

Electronic Supplementary Information

Theoretical Studies on N–X (X = Cl, O) Bond Activation Mechanism in Catalytic C–H Amination

Yang Yu^a, Gen Luo^{b,*}, Jimin Yang^a, and Yi Luo^{a,*}

^aState Key Laboratory of Fine Chemicals, School of Chemical Engineering, Dalian University of Technology, Dalian 116024, China

^bInstitutes of Physical Science and Information Technology, Anhui University, Hefei 230601, China.

E-mail: luogen@ahu.edu.cn (G.L.); luoyi@dlut.edu.cn (Y.L.).

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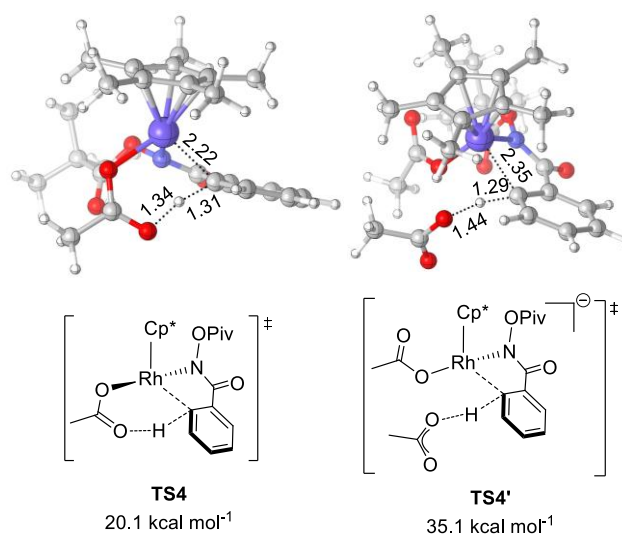


Fig. S1 Transition state structures and corresponding free energy barriers for the intramolecular CMD and intermolecular metalation/deprotonation of **A** by Rh catalyst, respectively (bond distance in angstrom).

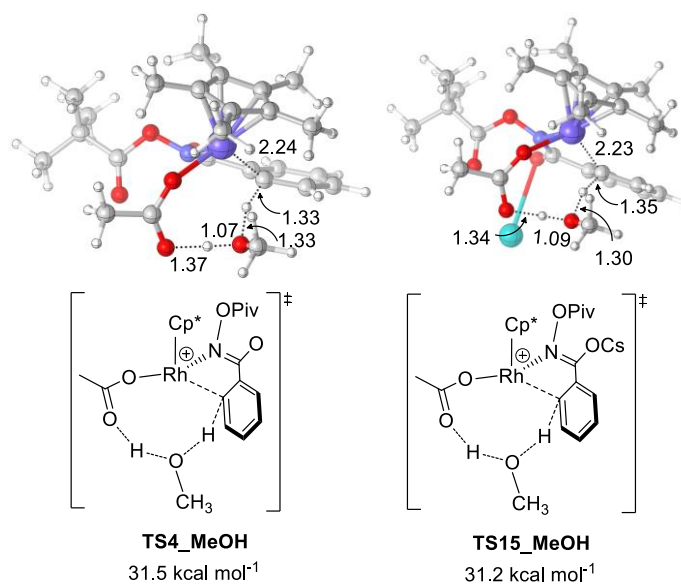


Fig. S2 Transition state structures and corresponding free energy barriers for the methanol-assisted C-H activation of **A** and **A'** by Rh catalyst, respectively (bond distance in angstrom).

