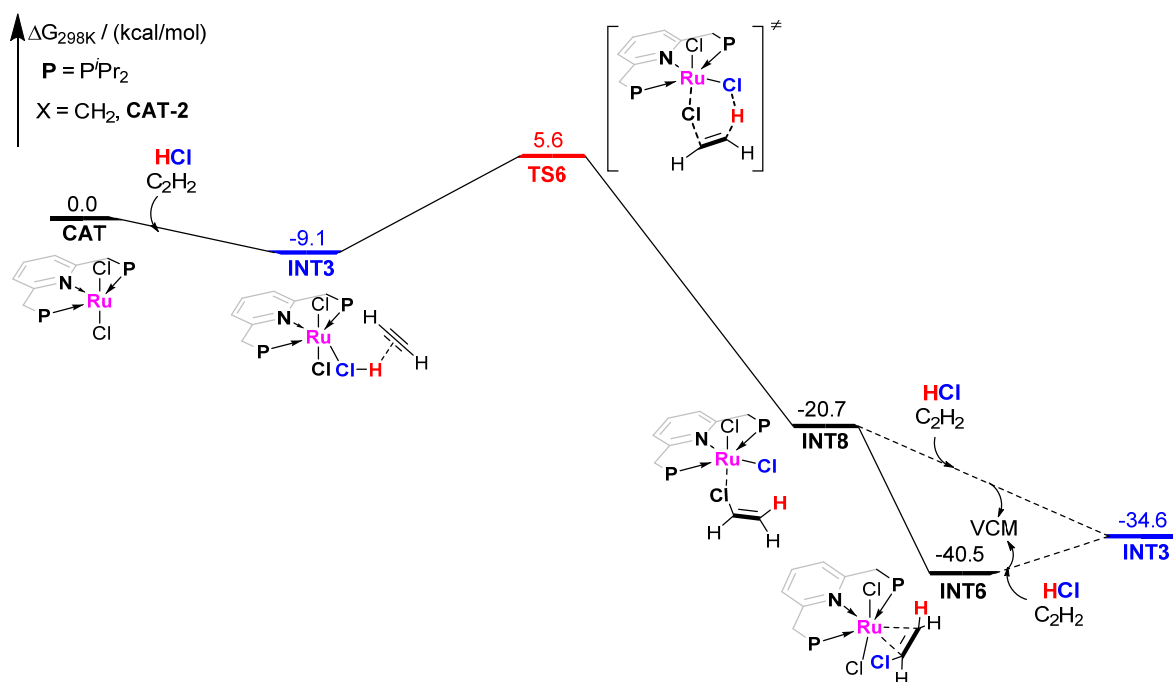


Figure S3. The Gibbs free energy profile for molecular complex **CAT-2** catalyzed acetylene hydrochlorination mechanism *pathway-3*.

The xyz coordinates for intermediates and transition states (unit: Angstrom)

1. For CAT-1

CAT-1

```

Ru -0.00000900 -0.56769000 0.09728000
Cl -0.00006500 -1.44317700 -2.14949700
P 2.29675600 -0.26735500 -0.02390700
P -2.29678900 -0.26733600 -0.02393900
O 2.32054800 1.42294600 -0.35728600
O -2.32053700 1.42284800 -0.35792400
N 0.00000400 1.40525800 -0.34752200
C 1.17008100 2.08788900 -0.47987700
C 1.20546700 3.45760900 -0.74302900
H 2.17519300 3.94403100 -0.83625000
C 0.00001900 4.14264400 -0.87334900
H 0.00002500 5.21515200 -1.07793900
C -1.20543600 3.45756000 -0.74334900
  
```

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 C -1.17006400 2.08784100 -0.48019200
 C 3.24439900 -0.86403400 -1.49885000
 H 2.51772100 -0.70768200 -2.31180600
 C 4.51939000 -0.07145700 -1.79155200
 H 5.29344300 -0.23293200 -1.02402900
 H 4.32120000 1.00766700 -1.85670800
 H 4.94311000 -0.39989600 -2.75452100
 C 3.49171000 -2.37250100 -1.38731700
 H 3.89842700 -2.75047000 -2.33871600
 H 2.55809600 -2.91892700 -1.18734100
 H 4.22289600 -2.61117900 -0.59852300
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 H 4.49465700 -0.41640600 0.94059100
 C 3.23283800 -1.67426000 2.16635400
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 H -4.14831900 0.73496700 3.13651800
 H -3.68206200 1.78150000 1.77030900
 H -2.42309600 0.96859300 2.74326100
 C -3.23302200 -1.67353700 2.16673200
 H -2.25588200 -1.63167700 2.66831600
 H -3.24848700 -2.55829400 1.51203600
 H -4.01446000 -1.81266600 2.93113500
 C1 0.00009600 -0.15084800 2.47967000

CAT-1 + C₂H₂

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 P -2.29983600 -0.18669600 -0.06777700
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 H -0.00001400 5.40352400 -0.26574200
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 H 4.31335100 1.36360600 -1.69964400
 H 4.99760800 0.08904200 -2.73945300
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 H 3.99675900 -2.32267300 -2.63449300
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 C -4.54140300 0.29023800 -1.75628100
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CAT-1 + HCl

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 Cl 0.16875198 0.10368038 2.39737288

INT3

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 O 2.49030500 -1.55519200 -0.44393100
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 H 4.18976100 -1.17378600 3.13733700
 H 3.77836000 -2.09457400 1.66796000
 H 2.47762100 -1.44651000 2.70616500
 C 3.17392500 1.28092100 2.40016300
 H 2.20137400 1.13906700 2.89277600
 H 3.13253400 2.22273400 1.82928900
 H 3.94826700 1.39560400 3.17548000
 Cl -0.18889800 2.50858200 1.23400700
 H -0.37911200 3.34772600 0.23341100
 Cl 0.05230900 -0.59289500 2.50099300
 C -0.69851400 4.26143400 -1.60937200
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 C -0.86908500 5.27022700 -0.95799600

H -1.02299200 6.17054600 -0.39128600

INT4

Ru 0.00001500 0.19080700 0.17383700
Cl 0.00009200 0.19796000 2.70484300
P 2.27412600 -0.17755200 0.10307900
P -2.27389000 -0.17844900 0.10316400
O 2.31034900 -1.91663000 -0.00252500
O -2.30945600 -1.91755000 -0.00188800
N 0.00046200 -1.94960000 0.01423500
C 1.16970300 -2.61186300 -0.10644800
C 1.21365000 -3.99293000 -0.31920300
H 2.17803000 -4.49074800 -0.40935500
C 0.00095500 -4.67582800 -0.42153600
H 0.00114400 -5.75458500 -0.59327900
C -1.21200400 -3.99340700 -0.31892700
H -2.17620000 -4.49161400 -0.40887500
C -1.16853500 -2.61234600 -0.10615500
C 3.30609000 0.00813900 1.64109800
H 2.63834500 -0.36410500 2.43487500
C 4.58853700 -0.82569100 1.66818700
H 5.31937500 -0.47663900 0.92229700
H 4.38436000 -1.88822500 1.47491400
H 5.06850000 -0.73981000 2.65700400
C 3.55850400 1.49984400 1.89510300
H 3.99731300 1.64510100 2.89509000
H 2.63140600 2.08993900 1.83641700
H 4.26691300 1.91525600 1.16146000
C 3.44332400 0.28761300 -1.27265000
H 4.44748300 0.26270200 -0.81852900
C 3.13737900 1.72387600 -1.72109500
H 3.92786900 2.06875200 -2.40713600
H 3.08218700 2.43032900 -0.88037400
H 2.17216100 1.76041900 -2.24123400
C 3.42151000 -0.70442700 -2.44027800
H 2.41904600 -0.75529200 -2.88695300
H 3.71745600 -1.71383500 -2.12204600
H 4.13012500 -0.36522500 -3.21364200
C -3.30588400 0.00734100 1.64117100
H -2.63794500 -0.36442600 2.43500500
C -4.58801300 -0.82697000 1.66857300
H -5.06795000 -0.74099000 2.65739400
H -4.38346000 -1.88948300 1.47558000
H -5.31904000 -0.47840300 0.92264000
C -3.55885500 1.49900800 1.89477600

H -4.26740600 1.91396400 1.16101200
 H -2.63199200 2.08945700 1.83596700
 H -3.99775200 1.64435400 2.89471300
 C -3.44334200 0.28580500 -1.27265700
 H -4.44744900 0.26046200 -0.81844600
 C -3.42109200 -0.70652700 -2.44002500
 H -4.12995300 -0.36790800 -3.21341800
 H -3.71647600 -1.71601500 -2.12151700
 H -2.41863800 -0.75697400 -2.88677300
 C -3.13826700 1.72210500 -1.72157400
 H -2.17327800 1.75898600 -2.24211900
 H -3.08304700 2.42881700 -0.88107300
 H -3.92919900 2.06641500 -2.40738900
 C -0.00108100 3.16995900 -0.62980800
 H -0.00121500 2.95460100 -1.69876500
 C -0.00057700 2.25719200 0.34178500
 H -0.00048700 2.68497900 1.36224100
 Cl -0.00163400 4.92701600 -0.32173000
 H 0.00002900 -1.05989300 3.02457400
 Cl -0.00003700 0.20675200 -2.24129600

INT5

Ru 0.00000300 0.19188000 0.21812100
 Cl -0.00032100 0.68793100 2.70936700
 P 2.29420700 -0.19789700 0.18517500
 P -2.29428100 -0.19761100 0.18509300
 O 2.30456600 -1.92299800 -0.02292200
 O -2.30492800 -1.92270600 -0.02301300
 N -0.00019200 -1.96947600 -0.06291900
 C 1.17280400 -2.61374200 -0.19697200
 C 1.21488100 -3.97859200 -0.49463800
 H 2.17795900 -4.47482600 -0.60325400
 C -0.00034400 -4.64870000 -0.64311800
 H -0.00040400 -5.71500300 -0.88009800
 C -1.21549000 -3.97845100 -0.49465300
 H -2.17862500 -4.47457100 -0.60328600
 C -1.17325700 -2.61360000 -0.19699600
 C 3.24364100 -0.06903400 1.76539800
 H 2.51555200 -0.41271500 2.51775200
 C 4.49439000 -0.94607000 1.83271400
 H 5.26209900 -0.62544200 1.11052300
 H 4.26039800 -2.00193300 1.63633700
 H 4.94193600 -0.87382800 2.83718300
 C 3.52788200 1.41446700 2.03700900

H 3.91956500 1.53576800 3.05892500
 H 2.61440500 2.02134100 1.95261500
 H 4.28209600 1.81658800 1.34227500
 C 3.49651600 0.31269400 -1.14362800
 H 4.48281900 0.30024400 -0.65066100
 C 3.17961000 1.74674500 -1.58755700
 H 3.98971500 2.11580900 -2.23662200
 H 3.07504000 2.44221700 -0.74272600
 H 2.23757600 1.77160400 -2.14916200
 C 3.53581500 -0.66076400 -2.32634700
 H 2.55015400 -0.73025500 -2.80721800
 H 3.84705000 -1.66801500 -2.01760800
 H 4.25857300 -0.28964700 -3.07109100
 C -3.24391700 -0.06858700 1.76518200
 H -2.51595300 -0.41229900 2.51763800
 C -4.49474800 -0.94551800 1.83236400
 H -4.94243100 -0.87317600 2.83676600
 H -4.26081500 -2.00141200 1.63608700
 H -5.26232800 -0.62487100 1.11004400
 C -3.52808100 1.41494500 2.03670200
 H -4.28222600 1.81707900 1.34190300
 H -2.61456100 2.02175600 1.95234200
 H -3.91982100 1.53631800 3.05858800
 C -3.49629900 0.31318900 -1.14389400
 H -4.48269100 0.30095700 -0.65110200
 C -3.53558600 -0.66028000 -2.32660400
 H -4.25812100 -0.28902100 -3.07149400
 H -3.84710300 -1.66745500 -2.01790100
 H -2.54984800 -0.72999700 -2.80728700
 C -3.17897800 1.74715900 -1.58778600
 H -2.23682200 1.77179600 -2.14919600
 H -3.07441600 2.44262000 -0.74294500
 H -3.98886500 2.11640500 -2.23702000
 C 0.00040800 3.05845000 -0.92016200
 H 0.00047300 2.73775600 -1.96127800
 C 0.00024000 2.26044800 0.14438800
 H 0.00015700 2.73926900 1.13155000
 C1 0.00052100 4.82842000 -0.77954600
 H 0.00087300 -0.68860500 1.53321400
 C1 0.00020600 0.04828700 -2.20191700