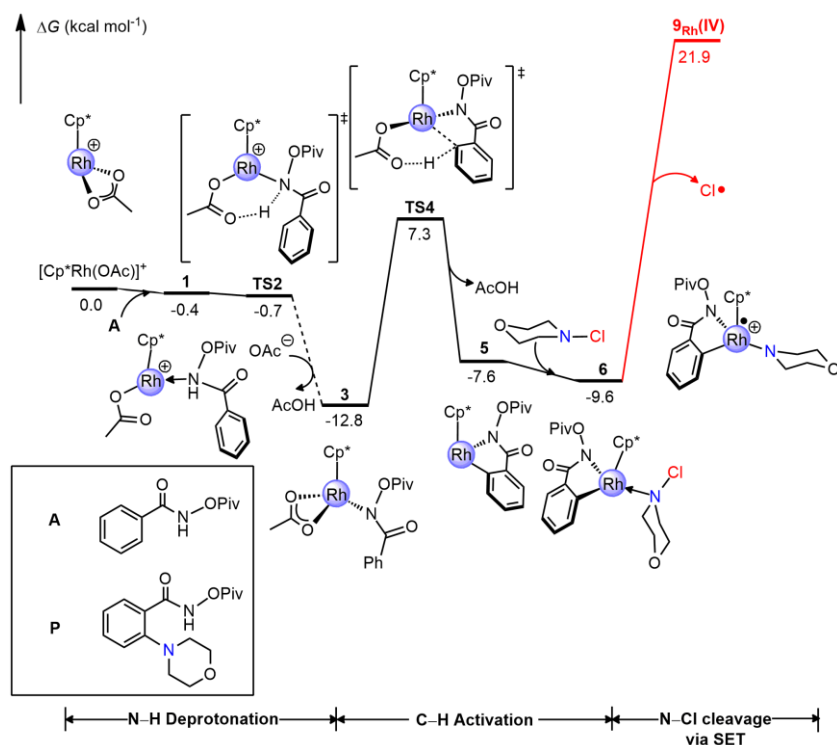


Fig. S3 Free energy profile for the Rh-catalysed C-H amination of **A** with *N*-chloromorpholine via SET process.

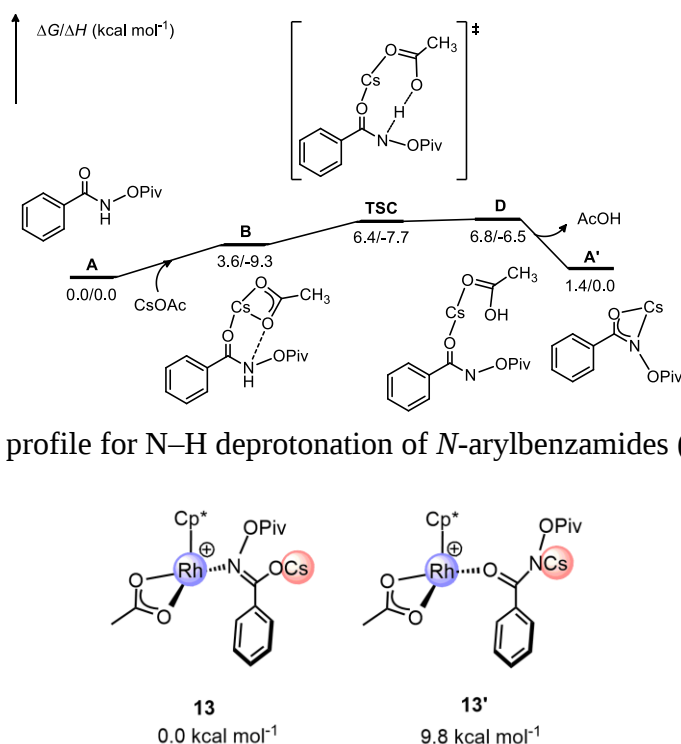


Fig. S5 Comparison of two isomers of different coordinating sites of N and O atoms with Rh center.

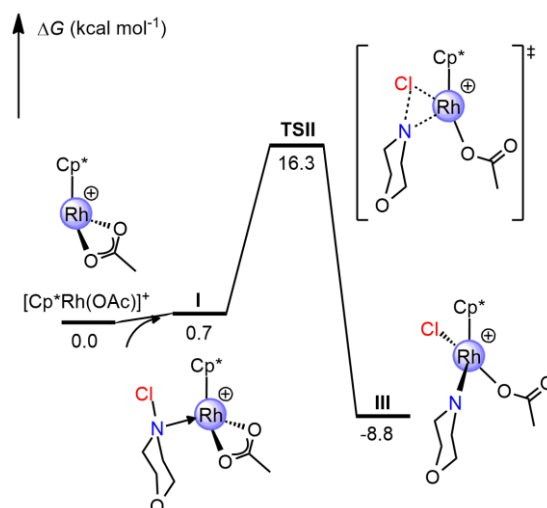


Fig. S6 Free energy profile for the Rh-catalysed amination starting from initial N-Cl cleavage.