INT6

Ru 0.04502100 -0.41881300 0.07023900
 C1 0.02924000 -0.47997300 -2.36962600

P 2.36648600 -0.19811200 -0.06509700
 P -2.21628700 0.22031600 0.07596400
 O 2.50438000 1.47868600 -0.38763800
 O -2.06224900 1.92947200 0.09855200
 N 0.22475100 1.70145700 -0.09644100
 C 1.43190200 2.26955700 -0.30833600
 C 1.59890400 3.64846400 -0.44972200
 H 2.60023700 4.04434200 -0.61053900
 C 0.46657800 4.45709700 -0.38281100
 H 0.56243900 5.53970100 -0.48934900
 C -0.78838800 3.88546700 -0.18986700
 H -1.70561600 4.47037200 -0.14728600
 C -0.86694000 2.49694200 -0.05947500
 C 3.31483100 -0.86038800 -1.52050900
 H 2.53093600 -0.93365100 -2.29064600
 C 4.40686400 0.09706600 -2.00760200
 H 5.18133000 0.26655400 -1.24139100
 H 3.99622100 1.07202800 -2.29828600
 H 4.90410500 -0.34363200 -2.88668600
 C 3.88256000 -2.25998700 -1.25332600
 H 4.28981300 -2.66585500 -2.19273900
 H 3.12509800 -2.96847700 -0.89318600
 H 4.70700400 -2.23610000 -0.52394200
 C 3.54821000 -0.30672600 1.37515900
 H 4.54860300 -0.27613500 0.90861500
 C 3.39252100 -1.62850000 2.13862100
 H 4.16413700 -1.68591700 2.92289500
 H 3.51440100 -2.51045700 1.49453200
 H 2.40693900 -1.67259600 2.62255000
 C 3.41164200 0.89941500 2.31291600
 H 2.39744300 0.95029900 2.73364900
 H 3.63484900 1.84356500 1.79809400
 H 4.12489800 0.78825900 3.14559500
 C -3.18612200 -0.03395200 -1.50749400
 H -2.60121600 -0.82786600 -1.99205600
 C -3.10859300 1.20477200 -2.40624600
 H -3.57882200 0.96807100 -3.37414800
 H -2.06577600 1.48515900 -2.60632300
 H -3.63546100 2.06574200 -1.96837400
 C -4.62241400 -0.52596200 -1.32501800
 H -5.27738000 0.24503800 -0.88940600
 H -4.68006600 -1.42819800 -0.70005700
 H -5.03685600 -0.78572900 -2.31230700
 C -3.41639700 0.07024900 1.49822100

H -4.39233400 0.31460600 1.05152900
 C -3.13520500 1.08271400 2.61532100
 H -3.87919500 0.93882900 3.41598700
 H -3.21473900 2.11720600 2.25669600
 H -2.13334400 0.93009600 3.03847500
 C -3.46830400 -1.36257200 2.04135400
 H -2.54863000 -1.58336500 2.60138100
 H -3.58982800 -2.11783000 1.25161100
 H -4.31988500 -1.45861500 2.73300300
 C 0.60567500 -2.54878800 0.09471000
 C -0.76636700 -2.43514500 0.32467700
 H -1.16378100 -2.52264400 1.33345900
 Cl 0.09043700 -0.32339600 2.51452000
 H 0.94590300 -2.87762100 -0.88921300
 H 1.24883800 -2.76017600 0.94899800
 Cl -1.92027700 -3.10039900 -0.86020700

INT7

Ru	0.14617400	-0.47040600	0.12803300
Cl	0.07688800	-0.79809500	-2.26971000
P	2.45818200	-0.39575700	-0.07518500
P	-2.15402500	0.25254100	0.02033100
O	2.73313600	1.25300500	-0.39550200
O	-1.80895800	1.97399600	-0.01174900
N	0.44947000	1.60269800	-0.26676400
C	1.69314400	2.10346300	-0.44022400
C	1.94075200	3.45758400	-0.64796900
H	2.96533300	3.79693000	-0.78738500
C	0.84371900	4.32328700	-0.65550900
H	0.99806300	5.39205400	-0.81686700
C	-0.44069300	3.83293700	-0.44982800
H	-1.32212800	4.47128600	-0.43635600
C	-0.60522500	2.45451200	-0.24472100
C	3.31050400	-1.07042700	-1.57703900
H	2.68821400	-0.63998500	-2.37911600
C	4.74816400	-0.55223800	-1.70522200
H	5.42603900	-1.03241800	-0.98151700
H	4.80386900	0.53712500	-1.56980100
H	5.12284200	-0.78988700	-2.71347300
C	3.22043900	-2.59639100	-1.69072600
H	3.80218200	-2.92436400	-2.56643300
H	2.18144400	-2.91503000	-1.85217900
H	3.63898400	-3.11249800	-0.81081700
C	3.58328400	-0.70951500	1.36888400
H	4.56755900	-0.93418900	0.92499700

C	3.09046700	-1.94325200	2.13979300
H	3.77773000	-2.14962100	2.97513100
H	3.06079300	-2.84526100	1.50890800
H	2.08678000	-1.75905400	2.55349800
C	3.71864900	0.52505200	2.27035500
H	2.74231600	0.80774300	2.68862900
H	4.13247500	1.38092900	1.71942400
H	4.40149300	0.28471600	3.10098400
C	-3.09218200	0.22528900	-1.60814900
H	-2.81417900	-0.76067400	-2.00656500
C	-2.60115800	1.31998400	-2.56238700
H	-3.03743800	1.12457200	-3.55521100
H	-1.50825800	1.30487200	-2.67630900
H	-2.92222000	2.32080200	-2.23709600
C	-4.61141200	0.26966900	-1.42959200
H	-4.94690100	1.21502400	-0.97215700
H	-4.95893600	-0.58483000	-0.83346700
H	-5.07948500	0.19786400	-2.42423400
C	-3.32944200	0.33293200	1.49096900
H	-4.32054000	0.31103700	1.01425400
C	-3.17789900	1.64555400	2.27697400
H	-3.89030700	1.61665600	3.11735500
H	-3.39650500	2.53200500	1.66853600
H	-2.16277800	1.73848500	2.68952200
C	-3.23381600	-0.86862300	2.43610900
H	-2.26946400	-0.86605300	2.96444300
H	-3.37804000	-1.81141700	1.89344900
H	-4.03345200	-0.77504500	3.18883400
C	0.44539300	-2.38692900	0.30351700
H	1.14686800	-3.10726600	-0.11098700
C	-0.72441300	-2.33661300	0.96065700
H	-0.81938900	-2.24379500	2.05162500
Cl	-3.36751600	-2.67566200	-0.42161600
H	-1.69271100	-2.68036300	0.42020500
Cl	0.20899300	0.18285100	2.44206900

INT8

Ru 0.02299100 -0.24389600 0.30040000
 Cl -0.05320900 -1.55804000 -1.89012200
 P 2.30857100 -0.02917000 0.04759800
 P -2.25684400 0.12404000 0.22703700
 O 2.34609500 1.38094600 -0.96481000
 O -2.28478200 1.54208600 -0.77304000
 N 0.02943900 1.45822500 -0.89458900
 C 1.20636600 2.00686800 -1.28419300

C 1.25542100 3.19450400 -2.01736500
 H 2.22431200 3.59600000 -2.31033500
 C 0.05168500 3.82302700 -2.33436000
 H 0.06039000 4.75524500 -2.90332400
 C -1.16256800 3.27528100 -1.92192100
 H -2.12259200 3.74125500 -2.13862500
 C -1.13531700 2.08583800 -1.19045500
 C 3.23103900 -1.19563500 -1.06390600
 H 2.53720600 -1.31569900 -1.91001700
 C 4.55819600 -0.66294500 -1.60617900
 H 5.32205700 -0.58147600 -0.81727900
 H 4.43726100 0.32608300 -2.07140500
 H 4.95297600 -1.35450100 -2.36861400
 C 3.36174800 -2.55328200 -0.36012200
 H 3.70019800 -3.31768200 -1.07790400
 H 2.40643300 -2.88245700 0.07786400
 H 4.10580900 -2.51070800 0.45092900
 C 3.53920000 0.41326600 1.37329400
 H 4.51608900 0.10132400 0.96957900
 C 3.23425800 -0.42047600 2.62726800
 H 4.04436100 -0.28151100 3.36155100
 H 3.15058900 -1.49444200 2.40772100
 H 2.28304000 -0.10626800 3.07587200
 C 3.60382100 1.91587200 1.66535100
 H 2.63970300 2.28136300 2.04362200
 H 3.87226300 2.49341400 0.76935300
 H 4.37173500 2.09860500 2.43499900
 C -3.33325200 -1.04245500 -0.78964700
 H -2.74898200 -1.97440200 -0.74420000
 C -3.41822900 -0.59563700 -2.25413600
 H -3.90266400 -1.38587900 -2.85064300
 H -2.42918600 -0.40235700 -2.68979700
 H -4.01517900 0.32290600 -2.35237400
 C -4.72471700 -1.34073600 -0.22471000
 H -5.38718700 -0.46283800 -0.27772900
 H -4.69147800 -1.68621200 0.81827500
 H -5.19255700 -2.14016300 -0.82222100
 C -3.31804400 0.70110300 1.64271500
 H -4.35770300 0.55849900 1.31417500
 C -3.13515300 2.18539100 1.97648400
 H -3.79863500 2.44301700 2.81856700
 H -3.40207000 2.82543200 1.12366300
 H -2.09984600 2.40093600 2.26886800
 C -3.03652000 -0.21933100 2.83953400

H -2.00271700 -0.08988400 3.18836800
 H -3.16457600 -1.28450300 2.59056900
 H -3.72879900 0.02260300 3.66196900
 Cl 0.17928900 1.24783800 2.16951400
 C -0.65458400 -3.22087400 -2.02172900
 H -0.86622500 -3.45399700 -3.06699700
 C -0.80554100 -4.02941500 -0.98155300
 H -1.18355200 -5.03919500 -1.16621900
 Cl 0.02968600 -2.20154800 1.75193800
 H -0.56946000 -3.70841500 0.04071100

TS1

Imaginary vibration: -330.39 cm⁻¹

Ru 0.03974000 -0.19436300 0.24671100
 Cl -0.05480800 -1.60264300 -2.02157100
 P 2.33090200 0.00639100 0.02811600
 P -2.23305000 0.28261000 0.07280200
 O 2.44532200 1.50324000 -0.82053600
 O -2.14958600 1.89223600 -0.55098800
 N 0.14236000 1.68328000 -0.73981900
 C 1.34195300 2.23088600 -1.03918000
 C 1.46418300 3.51777200 -1.56540500
 H 2.45569800 3.90453200 -1.79549900
 C 0.30001300 4.26202000 -1.75466900
 H 0.36149100 5.27463500 -2.15898900
 C -0.94003700 3.72405500 -1.41529400
 H -1.87248900 4.27500100 -1.52821700
 C -0.97543600 2.42716000 -0.89729500
 C 3.25707900 -1.03344100 -1.20719500
 H 2.59445600 -0.98801300 -2.08601900
 C 4.62155600 -0.46046300 -1.60068900
 H 5.36184300 -0.57073000 -0.79299000
 H 4.55531300 0.60378900 -1.86730300
 H 5.01143400 -1.00807100 -2.47392800
 C 3.34287600 -2.49629400 -0.75872600
 H 3.84278300 -3.09138000 -1.53945700
 H 2.35145600 -2.93900700 -0.59038500
 H 3.93558100 -2.60642200 0.16330900
 C 3.52833600 0.28827900 1.42715900
 H 4.52599400 0.07030800 1.01329000
 C 3.23107300 -0.70844200 2.55729700
 H 3.97584100 -0.58232200 3.35933100
 H 3.28596500 -1.75466000 2.21990900
 H 2.22992900 -0.53352900 2.97537300
 C 3.51887200 1.74029300 1.91930000

H 2.52691800 2.01600700 2.30270600
 H 3.79557300 2.44052300 1.11894100
 H 4.25046400 1.84720000 2.73678100
 C -3.27943500 -0.41703700 -1.30920400
 H -2.57160800 -0.43249100 -2.15377000
 C -4.46547600 0.48087900 -1.68066600
 H -4.94228000 0.09412800 -2.59576800
 H -4.15465400 1.51732800 -1.86630700
 H -5.23487400 0.48789500 -0.89250200
 C -3.72937200 -1.85668400 -1.03559100
 H -4.32007100 -1.93287400 -0.10805600
 H -2.89145800 -2.56344800 -0.97736800
 H -4.37863500 -2.19773300 -1.85770300
 C -3.42542400 0.51778600 1.48958400
 H -4.42820500 0.36749700 1.05693400
 C -3.36626100 1.92608600 2.09198900
 H -4.10414500 1.99802100 2.90775300
 H -3.60032000 2.69813400 1.34651800
 H -2.36890500 2.12954300 2.50485600
 C -3.17483000 -0.56994600 2.54361900
 H -2.15678200 -0.49080800 2.95046700
 H -3.30411900 -1.58530600 2.13885100
 H -3.89615200 -0.45272100 3.36806000
 C -0.79741700 -2.70769700 0.80402900
 H -1.86220200 -2.54847700 0.74098100
 C 0.29248000 -2.11063100 1.16142700
 H 1.25929600 -2.59535300 1.27351800
 Cl -0.67034200 -4.44456500 -0.40141000
 H -0.27682600 -2.85573600 -1.49206500
 Cl 0.07788700 1.03234200 2.30519800