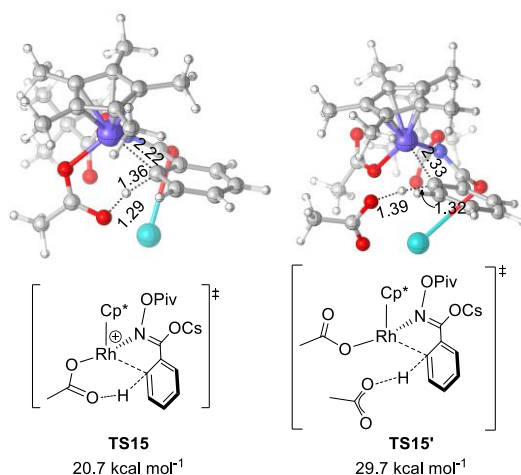


Fig. S7 Transition state structures and corresponding free energy barriers for the intramolecular CMD and intermolecular metalation/deprotonation of A' by the Rh catalyst, respectively (bond distance in angstrom).

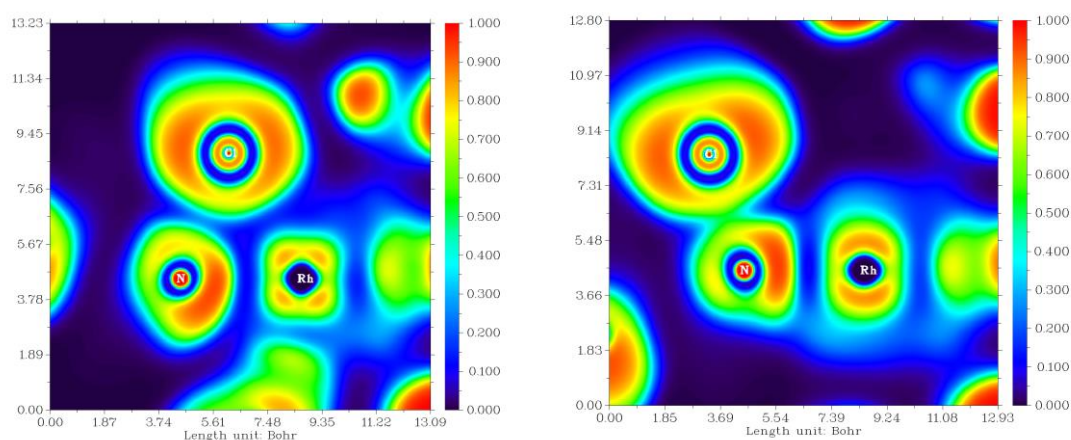


Fig. S8 ELF plots for oxidative addition TS TS18'_{Rh-Cl} (left) and S_N2-type TS TS18_{Rh-Cl} (right). ELF plots were generated by Multiwfn software.

Table S1 DFT test based on Rh-catalysed N–Cl bond cleavage process ($\Delta G^\ddagger$, kcal mol⁻¹)^a

DFT	$\Delta G^\ddagger_{(\text{S}_{\text{N}}2\text{-type})}$	$\Delta G^\ddagger_{(\text{Oxidative Addition})}$
M06-D3	7.9	42.7
M06L	4.8	29.0
ω B97XD	10.0	66.6
TPSSh	18.4	45.5

^a DFT/BSII(SMD)//B3LYP–D3/BSI.**Table S2** Computed free energy barriers for Ru-catalysed N–Cl and N–O bond cleavages, assembling with C₂H₄ ligand instead of *p*-cymene ($\Delta G^\ddagger$, kcal mol⁻¹)

Process	$\Delta G^\ddagger_{(\text{N-Cl Cleavage})}$	$\Delta G^\ddagger_{(\text{N-O Cleavage})}$
Oxidative addition	4.5	2.1
S _N 2-type	5.6	3.3

Cartesian coordinates and electronic energies (a.u., calculated at the level of M06-D3/BSII(SMD)//B3LYP-D3/BSI) for all of the stationary points and the imaginary frequencies (cm⁻¹) of transition states

A, E=-746.440638081 a.u.

C	-0.79551500	0.20568300	-0.58953600
O	-0.27743500	1.23994600	-0.96596500
N	-0.08062400	-1.00484500	-0.47758400
H	-0.23182100	-1.47443800	0.41400600
C	-2.24060400	0.07573900	-0.24332600
C	-2.90601500	-1.15758600	-0.21362000
C	-2.93972700	1.25170700	0.05611000
C	-4.25535900	-1.21100900	0.13010400
H	-2.37884400	-2.06533500	-0.48691600
C	-4.28594700	1.19324200	0.40182000
H	-2.40669300	2.19475200	0.01201500
C	-4.94445000	-0.03816300	0.44208400
H	-4.77086500	-2.16601400	0.14525800
H	-4.82371400	2.10563700	0.63929100
H	-5.99565300	-0.08263500	0.70984100
O	1.30074400	-0.82596200	-0.67310200
C	1.95188800	-0.35571000	0.45032400
O	1.41064700	-0.31613100	1.52911700
C	3.36456200	0.09305500	0.10742800
C	3.22796500	1.43605000	-0.64741200

H	4. 22358000	1. 79638100	-0. 92481200
H	2. 62392200	1. 32095600	-1. 54914500
H	2. 74948500	2. 19077200	-0. 01732600
C	4. 06324300	-0. 94640400	-0. 78966300
H	5. 07914900	-0. 60522300	-1. 01096600
H	4. 13512100	-1. 91789000	-0. 29047300
H	3. 53157000	-1. 08302600	-1. 73298300
C	4. 14633800	0. 28986600	1. 41267600
H	3. 64425400	1. 00592100	2. 06650200
H	4. 24584100	-0. 65162600	1. 96042900
H	5. 14911700	0. 66403300	1. 18605800

B, E=-995.118358269 a.u.

C	-1. 23589200	1. 17171100	-0. 42118600
O	-0. 88943700	1. 39385900	-1. 58091100
N	-0. 33877500	1. 03734200	0. 61771900
H	-0. 49298400	0. 24765800	1. 28933700
C	-2. 67299800	1. 04262700	-0. 02067800
C	-3. 09407000	0. 31567700	1. 10432400
C	-3. 62220100	1. 64158500	-0. 86001300
C	-4. 45691200	0. 20854700	1. 38225300
H	-2. 37765800	-0. 19498800	1. 74057200
C	-4. 97934300	1. 53947500	-0. 56884000
H	-3. 27092500	2. 18279600	-1. 73171300
C	-5. 39862400	0. 82249400	0. 55484000
H	-4. 78224300	-0. 36024900	2. 24795100
H	-5. 70976000	2. 01629700	-1. 21543600
H	-6. 45737800	0. 73942300	0. 78220800
O	0. 98956600	0. 84058900	0. 16256300
C	1. 78954600	1. 96100700	0. 24368900
O	1. 39322300	3. 04209300	0. 58354200
C	3. 22210900	1. 58282200	-0. 14027400
C	3. 23838600	0. 99637000	-1. 56697000
H	4. 27354600	0. 83186600	-1. 88222000
H	2. 72221600	0. 03417400	-1. 60503400
H	2. 76223300	1. 67185400	-2. 28391600
C	3. 74717500	0. 53548400	0. 86632100
H	4. 77820100	0. 27050700	0. 60889100
H	3. 75256600	0. 94398400	1. 88196900
H	3. 14327800	-0. 37593200	0. 87077600
C	4. 07974300	2. 85414300	-0. 09095000
H	3. 71817100	3. 60300800	-0. 80050100
H	4. 05538500	3. 30266700	0. 90469100
H	5. 11696300	2. 60848900	-0. 33892400