TS2

Imaginary vibration: -492.46 cm⁻¹

Ru 0.02495100 0.20198600 -0.00220300
 Cl -0.05369200 1.13573500 -2.40872100
 P -2.20742400 -0.41803500 -0.05409000
 P 2.33098800 0.03050000 -0.07626000
 O -2.05024600 -2.14291100 -0.11492500
 O 2.52430900 -1.64794100 -0.44361700
 N 0.23480700 -1.91475500 -0.32370700
 C -0.84883100 -2.71295600 -0.25382600
 C -0.75018900 -4.10542100 -0.33057400
 H -1.65493400 -4.70878200 -0.27408300
 C 0.52068900 -4.66276900 -0.46506600
 H 0.63334300 -5.74761600 -0.52389900

C 1.65091000 -3.84597200 -0.51157700
 H 2.66139400 -4.24262800 -0.59714100
 C 1.46143700 -2.46495200 -0.42456200
 C -3.23084200 -0.24681000 -1.60754900
 H -2.49704500 -0.46410000 -2.40184500
 C -4.37424500 -1.26134000 -1.70555600
 H -5.16091400 -1.06334000 -0.96039200
 H -4.01925700 -2.29051000 -1.56246600
 H -4.84414000 -1.19243500 -2.70025600
 C -3.72404000 1.19094000 -1.79545900
 H -4.31915200 1.26279100 -2.71981700
 H -2.88994200 1.89852100 -1.88862900
 H -4.36970000 1.51690500 -0.96433000
 C -3.44040600 -0.23312500 1.33427500
 H -4.43217800 -0.25650100 0.85304800
 C -3.24205600 1.13997900 1.99027500
 H -4.01307700 1.29301400 2.76243600
 H -3.32355400 1.96568100 1.26813100
 H -2.25037200 1.20212600 2.45926900
 C -3.37188400 -1.37574900 2.35325000
 H -2.37966000 -1.41599200 2.82324200
 H -3.57771000 -2.34921800 1.88772400
 H -4.12475900 -1.20146700 3.13943800
 C 3.27528100 0.72133300 -1.51925700
 H 2.59925700 0.51498300 -2.36417900
 C 4.61795900 0.03970100 -1.78972500
 H 5.04479500 0.42206100 -2.73137100
 H 4.50701000 -1.04971800 -1.88034100
 H 5.35080300 0.24563800 -0.99362100
 C 3.40391700 2.24274200 -1.37524700
 H 4.10987200 2.51360300 -0.57453400
 H 2.43876900 2.72267100 -1.15419700
 H 3.78777100 2.67688100 -2.31193600
 C 3.49318200 0.20498000 1.37180800
 H 4.49578800 0.34125700 0.93371200
 C 3.51856000 -1.04547500 2.25760000
 H 4.21744400 -0.88176000 3.09423600
 H 3.85422900 -1.93020000 1.69907300
 H 2.52162000 -1.24709200 2.67353900
 C 3.11922000 1.46616800 2.16390000
 H 2.12590100 1.35053200 2.61949300
 H 3.10872600 2.36948500 1.53545800
 H 3.85723200 1.63001600 2.96551200
 C -0.97267100 3.14058700 0.00127200

H -1.90498100 2.91573100 -0.51800700
 C -0.06293600 2.23081900 0.40447600
 H 0.77863400 2.67022000 0.95725200
 Cl -0.86290400 4.87238000 0.35025700
 H -0.11658200 2.10768100 -1.38280000
 Cl 0.04245400 -0.32922000 2.35422700

TS3

Imaginary vibration: -292.52 cm⁻¹

Ru -0.09111700 -0.14328200 0.31389600
 Cl 0.00872100 -2.25264400 1.72270900
 P -2.40866200 -0.29202200 0.24812400
 P 2.04940200 0.75586200 0.39941100
 O -2.77875700 1.25258600 -0.41223100
 O 1.67594400 2.40054400 -0.01169200
 N -0.54172100 1.81378600 -0.25383200
 C -1.81338300 2.15733900 -0.56877600
 C -2.14459700 3.43345300 -1.02695200
 H -3.18222300 3.65022400 -1.27513500
 C -1.12549700 4.37631400 -1.14278500
 H -1.35353500 5.38223900 -1.50180900
 C 0.18183500 4.04305500 -0.79674600
 H 1.00998000 4.74643800 -0.86600300
 C 0.43615000 2.74303100 -0.35270600
 C -3.37126600 -0.14209100 1.83490200
 H -2.74546700 0.54640800 2.42761500
 C -4.76216800 0.47302900 1.65887400
 H -5.42548800 -0.18050000 1.06993900
 H -4.71642600 1.45003800 1.15870900
 H -5.23395600 0.61140300 2.64541600
 C -3.42091200 -1.49348500 2.55755600
 H -3.89830000 -1.37137600 3.54294500
 H -2.41759600 -1.91287900 2.71261200
 H -4.01747700 -2.23007400 1.99524000
 C -3.47395600 -1.39921700 -0.81450000
 H -4.37885700 -1.57930800 -0.21100700
 C -2.75981600 -2.73776100 -1.03625400
 H -3.45271900 -3.45487900 -1.50417400
 H -2.39752000 -3.18280900 -0.09643900
 H -1.90479400 -2.59026600 -1.71091700
 C -3.88919600 -0.74712200 -2.13700900
 H -3.00046700 -0.49682100 -2.73325300
 H -4.47347300 0.16923000 -1.97642300
 H -4.50949100 -1.45806600 -2.70730100

C 2.75875400 1.07915000 2.08988300
 H 1.89187800 1.56266900 2.57191000
 C 3.94060600 2.04972800 2.12470700
 H 4.17120100 2.31712600 3.16892100
 H 3.71602100 2.97874900 1.58059200
 H 4.85070600 1.60731600 1.69269200
 C 3.02647500 -0.23204500 2.83949500
 H 3.88519900 -0.77856500 2.42064800
 H 2.15136000 -0.89682000 2.81583800
 H 3.26170100 -0.01585300 3.89393400
 C 3.50616600 0.67877800 -0.77071300
 H 3.94297400 1.68031600 -0.61775000
 C 3.02540000 0.57060300 -2.22015800
 H 3.88862900 0.67551100 -2.89796200
 H 2.29415600 1.35057900 -2.47198900
 H 2.54296600 -0.39705200 -2.40963500
 C 4.58935800 -0.35995200 -0.45914800
 H 4.28634900 -1.36995400 -0.76071700
 H 4.88480200 -0.37941800 0.59872000
 H 5.48993500 -0.11059700 -1.04338800
 C 2.00821900 -2.53807400 -0.26229600
 H 2.75186300 -2.27128100 0.48608100
 C 0.70105200 -2.23608400 -0.17607100
 H -0.04863200 -2.65758700 -0.83895900
 Cl 2.64285800 -3.40438200 -1.63844600
 H -0.17416600 0.40792700 1.80367300
 Cl -0.30780700 -0.38348300 -2.28230300

TS4

Imaginary vibration: -331.47 cm⁻¹

Ru 0.12100600 -0.39317600 0.14174800
 Cl 0.01102900 -0.75870500 -2.25377000
 P 2.43162500 -0.40508900 -0.06579700
 P -2.10213700 0.41869600 0.07357200
 O 2.75603000 1.24283700 -0.37851200
 O -1.78163300 2.10422500 -0.10905200
 N 0.48172100 1.65824200 -0.26388100
 C 1.74271800 2.11844400 -0.43807500
 C 2.03020400 3.46276300 -0.67141500
 H 3.06658000 3.76673900 -0.80593900
 C 0.96329800 4.36063200 -0.71891600
 H 1.15223700 5.42029500 -0.90124300
 C -0.34047900 3.91002800 -0.53261400
 H -1.20475800 4.57104900 -0.55843900
 C -0.54342500 2.54517200 -0.30290800

C 3.24730500 -1.10083100 -1.57722400
 H 2.62912600 -0.64857600 -2.37079700
 C 4.70132600 -0.64041200 -1.72885700
 H 5.37053000 -1.14437500 -1.01322700
 H 4.80096100 0.44647100 -1.59659400
 H 5.05330500 -0.89407200 -2.74148600
 C 3.08711600 -2.62132400 -1.68474000
 H 3.60316600 -2.97380000 -2.59158500
 H 2.02690100 -2.89281300 -1.78375700
 H 3.53265100 -3.15399300 -0.82818800
 C 3.57119000 -0.74011400 1.36251100
 H 4.55176100 -0.95891500 0.90775000
 C 3.08475900 -1.98266600 2.12403700
 H 3.77076300 -2.18748400 2.96088800
 H 3.06760500 -2.88112400 1.48770100
 H 2.07773200 -1.80946100 2.53467100
 C 3.71543300 0.48233000 2.27914200
 H 2.74223100 0.76211500 2.70688500
 H 4.12966600 1.34367100 1.73710900
 H 4.40210600 0.22862000 3.10278400
 C -3.10668400 0.11523400 -1.47402300
 H -2.73148500 -0.86768500 -1.79999900
 C -2.77387700 1.15977900 -2.54847100
 H -3.25137700 0.84626700 -3.49028600
 H -1.69255900 1.22419700 -2.73016900
 H -3.16017500 2.15417700 -2.27815900
 C -4.61615600 -0.00276400 -1.24786000
 H -5.06546000 0.94939500 -0.92092900
 H -4.85838200 -0.79954400 -0.53203400
 H -5.08291000 -0.27851300 -2.20668700
 C -3.28394500 0.56374300 1.50882400
 H -4.23056200 0.83981600 1.01860000
 C -2.90562800 1.68432900 2.48648100
 H -3.66839800 1.71849900 3.28152100
 H -2.88143000 2.66452600 1.99183500
 H -1.92657200 1.49234500 2.94586800
 C -3.48247800 -0.77798400 2.22421400
 H -2.59675700 -1.00915600 2.83526800
 H -3.67266700 -1.60777600 1.52551900
 H -4.34648900 -0.69442500 2.90214700
 C 0.32420700 -2.36667200 0.36345600
 H 1.07848300 -3.11582100 0.14213700
 C -0.92086100 -2.24294400 0.77861100
 H -1.29058300 -2.26005300 1.80966100

C1 -3.28580900 -3.15903400 -0.62990100
H -1.87762700 -2.66145000 0.03620400
C1 0.22092200 0.12725900 2.49567500

TS5

Imaginary vibration: -484.60 cm⁻¹

Ru 0.14991400 -0.41574600 0.08167200
C1 0.31112200 0.11014500 2.47380300
P -2.10837400 0.28645100 0.03176800
P 2.49403000 -0.22125200 0.04998100
N 0.39759000 1.71127600 -0.23599500
C -0.68264400 2.48304800 -0.46247800
C -0.57683100 3.86542700 -0.63666900
H -1.47748500 4.44883100 -0.82079000
C 0.69065100 4.43923600 -0.54895500
H 0.80671800 5.51789700 -0.67479500
C 1.81122500 3.64831300 -0.29472700
H 2.81691000 4.05785900 -0.21489900
C 1.61676000 2.27471900 -0.14186000
C -2.87644000 0.52651400 1.71663100
H -1.99708200 0.39466900 2.36330000
C -3.42051400 1.93221700 1.98851100
H -4.29159800 2.18796100 1.36902400
H -2.65336100 2.70252200 1.82748100
H -3.73165900 1.98943900 3.04439700
C -3.86755400 -0.59387900 2.05565200
H -4.08687000 -0.56117600 3.13488800
H -3.45965000 -1.58994100 1.82591400
H -4.82354100 -0.48512100 1.52089400
C -3.49927800 -0.24790700 -1.07562300
H -3.85994900 -1.14092900 -0.54064000
C -3.09546000 -0.69579900 -2.47951200
H -4.00702200 -1.00875700 -3.01472600
H -2.40288000 -1.54199600 -2.44538000
H -2.61966300 0.11443800 -3.04915700
C -4.60862600 0.81196300 -1.13002200
H -4.24149500 1.74692700 -1.57790000
H -5.03201100 1.04503000 -0.14522300
H -5.42728300 0.43265800 -1.76166700
C 3.57729400 -0.77396600 1.47216300
H 4.54494000 -1.00015900 0.99349800
C 3.02846700 -2.06868400 2.08432400
H 3.74040100 -2.45023000 2.83318900
H 2.88915800 -2.85704600 1.32841400