C	0.76904100	-1.73285900	2.03280400
O	-0.41476900	-1.38415800	1.67201000
O	1.57391500	-2.37003000	1.31364400
Cs	0.18721200	-1.88299000	-1.25182300
C	1.22045300	-1.27138500	3.41718800
H	0.41456400	-1.39182400	4.14574000
H	2.11226700	-1.81018600	3.74121100
H	1.45785600	-0.20149300	3.36877000

TSC, E=-995.110717067 a.u., Imaginary frequency = 405i

C	-1.29375300	0.75315400	-0.54328300
O	-0.88065000	0.45258200	-1.67986800
N	-0.52377400	0.98543200	0.55416800
H	-0.55188700	-0.02591400	1.46960200
C	-2.76359900	0.80928500	-0.24235000
C	-3.26912300	1.33196800	0.95576500
C	-3.64871200	0.30251900	-1.20119200
C	-4.64249900	1.32916700	1.19385400
H	-2.58214500	1.74942100	1.68274800
C	-5.02114000	0.30293500	-0.96291300
H	-3.23407200	-0.07431100	-2.13015300
C	-5.52029400	0.81305300	0.23791500
H	-5.02966000	1.73778800	2.12254400
H	-5.70253400	-0.08962500	-1.71226400
H	-6.59027200	0.81575500	0.42485600
O	0.87783000	0.86285700	0.19163800
C	1.46274000	2.02575200	-0.21330000
O	0.88438800	3.07571300	-0.33285700
C	2.95209600	1.79012600	-0.51058000
C	3.06333100	0.93407900	-1.78991100
H	4.11140900	0.86168900	-2.09837300
H	2.69657200	-0.08151400	-1.61854300
H	2.48811500	1.36991400	-2.61160700
C	3.63092500	1.06526400	0.66742500
H	4.69358600	0.91741900	0.44671800
H	3.56009200	1.65864700	1.58432200
H	3.17994000	0.09030200	0.86557400
C	3.61338600	3.15448800	-0.74861900
H	3.13805900	3.68084000	-1.57910300
H	3.52643100	3.78966400	0.13656700
H	4.67552300	3.01808700	-0.97616900
C	0.89503000	-1.12979600	2.41677900
O	-0.32578700	-1.05278700	1.91418400
O	1.67318400	-2.02937500	2.09708700

Cs	0.52817200	-2.14733100	-0.80593000
C	1.26999400	-0.04373100	3.40394300
H	0.62241100	-0.10979000	4.28381500
H	2.31303000	-0.14134500	3.70481700
H	1.10035100	0.93664000	2.94891900

D, E=-995.111854046 a.u.

C	-1.32456600	0.69625700	-0.51052100
O	-0.90102900	0.33224200	-1.62996300
N	-0.58264200	1.00349400	0.57824600
H	-0.56431900	-0.14910700	1.59694500
C	-2.80246000	0.74747600	-0.23293100
C	-3.33477100	1.33813900	0.92121900
C	-3.66637000	0.16922100	-1.16979100
C	-4.71162900	1.33223800	1.13830000
H	-2.66315000	1.80919800	1.62960500
C	-5.04278900	0.16550500	-0.95288100
H	-3.23176100	-0.25864200	-2.06698600
C	-5.56815100	0.74407000	0.20463200
H	-5.11871600	1.79465600	2.03282200
H	-5.70683600	-0.28336300	-1.68622900
H	-6.64100600	0.74423500	0.37476100
O	0.83359100	0.89431000	0.22575900
C	1.38863200	2.04564300	-0.23935200
O	0.78642500	3.07462300	-0.41849500
C	2.88587800	1.84166700	-0.53085800
C	3.01348700	1.01268100	-1.82644300
H	4.06313300	0.96125500	-2.13419900
H	2.66033500	-0.01155100	-1.67828900
H	2.43310400	1.45667100	-2.63988200
C	3.58306100	1.11168100	0.63168300
H	4.64823300	0.99003500	0.40673100
H	3.50190900	1.68669500	1.55928000
H	3.15488100	0.12380200	0.81514400
C	3.52217900	3.22206500	-0.74639700
H	3.03172400	3.75487900	-1.56339900
H	3.42898500	3.83870400	0.15147500
H	4.58560200	3.10968600	-0.98153200
C	0.95630700	-1.09723400	2.45193400
O	-0.27613500	-1.10683700	1.93844500
O	1.75265000	-1.98812200	2.18103100
Cs	0.61613500	-2.13753300	-0.80256800
C	1.27399900	0.05494300	3.37631400
H	0.65301800	-0.01927200	4.27477900

H	2.32720700	0.03651900	3.65482700
H	1.02787900	0.99959200	2.88400700

A', E=-766.059068362 a.u.

C	0.63576200	-1.16343400	0.43817600
O	0.17542900	-0.41579100	1.35355100
N	-0.00945200	-1.91703800	-0.44162700
C	2.13531400	-1.18274500	0.20873400
C	2.72489600	-1.73976300	-0.93666500
C	2.95656800	-0.56734000	1.16341600
C	4.10494900	-1.67256400	-1.12111700
H	2.08478700	-2.22002500	-1.66766200
C	4.33881500	-0.50359800	0.97954700
H	2.47923000	-0.15631800	2.04775400
C	4.91725100	-1.05242200	-0.16652000
H	4.55107300	-2.10609800	-2.01209400
H	4.96555700	-0.03421500	1.73357900
H	5.99266100	-1.00433900	-0.31301300
O	-1.43304000	-1.87711500	-0.12517500
C	-2.10991100	-0.79617400	-0.47122900
O	-1.67200100	0.16077400	-1.10492100
C	-3.53849900	-0.81340900	0.09040700
C	-3.47926500	0.09279000	1.34281600
H	-4.44486400	0.08853600	1.85932900
H	-2.70159000	-0.25384300	2.02905100
H	-3.25006700	1.12520200	1.05640400
C	-4.00025100	-2.22160300	0.49169400
H	-5.02574300	-2.17602400	0.87469600
H	-3.98500500	-2.90088200	-0.36538500
H	-3.35681700	-2.64531200	1.26460000
C	-4.49425200	-0.21148900	-0.95067100
H	-4.13300700	0.76317900	-1.28640300
H	-4.57932000	-0.86085600	-1.82805400
H	-5.49381800	-0.09102900	-0.51990800
Cs	0.27730400	2.07161600	-0.13055800

CsOAc, E=-248.661094842 a.u.

C	-1.97933900	0.00963700	-0.00285600
O	-1.40683200	-1.12112600	-0.00191900
O	-1.40359000	1.13729200	-0.00173700
Cs	1.22066100	-0.00144300	0.00032600
C	-3.51610600	-0.00382400	0.00127600
H	-3.87362600	-0.48481100	0.91882600
H	-3.92424500	1.00656800	-0.06230000

H	-3.88242300	-0.60661300	-0.83574400
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AcOH, E=-229.042220693 a.u.

C	-0.09200100	0.12530200	-0.00002600
O	-0.64360600	1.20237100	0.00000500
C	1.39584600	-0.11062900	-0.00000700
H	1.68002900	-0.69345100	-0.88079500
H	1.91528900	0.84629400	-0.00065000
H	1.68015900	-0.69223200	0.88155600
O	-0.77875300	-1.04573400	0.00000000
H	-1.71967700	-0.80175000	0.00004400

OAc⁻, E=-228.579049837 a.u.

C	0.22053300	0.00193200	-0.00021300
O	0.81011000	-1.10780300	-0.00001100
C	-1.35419300	-0.05721600	-0.00005700
H	-1.74737400	0.47141400	-0.87941100
H	-1.73141400	-1.08694600	-0.00058900
H	-1.74711100	0.47034100	0.88006500
O	0.69337200	1.16741500	0.00020600

[Cp^{*}Rh(OAc)]⁺, E=-728.788068678 a.u.