H 2.06467100 -1.88130100 2.57695800
 C 3.80358000 0.32015600 2.52058500
 H 2.85525400 0.60427000 2.99516900
 H 4.25759700 1.21793900 2.07912100
 H 4.48500700 -0.06547300 3.29627600
 C 3.57139400 -0.59632700 -1.42297700
 H 4.59571100 -0.46260900 -1.03286700
 C 3.37644500 0.37394200 -2.59074600
 H 3.59426400 1.40871800 -2.29053600
 H 2.35145000 0.32309400 -2.98000200
 H 4.07333400 0.10412700 -3.40111700
 C 3.38270500 -2.06425100 -1.82659000
 H 2.37014100 -2.21707800 -2.22646600
 H 3.54170200 -2.75358700 -0.98182800
 H 4.10944200 -2.33167600 -2.60987400
 C -0.32924800 -2.21982400 0.64077700
 H -0.49248900 -2.49344600 1.68812300
 C 0.12568300 -3.13089700 -0.30126200
 H -0.04202000 -2.95639700 -1.36479000
 Cl -2.35993700 -3.43769800 -0.06034500
 H 0.82606100 -3.92965100 -0.01029000
 Cl 0.11453100 -0.67278300 -2.35516100
 O -1.88810400 1.90300600 -0.50810000
 O 2.67264100 1.48047400 0.09610600

TS6

Imaginary vibration: -745.73 cm⁻¹

Ru -0.03590700 0.25112700 0.21085000
 Cl 0.06267700 1.29534100 -2.03496200
 P -2.32959400 0.07699400 -0.03558900
 P 2.23804000 -0.20088700 0.17816700
 O -2.40875800 -1.48893900 -0.76488300
 O 2.19465200 -1.84646500 -0.34352900
 N -0.10451800 -1.65314700 -0.57302100
 C -1.29396600 -2.21063400 -0.91175500
 C -1.38863200 -3.51232900 -1.40867800
 H -2.37083800 -3.90595500 -1.66541000
 C -0.21775600 -4.25491400 -1.54499100
 H -0.26214600 -5.27649800 -1.92846800
 C 1.00914700 -3.69942500 -1.18749100
 H 1.94948300 -4.24214200 -1.26990500
 C 1.02703100 -2.39228000 -0.69741300
 C -3.20989700 1.04025000 -1.35188600
 H -2.48376000 1.00235200 -2.17853000
 C -4.53245200 0.43002800 -1.81780800

H -5.31207100 0.48832900 -1.04145700
 H -4.41316800 -0.62396400 -2.10693600
 H -4.90590700 0.98427300 -2.69459600
 C -3.34420300 2.50411600 -0.91586800
 H -3.67815200 3.11692100 -1.76854200
 H -2.38650700 2.91011400 -0.55829500
 H -4.09045500 2.62185000 -0.11391600
 C -3.57363200 -0.10388500 1.33863400
 H -4.55415900 0.08708700 0.87239400
 C -3.30770800 0.97580300 2.39908900
 H -4.11306300 0.95582000 3.15112100
 H -3.27335600 1.98847000 1.97084700
 H -2.34911600 0.78703700 2.90139500
 C -3.58961800 -1.51342500 1.93977200
 H -2.60915200 -1.76258600 2.36894800
 H -3.85056500 -2.27167700 1.18818300
 H -4.34206000 -1.55449800 2.74460400
 C 3.31565900 0.54225500 -1.17272300
 H 2.86018600 1.53637300 -1.29381500
 C 3.12786200 -0.22538100 -2.48765600
 H 3.60861500 0.33230600 -3.30819500
 H 2.06646200 -0.34269200 -2.74054700
 H 3.59222200 -1.22101400 -2.43274900
 C 4.79941800 0.72387600 -0.84721100
 H 5.30740300 -0.24200300 -0.69804900
 H 4.96730300 1.34313300 0.04612400
 H 5.29627800 1.22680100 -1.69324300
 C 3.33824100 -0.36460000 1.67009700
 H 4.36872000 -0.39100300 1.28839200
 C 3.10878800 -1.64927500 2.47204500
 H 3.82407100 -1.67705900 3.31106700
 H 3.27541300 -2.54144500 1.85210600
 H 2.08936900 -1.68837300 2.87528700
 C 3.14829900 0.90529700 2.51080900
 H 2.12473200 0.95012000 2.90928300
 H 3.32167800 1.82226800 1.92321300
 H 3.85942100 0.90925900 3.35241200
 C1 -0.19448700 -0.69139500 2.43821300
 C 1.33715900 3.55758000 -1.94833800
 H 1.36355300 3.27209300 -2.98364400
 C 1.40091500 4.04348200 -0.80422300
 H 1.80624700 4.90067900 -0.27218400
 C1 -0.04034800 2.54307100 1.24019400
 H 0.70978900 3.29117100 0.11046300

2. For CAT-2

CAT-2

Ru 0.00000300 -0.39224100 -0.06505800
Cl 0.00006100 -0.38499300 -2.49020800
P 2.32174500 -0.18409500 -0.08007400
P -2.32172600 -0.18398700 -0.07995000
N 0.00004300 1.64372500 -0.27117200
C 1.17445100 2.34065100 -0.33136800
C 1.19429500 3.72990700 -0.20200000
H 2.15610600 4.24488600 -0.20948700
C 0.00028000 4.43867500 -0.09400800
H 0.00037600 5.52387700 0.02556400
C -1.19385300 3.73008900 -0.20174000
H -2.15559100 4.24520900 -0.20899900
C -1.17426000 2.34080600 -0.33102300
C 3.28564600 -1.11014400 -1.37673200
H 2.82783500 -0.71443200 -2.29861700
C 4.78652000 -0.81851400 -1.39016400
H 5.28972400 -1.22074000 -0.49712500
H 4.99968200 0.26129500 -1.44037400
H 5.25720500 -1.28816100 -2.26973200
C 2.95846900 -2.60676800 -1.33053200
H 3.40979000 -3.11676800 -2.19715800
H 1.87108600 -2.76662900 -1.37127000
H 3.34266000 -3.09055100 -0.42026600
C 3.34531800 -0.15843500 1.48093300
H 4.31931000 0.27207100 1.18619600
C 3.57632000 -1.55889800 2.05745300
H 4.15009400 -1.48422500 2.99611100
H 4.14894000 -2.19872500 1.37115900
H 2.61793600 -2.04969100 2.27741500
C 2.68834800 0.77474800 2.50635300
H 1.69752300 0.39568700 2.79381400
H 2.56541500 1.79880900 2.12102500
H 3.31351400 0.83474900 3.41218200
C -3.28555400 -1.10948400 -1.37705800
H -2.82754400 -0.71348500 -2.29872300
C -4.78639000 -0.81767800 -1.39060200
H -5.25700600 -1.28695600 -2.27040500
H -4.99941300 0.26217400 -1.44045800
H -5.28977300 -1.22015900 -0.49777800
C -2.95855400 -2.60616100 -1.33135200
H -3.34299700 -3.09023900 -0.42135100

H -1.87118300 -2.76613300 -1.37192500
 H -3.40975400 -3.11578600 -2.19826300
 C -3.34546100 -0.15894000 1.48098000
 H -4.31938100 0.27174100 1.18625500
 C -2.68860900 0.77378100 2.50689100
 H -3.31405000 0.83361700 3.41254100
 H -2.56533800 1.79794300 2.12194200
 H -1.69795300 0.39442200 2.79452200
 C -3.57667800 -1.55960500 2.05692100
 H -2.61837700 -2.05059000 2.27680800
 H -4.14930000 -2.19908900 1.37031300
 H -4.15054700 -1.48522500 2.99554400
 Cl -0.00003800 -1.61705100 1.98928400
 C 2.43638200 1.58158400 -0.63879400
 H 2.51974500 1.54186200 -1.73868900
 H 3.32275100 2.10943500 -0.25827600
 C -2.43651700 1.58198400 -0.63782200
 H -3.32244400 2.10967600 -0.25605100
 H -2.52109600 1.54307200 -1.73765000

CAT-2 + C₂H₂

Ru 0.00012000 -0.45826800 0.04018200
 Cl -0.00023100 -1.00127100 -2.37095700
 P 2.34551900 -0.22413300 -0.07870400
 P -2.34527700 -0.22471600 -0.07877900
 N -0.00011500 1.55947700 -0.68059600
 C 1.17213400 2.22098300 -0.80087200
 C 1.20020500 3.61682800 -0.85754500
 H 2.15862500 4.13398200 -0.91893800
 C -0.00117000 4.32292800 -0.84774300
 H -0.00160400 5.41512000 -0.86867600
 C -1.20197200 3.61584900 -0.85882100
 H -2.16075000 4.13221000 -0.92126900
 C -1.17280400 2.22004700 -0.80219200
 C 3.30395400 -1.35993100 -1.20929700
 H 2.60722000 -1.45762200 -2.05830700
 C 4.63601600 -0.79638100 -1.71060200
 H 5.35546200 -0.64758100 -0.88890400
 H 4.51877000 0.16229400 -2.23702100
 H 5.09768000 -1.50318400 -2.42006100
 C 3.48410700 -2.74496500 -0.57903900
 H 3.86204400 -3.45348000 -1.33404800
 H 2.53848600 -3.14178200 -0.18381700
 H 4.21638100 -2.72355800 0.24370600
 C 3.46240700 -0.00738000 1.41339200

H 4.47853300 -0.23757800 1.04826000
 C 3.08747500 -1.02378100 2.50098100
 H 3.84061600 -1.00466600 3.30590400
 H 3.03191800 -2.05157400 2.11563400
 H 2.11044300 -0.76516100 2.93142800
 C 3.46584900 1.41920500 1.97459000
 H 2.45140000 1.72571600 2.26588500
 H 3.86701500 2.15183700 1.25878900
 H 4.10599600 1.45775100 2.87172800
 C -3.30381700 -1.36255000 -1.20725000
 H -2.60653800 -1.46300300 -2.05548700
 C -4.63489500 -0.79891800 -1.71105500
 H -5.09721400 -1.50751200 -2.41829900
 H -4.51600300 0.15774700 -2.24072400
 H -5.35454600 -0.64622900 -0.89023700
 C -3.48578600 -2.74579500 -0.57358700
 H -4.21872100 -2.72156500 0.24848000
 H -2.54083800 -3.14246600 -0.17658400
 H -3.86376200 -3.45588000 -1.32710300
 C -3.46193700 -0.00507800 1.41299400
 H -4.47824900 -0.23506800 1.04819900
 C -3.46423900 1.42244900 1.97186700
 H -4.10469800 1.46307800 2.86869200
 H -3.86438700 2.15431300 1.25469800
 H -2.44961700 1.72846100 2.26310700
 C -3.08783800 -1.01998200 2.50230100
 H -2.11041200 -0.76172200 2.93208700
 H -3.03357100 -2.04852500 2.11879700
 H -3.84079600 -0.99858800 3.30733800
 C -0.00029500 -2.65109900 0.19573000
 H -0.00067000 -3.30638600 -0.66131100
 C -0.00016200 -2.21877500 1.36227700
 H -0.00007000 -2.17864100 2.43982100
 Cl 0.00054100 0.72426000 2.20717800
 C 2.40943600 1.39270100 -1.00175200
 H 2.39797900 1.09453300 -2.06464400
 H 3.32202700 1.97746300 -0.83104500
 C -2.40902600 1.39054700 -1.00439000
 H -3.32252900 1.97473700 -0.83662200
 H -2.39486000 1.09046400 -2.06671700

CAT-2 + HCl

Ru -0.01166300 -0.42621600 0.04702400
 Cl -0.03646800 -0.93682900 -2.41015000

P 2.31158100 -0.06504600 -0.15820700
 P -2.33678500 -0.16637900 0.09193300
 N -0.08670700 1.63048200 -0.00807400
 C 0.97317600 2.34356300 -0.47937700
 C 0.97509800 3.73872300 -0.44579600
 H 1.84400700 4.27641800 -0.82757400
 C -0.12492100 4.42072200 0.06896700
 H -0.13886000 5.51212000 0.10186400
 C -1.20766400 3.68147700 0.53787600
 H -2.09193400 4.17447800 0.94405600
 C -1.17214100 2.28665200 0.49413900
 C 3.32086700 -1.04442700 -1.39162300
 H 2.60435300 -1.13405600 -2.22453400
 C 4.57902000 -0.33351300 -1.89658300
 H 5.31486300 -0.17940500 -1.09099300
 H 4.35982100 0.64447400 -2.35006500
 H 5.06956700 -0.94858600 -2.66924500
 C 3.63770700 -2.45870500 -0.89250800
 H 3.98329900 -3.08098500 -1.73415300
 H 2.75840000 -2.94649100 -0.44923400
 H 4.44285100 -2.45135800 -0.14184800
 C 3.45949700 0.31022000 1.26941300
 H 4.45506000 0.46207500 0.81632200
 C 3.52533800 -0.87167400 2.24652100
 H 4.25407900 -0.65215000 3.04441600
 H 3.83708700 -1.80488100 1.75897000
 H 2.54126300 -1.03450000 2.70759400
 C 3.05345500 1.59926000 1.99604300
 H 2.03194800 1.51439300 2.39431800
 H 3.10802000 2.48462900 1.34576200
 H 3.73702700 1.77128600 2.84381600
 C -3.22000900 0.21224900 -1.52194800
 H -3.02840000 -0.68146800 -2.13829400
 C -2.58369100 1.41074200 -2.23685900
 H -3.00427000 1.49758500 -3.25159600
 H -1.49734600 1.30080100 -2.33281600
 H -2.79985200 2.35355000 -1.71050200
 C -4.73166500 0.41857200 -1.37822100
 H -4.96336800 1.24591600 -0.68688400
 H -5.25700600 -0.47740300 -1.02061000
 H -5.16486600 0.68398100 -2.35664500
 C -3.53549800 -1.26164800 1.00967900
 H -4.49442200 -0.71716600 1.04105200
 C -3.09096800 -1.55692000 2.44359300

H -3.83336000 -2.21376900 2.92655500
 H -2.99575500 -0.64734200 3.05234800
 H -2.11241800 -2.05496900 2.45906600
 C -3.72254700 -2.56649400 0.22192300
 H -2.77783600 -3.12819400 0.17735400
 H -4.06523600 -2.39975300 -0.80987400
 H -4.47054600 -3.20169500 0.72318400
 Cl 0.03237600 -3.01285300 -0.05574300
 H 0.00235300 -2.53117100 -1.34252800
 Cl 0.05019500 -0.26638000 2.47015700
 C 2.12506400 1.56870300 -1.04642400
 H 1.87761600 1.27638600 -2.08154300
 H 3.03718500 2.18114400 -1.07201400
 C -2.33221300 1.46285500 0.98467000
 H -2.14322400 1.19874900 2.03742000
 H -3.27312400 2.02977400 0.92501500

INT1

Ru 0.05491100 0.14096700 0.27322400
 Cl -0.20551000 1.47820000 -1.81100500
 P -2.23390000 -0.42806500 0.13881700
 P 2.39599800 0.35695500 0.03564600
 N 0.29393200 -1.43945600 -1.15093800
 C -0.78242400 -2.17906100 -1.50329300
 C -0.62162500 -3.43633400 -2.09071800
 H -1.50219100 -4.03112000 -2.33648700
 C 0.66315500 -3.90240400 -2.36254400
 H 0.81205800 -4.89149000 -2.80161400
 C 1.75234000 -3.07151200 -2.10794500
 H 2.76703200 -3.37527600 -2.36838100
 C 1.53672600 -1.82166200 -1.52174800
 C -3.46775300 0.86373700 -0.40483700
 H -2.88455900 1.45358600 -1.12881200
 C -4.70938200 0.30584600 -1.10578300
 H -5.29819600 -0.34751700 -0.44117200
 H -4.46379900 -0.26420900 -2.01390600
 H -5.36744700 1.13615600 -1.41065800
 C -3.85125400 1.78825000 0.75583000
 H -4.36929100 2.67648200 0.36332800
 H -2.97101800 2.14034700 1.31022500
 H -4.52908100 1.28592700 1.46432100
 C -3.14545700 -1.40874600 1.45212300
 H -4.21545600 -1.24243300 1.23752300
 C -2.82799800 -0.84684800 2.84462700

H -3.47301500 -1.32901300 3.59750900
 H -2.98983800 0.23797300 2.90696000
 H -1.77945300 -1.05232900 3.09891600
 C -2.87031900 -2.91527300 1.38724500
 H -1.79693500 -3.12157700 1.50075700
 H -3.22100000 -3.36607400 0.44699400
 H -3.40426000 -3.42043200 2.20912400
 C 3.08101400 1.95745300 -0.64060400
 H 2.33794800 2.20649000 -1.41585300
 C 4.46232000 1.84119900 -1.28995100
 H 4.75261700 2.81070100 -1.72748300
 H 4.48672400 1.09708200 -2.10010200
 H 5.24062200 1.57145200 -0.55788500
 C 3.04318100 3.05907400 0.42323600
 H 3.80382300 2.89606100 1.20365300
 H 2.06041700 3.11939700 0.91166000
 H 3.25403400 4.03652500 -0.03983600
 C 3.64252300 -0.16262700 1.33981000
 H 4.57024200 0.37338400 1.07651200
 C 3.93897600 -1.66672100 1.33654800
 H 4.61600900 -1.90845200 2.17249800
 H 4.43651600 -1.99414600 0.41183400
 H 3.01441700 -2.24622600 1.46757500
 C 3.18417000 0.30623300 2.72717500
 H 2.31734400 -0.28510300 3.05112600
 H 2.90050000 1.36817000 2.74099900
 H 3.99799000 0.16334500 3.45688500
 C -0.32753300 2.08117900 1.28718300
 H -0.61432600 2.99421400 0.78615500
 C -0.06337600 1.25290700 2.17460000
 H 0.11235700 0.80270200 3.13791700
 Cl -1.88152900 4.28846000 -1.06396100
 H -1.20920600 3.19944000 -1.44240500
 Cl 0.43055500 -1.72811300 1.83232300
 C 2.64039000 -0.80735600 -1.39867200
 H 3.62960800 -1.28042800 -1.42914900
 H 2.55899100 -0.16438000 -2.29228100
 C -2.13456000 -1.54231900 -1.34953800
 H -2.24074400 -0.85307500 -2.20519600
 H -2.94297900 -2.28123000 -1.41503100

INT2

Ru 0.06658900 -0.18167100 -0.10687200

C1 0.12558300 -0.17198700 -2.57072500
 P 2.38075200 -0.66438800 -0.12622500
 P -2.08624400 0.79672700 -0.20491800
 N 0.73797200 1.84384200 -0.35186500
 C 2.06473300 2.10520100 -0.34736200
 C 2.53778300 3.39409800 -0.09090800
 H 3.61270400 3.57586700 -0.05863300
 C 1.62438600 4.42712500 0.11038900
 H 1.97217300 5.43802300 0.33483000
 C 0.26348100 4.16138000 -0.02169000
 H -0.47800900 4.95666900 0.06462000
 C -0.15609600 2.85382800 -0.28226700
 C 3.04705900 -1.83367200 -1.42126200
 H 2.40080700 -1.59521300 -2.28233000
 C 4.50928800 -1.59102900 -1.80454800
 H 5.19098800 -1.76015800 -0.95465600
 H 4.68378600 -0.57367100 -2.18379300
 H 4.80750100 -2.29151700 -2.60214800
 C 2.81017700 -3.29589100 -1.02858700
 H 3.02472200 -3.95264100 -1.88721100
 H 1.77267900 -3.47704400 -0.71520600
 H 3.47443900 -3.60649900 -0.20652800
 C 3.38633700 -1.04660000 1.41040200
 H 4.31949700 -1.50119400 1.03459400
 C 2.65150300 -2.07498600 2.28110400
 H 3.31628700 -2.42615300 3.08735400
 H 2.32492000 -2.95402600 1.70807300
 H 1.76541400 -1.61264100 2.73733700
 C 3.74910100 0.20261500 2.22124700
 H 2.84257900 0.73589200 2.54054200
 H 4.38980700 0.89669500 1.65778700
 H 4.30643400 -0.09554100 3.12471800
 C -3.21865800 0.38644600 -1.63423900
 H -2.50823700 0.35509900 -2.47686400
 C -4.29553000 1.43825900 -1.91478100
 H -4.86569900 1.15602100 -2.81529800
 H -3.87745900 2.43964100 -2.09550000
 H -5.01872600 1.51615400 -1.08704800
 C -3.82910100 -1.00705200 -1.47517700
 H -4.55414600 -1.04891500 -0.64741400
 H -3.06685100 -1.77301800 -1.28888200
 H -4.36632300 -1.28973500 -2.39488700
 C -3.23988500 0.92503800 1.27337100
 H -4.24175400 1.07748900 0.83749600

C -2.93288200 2.10924100 2.19661700
 H -3.61942100 2.08640100 3.05916300
 H -3.07336500 3.07963000 1.69808900
 H -1.90371100 2.05070800 2.57791100
 C -3.24400100 -0.39490700 2.05465200
 H -2.27741200 -0.53405900 2.55740200
 H -3.43219400 -1.26863100 1.41687000
 H -4.03435600 -0.37026300 2.82257000
 C -0.55539500 -2.24076700 -0.44475400
 H -0.67845000 -2.70258000 -1.41342700
 C -0.50382300 -2.08081500 0.79347900
 H -0.55115500 -2.29364700 1.85065400
 Cl -3.35107000 -4.06086100 0.59714000
 H -2.33996600 -3.25076500 0.43574900
 Cl 0.20923600 0.48729300 2.26254400
 C 2.98503700 0.98459200 -0.73669000
 H 2.91255300 0.89971600 -1.83483800
 H 4.02926100 1.20629400 -0.48325800
 C -1.58473600 2.54276900 -0.62736800
 H -2.26845400 3.30705000 -0.23848800
 H -1.64059800 2.58731900 -1.72883900

INT3

Ru -0.03202400 0.21975600 0.16167500
 Cl 0.12577100 0.90220000 -2.21398400
 P -2.36548700 0.30443700 -0.16159400
 P 2.21758900 -0.43605100 0.21488600
 N -0.29387000 -1.77893500 -0.26727000
 C -1.43383600 -2.20797300 -0.87544900
 C -1.66703200 -3.56754000 -1.08965700
 H -2.59461100 -3.87558300 -1.57392900
 C -0.72020800 -4.50553100 -0.68577100
 H -0.88882800 -5.57253300 -0.84588200
 C 0.44635900 -4.05423800 -0.07439900
 H 1.21638200 -4.75318900 0.25497300
 C 0.64258700 -2.68721200 0.12971100
 C -3.11305000 1.64251000 -1.23056800
 H -2.35057900 1.71223200 -2.02352900
 C -4.45975100 1.27891000 -1.86060400
 H -5.25096800 1.16486600 -1.10189100
 H -4.41407600 0.34974100 -2.44788900
 H -4.78071900 2.08189100 -2.54492200
 C -3.17226000 2.99914100 -0.52097000

H -3.36047900 3.79619200 -1.25886700
 H -2.23202400 3.23310400 -0.00315300
 H -3.98985300 3.03852700 0.21539100
 C -3.63500200 -0.08436100 1.15428600
 H -4.61746400 0.02449500 0.66183000
 C -3.54192000 0.91226500 2.31808600
 H -4.34963300 0.71443600 3.04226800
 H -3.63952900 1.95526000 1.98793600
 H -2.57752200 0.80045400 2.83345600
 C -3.49855600 -1.52703600 1.65801100
 H -2.49842300 -1.69441400 2.08334200
 H -3.67490800 -2.26830500 0.86476000
 H -4.24187700 -1.71065200 2.45145800
 C 3.13338700 -0.67512700 -1.40984800
 H 3.08666700 0.31938800 -1.88290700
 C 2.38960600 -1.65498100 -2.32650700
 H 2.84735700 -1.63554200 -3.32879800
 H 1.33331900 -1.38513700 -2.43642800
 H 2.46248300 -2.68876500 -1.95375900
 C 4.59790000 -1.09977200 -1.25944100
 H 4.68970800 -2.04325900 -0.69541200
 H 5.21903100 -0.34423600 -0.75943800
 H 5.03522300 -1.27581400 -2.25601200
 C 3.53007600 0.23469500 1.36266700
 H 4.39106100 -0.44804600 1.27254900
 C 3.09418600 0.27442100 2.82894500
 H 3.91042800 0.69690000 3.43859300
 H 2.86107200 -0.72382200 3.22473400
 H 2.19499200 0.89002100 2.96285800
 C 3.94968800 1.63099100 0.88271500
 H 3.12691700 2.34697400 1.01603300
 H 4.24161400 1.65614100 -0.17723200
 H 4.80650100 1.99059300 1.47536400
 C1 0.27093600 2.61105400 0.97839900
 H 0.93696100 3.22351400 0.02092000
 C1 -0.23825500 -0.35393300 2.53071900
 C 1.97762400 3.62900900 -1.74621000
 H 1.50002800 2.77118300 -2.21574000
 C 2.46955500 4.56678800 -1.15496500
 H 2.91207700 5.39977500 -0.63995200
 C -2.42023400 -1.16613600 -1.31149200
 H -2.08300600 -0.75030900 -2.27585600
 H -3.41921500 -1.60282000 -1.44895600
 C 1.89193700 -2.17289400 0.79143900