Rh	-0.34975800	-0.00113400	-0.15249200
C	-2.82051800	-0.00948600	-0.18045800
O	-2.14289700	-1.10092200	-0.14758100
O	-2.14397500	1.08592800	-0.14183800
C	-4.30714900	-0.00089200	-0.25358200
C	1.15122200	-0.01330300	1.35681100
C	1.35609300	-1.18436000	0.51621000
C	1.60500700	-0.71944700	-0.80652700
C	1.34478100	1.17980100	0.54354800
C	1.59840300	0.74855300	-0.78953200
C	1.84063500	1.61510900	-1.98147400
H	2.92061900	1.69933800	-2.15611500
H	1.39420500	1.19037200	-2.88367500
H	1.44166000	2.62034400	-1.83943000
C	1.85396100	-1.55571500	-2.01846700
H	1.40471600	-1.11310800	-2.91062400
H	2.93463400	-1.62764600	-2.19448100
H	1.46265600	-2.56705800	-1.90041000
C	1.29210900	-2.60440300	0.98041700
H	1.09211600	-3.28913300	0.15523600
H	2.24975900	-2.88698900	1.43339100
H	0.51133600	-2.74293500	1.73147300

C	0.88042600	-0.03157600	2.82220900
H	0.32958100	-0.92565400	3.11961400
H	1.83795300	-0.03314000	3.36014100
H	0.32104900	0.85003100	3.14019500
C	1.26861200	2.58763800	1.04150700
H	0.48730200	2.70134700	1.79615400
H	2.22414200	2.86758400	1.50062300
H	1.06203200	3.29003900	0.23297900
H	-4.69282100	-1.01334900	-0.37265700
H	-4.62585300	0.63505600	-1.08460300
H	-4.70247900	0.44436200	0.66569500

1, E=-1475.25746311 a.u.

Rh	0.82880700	0.78087100	0.09549400
C	0.32092800	0.57907400	3.07475200
O	0.96423500	1.16421100	2.08870500
O	-0.45570700	-0.37796000	2.94269900
C	0.41722200	1.52512300	-1.91787800
C	0.66375600	2.60982200	-0.97086200
C	2.03092900	2.50289600	-0.49281100
C	1.59012600	0.72090200	-1.96632700
C	2.58613700	1.32085400	-1.07416800
C	3.94620200	0.75632700	-0.82942700
H	4.60911000	1.02730000	-1.66070400
H	4.38185800	1.13645900	0.09536700
H	3.91455000	-0.33492900	-0.77494900
C	2.67251600	3.43835000	0.48417900
H	2.15339500	3.39461800	1.44720800
H	3.71941500	3.18427600	0.65364600
H	2.62678000	4.46574800	0.11011800
C	-0.29881400	3.68869400	-0.60648200
H	-1.32221900	3.30951000	-0.56341900
H	-0.04788000	4.13132400	0.35894900
H	-0.26417800	4.48009200	-1.36646200
C	-0.83938200	1.30551300	-2.69660800
H	-1.68198700	1.83083200	-2.24679200
H	-0.70352900	1.68268900	-3.71726200
H	-1.09236900	0.24468400	-2.74665400
C	1.80132000	-0.48508200	-2.82366200
H	0.85502100	-0.98138500	-3.04540100
H	2.26150200	-0.18405900	-3.77255000
H	2.46118500	-1.20999100	-2.34339900
C	0.61126500	1.17690800	4.43156800
H	0.09949100	0.61020500	5.20868400