H 2.73040200 -2.87239000 0.65593700
H 1.68605800 -2.06741000 1.86881200

INT4

Ru 0.00018000 0.11195900 0.24306600
Cl 0.00028600 0.55177800 2.73795800
P 2.32427600 -0.16858500 0.20092500
P -2.32385500 -0.17009300 0.20127700
N 0.00085100 -2.08727500 0.35982200
C 1.17391200 -2.74094300 0.18922700
C 1.20277000 -4.05974600 -0.27082600
H 2.16162300 -4.55554800 -0.42941500
C 0.00115900 -4.72064900 -0.52401100
H 0.00126700 -5.74518200 -0.90268600
C -1.20059400 -4.06038900 -0.26977300
H -2.15932300 -4.55669900 -0.42751900
C -1.17202300 -2.74160900 0.19031600
C 3.33796500 0.54811900 1.60675600
H 2.73605300 0.27535300 2.49039600
C 4.73854700 -0.04442500 1.78434600
H 5.39613100 0.20423700 0.93693900
H 4.72543200 -1.14005700 1.89119100
H 5.21123900 0.36947900 2.69069800
C 3.37169300 2.07757200 1.51992900
H 3.77378600 2.50447000 2.45328700
H 2.37142000 2.49878700 1.34503400
H 4.02210400 2.41472000 0.69796700
C 3.41330600 0.09979800 -1.30565400
H 4.43520300 0.18749000 -0.89984100
C 3.04579600 1.41632600 -2.00332700
H 3.80680200 1.65384900 -2.76508100
H 2.97864200 2.26400900 -1.30854000
H 2.06971000 1.31928100 -2.49434200
C 3.39648500 -1.07285900 -2.29347400
H 2.37649900 -1.26261500 -2.65470500
H 3.79749500 -1.99970700 -1.85661100
H 4.02887600 -0.82418700 -3.16194800
C -3.33798400 0.54732000 1.60640500
H -2.73559400 0.27620600 2.49022700
C -4.73792600 -0.04644000 1.78492600
H -5.21103100 0.36832300 2.69067100
H -4.72365900 -1.14189500 1.89341200
H -5.39577900 0.20028100 0.93715600

C -3.37331500 2.07663500 1.51776000
 H -4.02463500 2.41209800 0.69583000
 H -2.37359400 2.49867600 1.34172100
 H -3.77525100 2.50422600 2.45087000
 C -3.41303900 0.09558200 -1.30557000
 H -4.43515200 0.18201100 -0.90000700
 C -3.39415200 -1.07787000 -2.29243700
 H -4.02714300 -0.83110200 -3.16101300
 H -3.79332700 -2.00511300 -1.85473600
 H -2.37384200 -1.26599100 -2.65361700
 C -3.04735800 1.41210000 -2.00425100
 H -2.07068700 1.31635100 -2.49436300
 H -2.98245900 2.26064200 -1.31029500
 H -3.80815300 1.64743500 -2.76689800
 C -0.00198900 2.92213400 -1.04093300
 H -0.00197500 2.55817100 -2.06808400
 C -0.00103000 2.16088000 0.05401100
 H -0.00120200 2.74501500 0.99517300
 Cl -0.00357800 4.70810700 -0.98656700
 H -0.00174900 -0.62086500 3.29188800
 Cl 0.00046100 -0.29005400 -2.14445400
 C 2.43228000 -2.00432600 0.57541700
 H 2.52545100 -2.06877600 1.67446600
 H 3.32314000 -2.49224700 0.15919000
 C -2.43035000 -2.00554200 0.57763100
 H -3.32153700 -2.49449600 0.16328600
 H -2.52178600 -2.06885800 1.67689800

INT5

Ru 0.03349500 0.14440700 0.22339000
 Cl -0.38274100 0.23350500 2.69911300
 P 2.38559500 0.02502000 0.06970200
 P -2.30592100 -0.37568100 0.13386200
 N 0.15503800 -2.05177300 -0.02008700
 C 1.33468900 -2.59053500 -0.39443000
 C 1.46180900 -3.97657400 -0.53677900
 H 2.41954200 -4.40342900 -0.83828800
 C 0.35334100 -4.79053700 -0.30946400
 H 0.43107800 -5.87357600 -0.42859700
 C -0.85415100 -4.20969200 0.07601000
 H -1.73638000 -4.82087100 0.27140600
 C -0.92215200 -2.82260700 0.23485400
 C 3.30612400 -0.14043800 1.68779700
 H 2.70046200 -0.87106300 2.25282000
 C 4.73465900 -0.67740600 1.57958100

H 5.38943600 0.00417800 1.01371900
 H 4.77825900 -1.66647000 1.09840900
 H 5.17094600 -0.78264100 2.58617400
 C 3.23773200 1.19954700 2.43162800
 H 3.67025700 1.09480400 3.43949700
 H 2.19913600 1.54280900 2.54088100
 H 3.81082800 1.97957600 1.90507200
 C 3.49369800 1.15267200 -0.95305000
 H 4.40262000 1.24389000 -0.33623300
 C 2.86784500 2.54253300 -1.09774500
 H 3.59716200 3.22389200 -1.56569900
 H 2.56517800 2.97049900 -0.13238000
 H 1.96783100 2.49879300 -1.72306300
 C 3.90434500 0.57997000 -2.31238300
 H 3.02418000 0.42488000 -2.95245900
 H 4.45384400 -0.36932100 -2.22430100
 H 4.56887200 1.29869300 -2.81897000
 C -3.48482100 0.37970300 1.36515800
 H -2.90413100 0.28069000 2.29516500
 C -4.80915700 -0.37341300 1.51634000
 H -5.39352900 0.07283700 2.33753000
 H -4.67005300 -1.43864400 1.75588500
 H -5.42758300 -0.30492400 0.60704500
 C -3.70240600 1.87633100 1.11687600
 H -4.36114200 2.05403900 0.25271300
 H -2.75635300 2.40620200 0.94348200
 H -4.19145800 2.32473200 1.99662600
 C -3.24642600 -0.51669500 -1.47286900
 H -4.28670700 -0.72498700 -1.16839900
 C -2.75490400 -1.68615000 -2.33508900
 H -3.33027800 -1.71196700 -3.27503800
 H -2.89113800 -2.65975400 -1.84138400
 H -1.69320100 -1.56497600 -2.59148600
 C -3.21174500 0.80445500 -2.25306300
 H -2.19549900 1.00117900 -2.61802800
 H -3.52556100 1.66244100 -1.64463000
 H -3.88814000 0.73828100 -3.12089700
 C -0.51007200 3.02213500 -0.64732600
 H -0.67495400 2.75252700 -1.69010400
 C -0.15925200 2.19009400 0.33108100
 H -0.03329200 2.61958700 1.33373400
 C1 -0.74714800 4.76697200 -0.38095400
 H 0.83306000 -0.56605400 1.33565300
 C1 0.26377300 0.19109100 -2.20509200

C -2.15824000 -2.13449200 0.74764600
 H -3.05587900 -2.74128600 0.56195500
 H -2.04858000 -2.01808900 1.83988500
 C 2.48429400 -1.66857000 -0.72641100
 H 3.44655700 -2.16859900 -0.54851900
 H 2.41320300 -1.45811100 -1.80347300

INT6

Ru 0.06736400 -0.40471900 0.14263600
 Cl 0.10615700 -0.69498900 -2.29206000
 P 2.40390400 -0.15122500 -0.12217000
 P -2.25168800 0.23002900 0.13673700
 N 0.19197300 1.75519200 -0.14969400
 C 1.28414300 2.30540100 -0.73095300
 C 1.38250300 3.68510800 -0.93360100
 H 2.27933200 4.09132200 -1.40293600
 C 0.33410400 4.51383700 -0.54534700
 H 0.38956900 5.59322500 -0.70282500
 C -0.78554000 3.93969600 0.05133100
 H -1.62705700 4.55016800 0.38091600
 C -0.82688200 2.55748300 0.24922200
 C 3.37975100 -1.33204800 -1.20684300
 H 2.59483300 -1.70198100 -1.88653900
 C 4.46133000 -0.63578800 -2.04232600
 H 5.20265800 -0.12117900 -1.40839100
 H 4.04695700 0.09276200 -2.75125000
 H 5.00777100 -1.38926300 -2.63254600
 C 3.99617500 -2.51343700 -0.44821500
 H 4.36679600 -3.25443800 -1.17472100
 H 3.28594600 -3.02504800 0.21206300
 H 4.85778100 -2.19465700 0.15852600
 C 3.53095400 0.29541000 1.30211700
 H 4.54378700 0.33934400 0.86082300
 C 3.50871700 -0.75947500 2.41694800
 H 4.23105700 -0.47749300 3.20039300
 H 3.78016500 -1.76160300 2.06334200
 H 2.50887500 -0.80534500 2.86999800
 C 3.17571100 1.67617600 1.86911100
 H 2.13789300 1.68518500 2.23274900
 H 3.30170800 2.48335600 1.13348000
 H 3.83520700 1.90227200 2.72273700
 C -2.91106100 0.68823900 -1.55506400
 H -1.98983500 1.04804500 -2.04188600
 C -3.95064700 1.81223700 -1.55152600
 H -4.26029800 2.02593300 -2.58779700

H -3.56309700 2.75059500 -1.12881000
 H -4.86111600 1.53479900 -0.99538200
 C -3.39478800 -0.52150800 -2.36087400
 H -4.38221300 -0.86647800 -2.01609700
 H -2.68393700 -1.35473500 -2.30679000
 H -3.49847600 -0.23379600 -3.41945100
 C -3.71987300 -0.39022200 1.12827900
 H -4.52898000 0.29100400 0.81022600
 C -3.51880200 -0.22846300 2.64096800
 H -4.39017000 -0.65011700 3.16788500
 H -3.42654000 0.82292300 2.94671400
 H -2.61445100 -0.75046700 2.98407100
 C -4.15618400 -1.82348900 0.80368700
 H -3.45636000 -2.55930100 1.22117900
 H -4.23392600 -2.02261700 -0.27045700
 H -5.14232800 -2.00785100 1.26021600
 C 0.70682700 -2.45747800 0.52570900
 C -0.68816600 -2.40990600 0.50996500
 H -1.25636500 -2.41384900 1.44017600
 Cl 0.06132300 -0.07615400 2.58128000
 H 1.20831400 -2.91706100 -0.32654900
 H 1.21850600 -2.48762300 1.48984000
 Cl -1.55421100 -3.28609000 -0.77628600
 C 2.36991100 1.37959900 -1.17341800
 H 2.09308300 0.99641400 -2.16944800
 H 3.33798200 1.89368800 -1.24138400
 C -1.97730300 1.89008400 0.92362000
 H -1.66569200 1.64817000 1.95268100
 H -2.86932700 2.52915900 0.95196100

INT7

Ru 0.04839700 -0.34933100 -0.08055300
 Cl 0.15512400 0.17764600 -2.47507400
 P 2.43365900 -0.50105000 -0.01379400
 P -2.15362000 0.57183000 -0.04117100
 N 0.54994700 1.77292800 0.09849600
 C 1.79463300 2.14779000 0.47888600
 C 2.16210700 3.49475200 0.50968400
 H 3.17364300 3.76776400 0.81257100
 C 1.22337200 4.46733000 0.17222300
 H 1.48797400 5.52667600 0.20040200
 C -0.05526900 4.06782500 -0.20290800
 H -0.81653400 4.79861900 -0.47832100
 C -0.36756400 2.70535500 -0.24953500
 C 3.35061500 -0.30260800 -1.62307200

H 2.77008800 0.47624600 -2.14253200
 C 4.80205900 0.15665700 -1.46396400
 H 5.40678700 -0.55913400 -0.88329800
 H 4.88106200 1.14068700 -0.97909700
 H 5.27182000 0.24544500 -2.45697500
 C 3.23787800 -1.58661600 -2.45142600
 H 3.71325600 -1.43906000 -3.43405900
 H 2.18625800 -1.84493400 -2.63298800
 H 3.74305000 -2.43841900 -1.96762000
 C 3.38199400 -1.84473100 0.89452200
 H 4.27856200 -2.00276800 0.27271700
 C 2.57889000 -3.14833000 0.92172700
 H 3.19776300 -3.96039500 1.33551200
 H 2.25148600 -3.45835900 -0.08171700
 H 1.68914300 -3.03609200 1.55546400
 C 3.84490000 -1.45044000 2.30073500
 H 2.98425900 -1.24007600 2.95115600
 H 4.50672600 -0.57198800 2.29317400
 H 4.41180800 -2.28549800 2.74329100
 C -3.55982500 -0.00912300 -1.11918400
 H -4.05532600 -0.75608200 -0.47758600
 C -3.11429200 -0.75204800 -2.37836000
 H -4.00993300 -1.12194900 -2.90197400
 H -2.50800100 -1.62990700 -2.12628200
 H -2.53836400 -0.11404800 -3.06245500
 C -4.53933800 1.12233500 -1.45308600
 H -4.10662600 1.83801700 -2.17047000
 H -4.87319100 1.68338000 -0.56691400
 H -5.43814100 0.69307000 -1.92362500
 C -2.98547800 0.94117700 1.58678400
 H -3.95678700 1.37618200 1.29280300
 C -2.22045300 1.98199600 2.41194500
 H -2.13680300 2.95227800 1.89941500
 H -1.21145200 1.62246200 2.65792500
 H -2.75517600 2.15745600 3.35949000
 C -3.24554700 -0.34243000 2.38594600
 H -2.29997900 -0.74095700 2.77801300
 H -3.72109400 -1.13460800 1.78913200
 H -3.90182300 -0.11021800 3.24057600
 C -0.08470300 -2.20122200 -0.72555300
 H 0.24537300 -2.62977200 -1.67162100
 C -0.88980200 -2.40717100 0.30463800
 H -0.63368200 -2.71195500 1.32495200
 Cl -3.73869000 -3.15486900 0.09975700

H -2.08176000 -2.61974700 0.12482500
 Cl 0.31008200 -0.51839000 2.35408000
 C 2.74897500 1.07492400 0.91282200
 H 3.78960800 1.41939800 0.85992000
 H 2.51503100 0.82704000 1.95920000
 C -1.70872300 2.23971700 -0.72802300
 H -1.63540000 2.07421100 -1.81588000
 H -2.48065000 2.99997600 -0.54554100

INT8

Ru 0.07967100 -0.35334000 0.17005800
 Cl 0.19087600 -1.17193100 -2.21284200
 P 2.39193300 0.02219500 -0.02490400
 P -2.27285400 -0.12280900 0.26247700
 N -0.03475400 1.65252000 -0.43545600
 C 1.04083900 2.25671900 -1.01243500
 C 1.01393700 3.60988900 -1.35332900
 H 1.89553400 4.06095400 -1.81116800
 C -0.13263300 4.36242800 -1.10661600
 H -0.17305200 5.42073000 -1.37292500
 C -1.22044000 3.73911600 -0.50127100
 H -2.13114900 4.29499300 -0.27314600
 C -1.14743000 2.38679200 -0.15740000
 C 3.47507300 -1.19639000 -0.94533700
 H 2.81787200 -1.49234100 -1.77960900
 C 4.75843400 -0.59761600 -1.52755500
 H 5.44903300 -0.26937400 -0.73458300
 H 4.56911100 0.26044500 -2.19013000
 H 5.28876700 -1.36079100 -2.12096200
 C 3.75810400 -2.45481300 -0.11688400
 H 4.15926200 -3.24518200 -0.77270200
 H 2.84396600 -2.83054600 0.36578100
 H 4.51591400 -2.26019900 0.65764400
 C 3.46832600 0.72192100 1.33310400
 H 4.48694800 0.74917500 0.90745900
 C 3.46243900 -0.19385900 2.56520600
 H 4.16364700 0.20089800 3.31912500
 H 3.76659700 -1.22102200 2.32675900
 H 2.45638900 -0.23309600 3.00371800
 C 3.06102800 2.15402500 1.70253300
 H 2.02146900 2.18023500 2.05795600
 H 3.16601800 2.85435700 0.86040600
 H 3.71018600 2.51886000 2.51555700

C -3.32516000 -0.25604300 -1.29432300
 H -3.19058900 -1.30488600 -1.60380000
 C -2.78477000 0.65190400 -2.40696200
 H -3.27807300 0.41034400 -3.36279500
 H -1.70253300 0.55279300 -2.54815000
 H -2.99822800 1.71048500 -2.19056500
 C -4.82377400 0.00182700 -1.10246900
 H -5.01941500 1.03471300 -0.77215300
 H -5.28889800 -0.68119100 -0.37897200
 H -5.34705900 -0.13208700 -2.06395300
 C -3.37261400 -0.88143700 1.58798100
 H -4.01049500 -1.56716400 1.00417600
 C -4.27489200 0.13494200 2.29870100
 H -4.97499300 -0.39582900 2.96447500
 H -4.87097600 0.74978400 1.60972500
 H -3.67547600 0.80929600 2.92886100
 C -2.59233400 -1.72380200 2.60153600
 H -1.92574700 -1.09499800 3.20626200
 H -1.95469400 -2.47115700 2.11239500
 H -3.30630200 -2.23510800 3.26919100
 Cl 0.04351600 0.50218900 2.43048900
 C -0.91871700 -2.46424700 -2.71173100
 H -1.12638600 -2.38784700 -3.78040000
 C -1.39277900 -3.37389400 -1.87199700
 H -2.07161800 -4.13661100 -2.26442400
 Cl 0.33082100 -2.66169300 0.94035400
 H -1.09980200 -3.38356300 -0.81419400
 C 2.25901900 1.41403100 -1.27455000
 H 2.14580600 0.90933500 -2.25000000
 H 3.15855300 2.04208100 -1.34709300
 C -2.27973700 1.71627400 0.56793700
 H -3.23748200 2.20803600 0.34686400
 H -2.08067400 1.81179700 1.64653600

TS1

Imaginary vibration: -327.06 cm⁻¹

Ru -0.01155000 0.16834700 0.26553900
 Cl -0.24782800 1.34157000 -2.16502000
 P -2.33419500 -0.21980500 0.04602600
 P 2.32190200 -0.08441800 0.15799200
 N 0.06779300 -1.78046700 -0.66040100
 C -1.02142900 -2.31352100 -1.27078400
 C -0.98624500 -3.58740900 -1.84332600
 H -1.88448700 -3.98189000 -2.32078700
 C 0.19394400 -4.32638000 -1.81066700

H 0.24439800 -5.31812800 -2.26504600
 C 1.30496300 -3.77718300 -1.17410800
 H 2.24394000 -4.32834500 -1.10465000
 C 1.21127400 -2.51367600 -0.58623900
 C -3.51567600 1.01697000 -0.74899000
 H -3.04073700 1.16821900 -1.73205600
 C -4.92130800 0.44929300 -0.97732000
 H -5.48059600 0.36510400 -0.03262200
 H -4.91336000 -0.54175100 -1.45600200
 H -5.49234000 1.12711900 -1.63246500
 C -3.57668200 2.38674500 -0.06585500
 H -4.32422800 3.01422900 -0.57847800
 H -2.61846700 2.91797300 -0.11621500
 H -3.88387400 2.31388100 0.98869300
 C -3.32298900 -1.08248600 1.37429400
 H -4.34533500 -1.18724400 0.97553500
 C -3.36368900 -0.21733200 2.64029900
 H -3.95418300 -0.72317300 3.42166900
 H -3.82957400 0.76217100 2.45640400
 H -2.34657200 -0.05512800 3.02560700
 C -2.77381100 -2.48587200 1.65955600
 H -1.73189800 -2.43588200 2.00423800
 H -2.82327800 -3.14052800 0.77626700
 H -3.37664900 -2.95858700 2.45249500
 C 3.15213400 0.31350300 -1.47884600
 H 2.39712600 -0.00142000 -2.21917700
 C 4.44381100 -0.46844300 -1.73567500
 H 4.86902900 -0.18045900 -2.71116600
 H 4.27847800 -1.55499300 -1.76014800
 H 5.21099700 -0.25790200 -0.97296800
 C 3.37183100 1.82115700 -1.64630000
 H 4.05841000 2.22131400 -0.88314300
 H 2.43078700 2.38416000 -1.59801700
 H 3.82245700 2.02812200 -2.63032800
 C 3.58007600 0.43970900 1.45891500
 H 4.51593600 0.61095900 0.90009500
 C 3.85028000 -0.63035000 2.52309900
 H 4.58122300 -0.24075200 3.25036000
 H 4.27125800 -1.55292800 2.09756200
 H 2.92751700 -0.88037300 3.06627700
 C 3.14965600 1.75600900 2.11538800
 H 2.16527900 1.64864300 2.59272200
 H 3.08105300 2.58121000 1.39307500
 H 3.88660800 2.04775300 2.88111600

C 0.41917000 2.81602000 0.42538800
 H 1.42992300 2.79038400 0.05148500
 C -0.41333300 2.08181100 1.08874400
 H -1.37857700 2.38087100 1.48639800
 Cl -0.26706600 4.39854700 -0.80343200
 H -0.34584000 2.65029600 -1.75265900
 Cl 0.18209200 -0.80557800 2.46079300
 C -2.26028500 -1.46952000 -1.34246200
 H -2.22020400 -0.86537600 -2.26475400
 H -3.15834300 -2.10036000 -1.41004200
 C 2.34183100 -1.94303800 0.21319700
 H 2.12728800 -2.16469200 1.27049100
 H 3.30136800 -2.40637300 -0.05060800

TS2

Imaginary vibration: -449.26 cm⁻¹

Ru 0.00002400 0.12782800 0.22923900
 Cl 0.00005500 0.43614800 2.88357300
 P 2.32472800 -0.15752900 0.19366900
 P -2.32465400 -0.15772600 0.19372800
 N 0.00009600 -2.08407300 0.38412900
 C 1.17441100 -2.73153600 0.19592400
 C 1.20261000 -4.04111000 -0.28860500
 H 2.16099200 -4.53350700 -0.45973800
 C 0.00012400 -4.69708400 -0.55176500
 H 0.00013400 -5.71477500 -0.94836800
 C -1.20237600 -4.04118400 -0.28847700
 H -2.16074600 -4.53364000 -0.45950200
 C -1.17419800 -2.73161800 0.19607100
 C 3.33982600 0.57187900 1.59223400
 H 2.72968300 0.32912300 2.47853800
 C 4.72972300 -0.04011500 1.78669800
 H 5.39203600 0.17203500 0.93286400
 H 4.69713700 -1.13162600 1.92547000
 H 5.20952600 0.39111100 2.68106900
 C 3.40004100 2.09845400 1.47056600
 H 3.80000500 2.53857700 2.39864200
 H 2.40911100 2.53355000 1.27652100
 H 4.06577800 2.40596000 0.64920800
 C 3.41319100 0.10396600 -1.31453400
 H 4.43259200 0.21352400 -0.90746400
 C 3.02709700 1.40617800 -2.02879600
 H 3.78760200 1.64805500 -2.78965900
 H 2.94215100 2.25950900 -1.34318200
 H 2.05494500 1.28888200 -2.52314200

C 3.41781800 -1.08226100 -2.28595000
 H 2.40123400 -1.29984300 -2.64088900
 H 3.84072900 -1.99381700 -1.83751700
 H 4.04112700 -0.83215400 -3.16043500
 C -3.33977800 0.57186800 1.59217600
 H -2.72947700 0.32955500 2.47849100
 C -4.72950200 -0.04039800 1.78700900
 H -5.20944400 0.39128600 2.68108400
 H -4.69659300 -1.13180300 1.92652700
 H -5.39186500 0.17097800 0.93302100
 C -3.40037100 2.09839300 1.47002700
 H -4.06634000 2.40548600 0.64870400
 H -2.40957600 2.53366000 1.27566100
 H -3.80026100 2.53871200 2.39804200
 C -3.41317200 0.10334300 -1.31449700
 H -4.43260900 0.21263400 -0.90744200
 C -3.41741700 -1.08297700 -2.28580800
 H -4.04080400 -0.83315000 -3.16031600
 H -3.84001200 -1.99464600 -1.83731000
 H -2.40075900 -1.30024900 -2.64072300
 C -3.02744700 1.40558400 -2.02890300
 H -2.05530400 1.28846100 -2.52331200
 H -2.94265200 2.25900200 -1.34338000
 H -3.78806300 1.64721100 -2.78973500
 C -0.00030800 2.94249100 -1.04043500
 H -0.00040500 2.59946800 -2.07508900
 C -0.00009100 2.15854600 0.03813900
 H 0.00000700 2.70606800 1.00103900
 Cl -0.00045600 4.72623300 -0.94793000
 H 0.00003300 -0.84241100 2.64465400
 Cl 0.00005600 -0.33242100 -2.14024900
 C -2.43027700 -1.99272200 0.58300500
 H -3.32257100 -2.48227700 0.17218500
 H -2.52211300 -2.04803700 1.68280600
 C 2.43050800 -1.99257500 0.58267700
 H 2.52257600 -2.04803400 1.68245200
 H 3.32273900 -2.48202900 0.17160500

TS3

Imaginary vibration: -292.36 cm⁻¹

Ru -0.04512500 -0.12302400 0.30066900
 Cl 0.10463600 -2.14279300 1.82704900
 P -2.39219500 -0.36628600 0.19263600

P 2.07707900 0.84799500 0.46870100
 N -0.57676300 1.83079400 -0.32010100
 C -1.77256100 2.05584300 -0.93048900
 C -2.13833500 3.33792300 -1.34702200
 H -3.10246300 3.47925100 -1.83692600
 C -1.26952700 4.40659700 -1.14571000
 H -1.53430000 5.41156900 -1.48133500
 C -0.06256100 4.16941600 -0.49393300
 H 0.64003500 4.97946400 -0.29420000
 C 0.25355600 2.87636900 -0.07178400
 C -3.27165100 0.34703000 1.68225300
 H -2.75037600 1.31148800 1.81316300
 C -4.76748800 0.61562300 1.50335000
 H -5.33682100 -0.32026400 1.39065000
 H -4.98140500 1.25258700 0.63190200
 H -5.16589200 1.13092200 2.39307700
 C -2.99411600 -0.50960700 2.92162600
 H -3.41356000 -0.02759200 3.81976100
 H -1.91621500 -0.65591500 3.07433400
 H -3.46136300 -1.50474600 2.83632400
 C -3.44164700 -1.84727300 -0.30119900
 H -3.90590100 -2.16343600 0.64861300
 C -2.57770900 -2.99975200 -0.82026000
 H -3.21875700 -3.84134200 -1.12937400
 H -1.89425100 -3.36559500 -0.04226000
 H -1.98057900 -2.68176500 -1.68894000
 C -4.55775200 -1.50819800 -1.29664800
 H -4.14139700 -1.23372900 -2.27756400
 H -5.20228600 -0.68644200 -0.95608400
 H -5.19771600 -2.39282400 -1.44849000
 C 3.11275400 0.65271700 2.02496200
 H 2.36915400 0.91977400 2.79636000
 C 4.29403800 1.62300900 2.12117600
 H 4.73650400 1.57585500 3.12980300
 H 4.00633200 2.66899300 1.93665400
 H 5.08873700 1.35911500 1.40610400
 C 3.55388100 -0.78547400 2.30538000
 H 4.27722600 -1.14323700 1.55633100
 H 2.69849400 -1.47229600 2.33087000
 H 4.05441000 -0.83370900 3.28639700
 C 3.28144300 1.07050900 -0.95216400
 H 4.09496500 1.69442100 -0.54351200
 C 2.62162800 1.82515600 -2.11446400
 H 3.34243400 1.91177500 -2.94416300

H 2.31791700 2.84600100 -1.84051300
 H 1.73952700 1.27899900 -2.48119400
 C 3.86619000 -0.25528500 -1.44297000
 H 3.08198700 -0.88688400 -1.88044900
 H 4.36249600 -0.82408400 -0.64344700
 H 4.61949300 -0.05748100 -2.22311800
 C 2.00067500 -2.65739200 -0.25846600
 H 2.83141000 -2.39268500 0.38634300
 C 0.72695700 -2.26210300 -0.10103500
 H -0.07505100 -2.67984400 -0.69832800
 Cl 2.44890700 -3.65798700 -1.62016700
 H -0.18294400 0.48060200 1.76563600
 Cl -0.05428800 -0.50956000 -2.31457700
 C 1.49636800 2.60383900 0.71740400
 H 2.26701400 3.35959100 0.50943900
 H 1.24113700 2.67265900 1.78879600
 C -2.68256200 0.88942300 -1.14182600
 H -3.72377700 1.21633000 -1.25802200
 H -2.35145900 0.37186900 -2.05967300

TS4

Imaginary vibration: -106.47 cm⁻¹

Ru 0.04716700 -0.34539700 -0.07930400
 Cl 0.14830900 0.18060700 -2.47553900
 P 2.43108900 -0.49666300 -0.01466300
 P -2.15684900 0.56760900 -0.03961000
 N 0.54306300 1.77382200 0.09846600
 C 1.78737200 2.15125500 0.47807300
 C 2.15240100 3.49897900 0.50785400
 H 3.16367800 3.77381700 0.80996400
 C 1.21191400 4.46976400 0.17038000
 H 1.47470200 5.52959000 0.19773300
 C -0.06627800 4.06773800 -0.20370700
 H -0.82901700 4.79702000 -0.47909200
 C -0.37624600 2.70475700 -0.24937500
 C 3.34702800 -0.29438500 -1.62443800
 H 2.76375600 0.48313500 -2.14287900
 C 4.79732500 0.16884800 -1.46712700
 H 5.40493800 -0.54572400 -0.88795100
 H 4.87413200 1.15257200 -0.98125100
 H 5.26562000 0.26007300 -2.46064800
 C 3.23666100 -1.57806300 -2.45358100
 H 3.71132700 -1.42924900 -3.43640700
 H 2.18538100 -1.83818600 -2.63465400
 H 3.74353400 -2.42921900 -1.97036100

C 3.38756500 -1.83568800 0.89272100
 H 4.28428200 -1.99025300 0.27025400
 C 2.58995700 -3.14268200 0.92138900
 H 3.21316900 -3.95237400 1.33343900
 H 2.26077900 -3.45351700 -0.08122200
 H 1.70110600 -3.03410500 1.55697100
 C 3.84994700 -1.43934900 2.29849300
 H 2.98886000 -1.23133300 2.94914500
 H 4.50890700 -0.55874700 2.29028300
 H 4.41969300 -2.27235400 2.74138500
 C -3.56568100 -0.01341900 -1.11586200
 H -4.06134600 -0.75889200 -0.47344300
 C -3.11954700 -0.75444500 -2.37610300
 H -4.01395500 -1.12653900 -2.90044100
 H -2.50819100 -1.62932900 -2.12620200
 H -2.54612000 -0.11335200 -3.05936700
 C -4.54677200 1.11688000 -1.44917100
 H -4.11445500 1.83263900 -2.16658300
 H -4.88017300 1.67785600 -0.56281600
 H -5.44567500 0.68757300 -1.91959000
 C -2.99090100 0.93615000 1.58801600
 H -3.96310400 1.37021400 1.29566600
 C -2.22689100 1.97664600 2.41449600
 H -2.14423200 2.94734700 1.90263500
 H -1.21748300 1.61777600 2.65973200
 H -2.76162000 2.15092600 3.36230100
 C -3.24797400 -0.34878100 2.38592400
 H -2.30090900 -0.74801400 2.77372500
 H -3.72550600 -1.13947000 1.78920400
 H -3.90167300 -0.11920500 3.24324400
 C -0.08517600 -2.20739300 -0.73174400
 H 0.23965100 -2.62692300 -1.68324200
 C -0.87068600 -2.41560700 0.30471600
 H -0.63152400 -2.72026900 1.32825500
 C1 -3.69038300 -3.18153600 0.09659300
 H -2.08777900 -2.64951800 0.12143800
 C1 0.30890500 -0.51658600 2.35762800
 C 2.74401400 1.08048700 0.91169000
 H 3.78381300 1.42756900 0.85909000
 H 2.51023500 0.83192000 1.95795200
 C -1.71744000 2.23705800 -0.72642300
 H -1.64482800 2.07200600 -1.81440300
 H -2.49005600 2.99628900 -0.54259700

TS5

Imaginary vibration: -456.19 cm⁻¹

Ru -0.13476000 -0.38967500 -0.00071700
Cl -0.37337500 -0.23654600 -2.44734700
P 2.12303900 0.37927300 -0.01436300
P -2.51201200 -0.28268300 -0.06791800
N -0.44263200 1.82327700 0.06128500
C 0.57269800 2.63070500 0.44602900
C 0.41557900 4.01967200 0.47242600
H 1.25248300 4.64797000 0.77995700
C -0.81309000 4.57614300 0.12449500
H -0.95905600 5.65832700 0.15036200
C -1.85149100 3.73157200 -0.25909700
H -2.82621300 4.12956900 -0.54454000
C -1.63362800 2.35094300 -0.29748600
C 2.69883900 0.80510900 -1.73635900
H 1.73859500 0.89484300 -2.26538200
C 3.44493300 2.13163200 -1.90177500
H 4.39863700 2.16804700 -1.35593300
H 2.83344000 2.98750800 -1.57729100
H 3.67204900 2.28536100 -2.96983600
C 3.42889600 -0.39282200 -2.35635700
H 3.49463000 -0.26044000 -3.44796000
H 2.89965100 -1.33779600 -2.16193600
H 4.45441200 -0.49839700 -1.96964300
C 3.56436900 -0.41925300 0.85649500
H 3.73999100 -1.31832400 0.24590200
C 3.23625900 -0.90696400 2.26811500
H 4.12585300 -1.41211400 2.67769400
H 2.41583100 -1.62938300 2.25900800
H 2.96648800 -0.08479400 2.94735700
C 4.81943700 0.46167000 0.85531900
H 4.66532700 1.40340600 1.40672600
H 5.16911200 0.70774300 -0.15522200
H 5.63547100 -0.07868600 1.36173600
C -3.53589900 -1.42682300 -1.16769600
H -4.43938400 -1.61513500 -0.56358900
C -2.82778400 -2.76248200 -1.40254900
H -3.49162700 -3.44367100 -1.95837000
H -2.55804300 -3.25560800 -0.45821700
H -1.91281800 -2.61171300 -1.99187200
C -3.97293700 -0.79801300 -2.49463100
H -3.09903700 -0.55381300 -3.11514700
H -4.57484700 0.11150300 -2.35194200

H -4.59472700 -1.51939600 -3.04925900
 C -3.55507100 -0.21972600 1.47865300
 H -4.59153100 -0.15708600 1.09716100
 C -3.27968100 1.01504300 2.34160700
 H -3.49313100 1.95215600 1.80600900
 H -2.23414000 1.03029100 2.67820200
 H -3.92908100 0.99042400 3.23213200
 C -3.39337600 -1.52441400 2.26769500
 H -2.36668400 -1.60525400 2.65326100
 H -3.61179200 -2.41160200 1.65226800
 H -4.08741500 -1.53720200 3.12346800
 C 0.33317300 -2.22802800 -0.36266300
 H 0.33329300 -2.66081900 -1.36596100
 C 0.04563600 -2.94236700 0.78449700
 H 0.42399900 -2.63252200 1.75725600
 Cl 2.44929600 -3.54185300 0.06589400
 H -0.71422900 -3.73784800 0.76926100
 Cl -0.03203100 -0.23146100 2.46387100
 C 1.85830800 1.98514500 0.87244200
 H 2.70223600 2.68134600 0.78377300
 H 1.75492700 1.68889800 1.93008700
 C -2.69672400 1.41534100 -0.79674400
 H -2.52484300 1.27625800 -1.87447100
 H -3.70215900 1.83693500 -0.65390400

TS6

Imaginary vibration: -777.69 cm⁻¹

Ru -0.01183000 -0.19409400 0.18877700
 Cl 0.16680600 -0.97224700 -2.17294100
 P 2.28352400 0.28063900 0.10208900
 P -2.35765000 -0.10778000 0.10071700
 N -0.17511800 1.74038800 -0.54144700
 C 0.89039900 2.34225700 -1.13969600
 C 0.78889500 3.62824900 -1.67479100
 H 1.66809200 4.07819000 -2.13826000
 C -0.42488200 4.30809400 -1.62558400
 H -0.52244200 5.30941800 -2.05030500
 C -1.51118100 3.68192800 -1.01944100
 H -2.48055000 4.17735700 -0.94970400
 C -1.36195900 2.40715000 -0.46983500
 C 3.49218500 -0.92683800 -0.66100400
 H 2.89580300 -1.29892900 -1.51000800
 C 4.77825600 -0.29549400 -1.20124300

H 5.39053700 0.13519600 -0.39271600
 H 4.58403900 0.49636300 -1.93965900
 H 5.39378200 -1.06389600 -1.69859800
 C 3.79806500 -2.11593200 0.25620800
 H 4.23714000 -2.93786100 -0.33291900
 H 2.89636000 -2.49420100 0.75589300
 H 4.52993800 -1.84499800 1.03244200
 C 3.20154400 1.14730800 1.47968800
 H 4.23079900 1.30063700 1.10846200
 C 3.24211700 0.28350600 2.74749400
 H 3.79815100 0.81309800 3.53892300
 H 3.73719000 -0.68256800 2.58287000
 H 2.22135100 0.09277900 3.10801800
 C 2.57655700 2.51802200 1.77208500
 H 1.52736300 2.40370200 2.08057600
 H 2.61950400 3.19552500 0.90635400
 H 3.12445100 3.00269100 2.59700300
 C -3.15688000 -0.51875600 -1.53459400
 H -2.43188000 -0.12381900 -2.26490300
 C -4.51981500 0.13123200 -1.77616200
 H -4.91179000 -0.16770000 -2.76278800
 H -4.46487600 1.23018400 -1.76609100
 H -5.26503200 -0.17763200 -1.02474800
 C -3.19896400 -2.04186900 -1.70578500
 H -3.92586200 -2.50650500 -1.01988600
 H -2.21114500 -2.48770900 -1.52254700
 H -3.50361000 -2.30033100 -2.73318200
 C -3.56772300 -0.78986100 1.37190900
 H -4.47015600 -1.04067900 0.78917900
 C -3.96986800 0.21072900 2.46011100
 H -4.67069500 -0.27462900 3.15947600
 H -4.47569200 1.09820100 2.05161300
 H -3.08916700 0.53658000 3.03238000
 C -3.01425500 -2.07615800 1.99280900
 H -2.12113300 -1.85398700 2.59357300
 H -2.72600700 -2.81567500 1.23307100
 H -3.77546500 -2.53203900 2.64752500
 C1 -0.29682100 0.52891000 2.50098800
 C 1.15945000 -3.33620100 -2.41103300
 H 1.14527100 -2.96262800 -3.41799400
 C 1.25337900 -3.94884200 -1.33141500
 H 1.59379700 -4.90110200 -0.93272700
 C1 0.20803500 -2.56994300 1.01411500
 H 0.74956900 -3.23312200 -0.27598000

C 2.17288200 1.56895500 -1.24013600
H 2.14126100 0.98046300 -2.17198600
H 3.03716500 2.24660800 -1.29275600
C -2.48788300 1.74076400 0.25906700
H -3.45897100 2.17078600 -0.02120500
H -2.32708600 1.91308500 1.33477700