H	1.68998700	1.18056500	4.61176300
H	0.27521800	2.21826700	4.44851100
C	-0.49218200	-1.76824800	-0.54830800
O	-1.09724200	-1.88469100	-1.59256200
N	-0.78266500	-0.63515800	0.32713800
H	-0.79430500	-0.80428500	1.36993600
C	0.66370800	-2.60144100	-0.13674700
C	1.28607600	-2.50009200	1.12204000
C	1.16851800	-3.49674400	-1.09563100
C	2.41943400	-3.26577800	1.39580500
H	0.87801200	-1.86907000	1.90434500
C	2.29713100	-4.25890500	-0.81220300
H	0.66292000	-3.57797500	-2.05154200
C	2.92942000	-4.13774800	0.43090700
H	2.89123000	-3.19422600	2.37055000
H	2.68253900	-4.95103500	-1.55407200
H	3.80832700	-4.73569000	0.65173200
O	-1.99250000	0.00997100	-0.02784900
C	-3.12193800	-0.74946400	0.33779900
O	-2.99811000	-1.78586800	0.92909300
C	-4.39487900	-0.08380900	-0.16206700
C	-4.45726000	-0.32703200	-1.69007100
H	-5.38367500	0.10212700	-2.08311700
H	-3.61260100	0.13996500	-2.20276900
H	-4.44854800	-1.39602100	-1.92022000
C	-4.37609500	1.42957400	0.13720400
H	-5.31688400	1.87385100	-0.20011500
H	-4.27598600	1.62284400	1.20979600
H	-3.55663100	1.93395400	-0.38244100
C	-5.58821600	-0.75711300	0.53566400
H	-5.59714000	-1.83296000	0.34816200
H	-5.55119900	-0.60421900	1.61784400
H	-6.52002300	-0.32732300	0.15741400

TS2, E=-1475.25084403 a.u., Imaginary frequency = 826i

Rh	0.82880700	0.78087100	0.09549400
C	0.32092800	0.57907400	3.07475200
O	0.96423500	1.16421100	2.08870500
O	-0.45570700	-0.37796000	2.94269900
C	0.41722200	1.52512300	-1.91787800
C	0.66375600	2.60982200	-0.97086200
C	2.03092900	2.50289600	-0.49281100
C	1.59012600	0.72090200	-1.96632700
C	2.58613700	1.32085400	-1.07416800

C	3.94620200	0.75632700	-0.82942700
H	4.60911000	1.02730000	-1.66070400
H	4.38185800	1.13645900	0.09536700
H	3.91455000	-0.33492900	-0.77494900
C	2.67251600	3.43835000	0.48417900
H	2.15339500	3.39461800	1.44720800
H	3.71941500	3.18427600	0.65364600
H	2.62678000	4.46574800	0.11011800
C	-0.29881400	3.68869400	-0.60648200
H	-1.32221900	3.30951000	-0.56341900
H	-0.04788000	4.13132400	0.35894900
H	-0.26417800	4.48009200	-1.36646200
C	-0.83938200	1.30551300	-2.69660800
H	-1.68198700	1.83083200	-2.24679200
H	-0.70352900	1.68268900	-3.71726200
H	-1.09236900	0.24468400	-2.74665400
C	1.80132000	-0.48508200	-2.82366200
H	0.85502100	-0.98138500	-3.04540100
H	2.26150200	-0.18405900	-3.77255000
H	2.46118500	-1.20999100	-2.34339900
C	0.61126500	1.17690800	4.43156800
H	0.09949100	0.61020500	5.20868400
H	1.68998700	1.18056500	4.61176300
H	0.27521800	2.21826700	4.44851100
C	-0.49218200	-1.76824800	-0.54830800
O	-1.09724200	-1.88469100	-1.59256200
N	-0.78266500	-0.63515800	0.32713800
H	-0.79430500	-0.80428500	1.36993600
C	0.66370800	-2.60144100	-0.13674700
C	1.28607600	-2.50009200	1.12204000
C	1.16851800	-3.49674400	-1.09563100
C	2.41943400	-3.26577800	1.39580500
H	0.87801200	-1.86907000	1.90434500
C	2.29713100	-4.25890500	-0.81220300
H	0.66292000	-3.57797500	-2.05154200
C	2.92942000	-4.13774800	0.43090700
H	2.89123000	-3.19422600	2.37055000
H	2.68253900	-4.95103500	-1.55407200
H	3.80832700	-4.73569000	0.65173200
O	-1.99250000	0.00997100	-0.02784900
C	-3.12193800	-0.74946400	0.33779900
O	-2.99811000	-1.78586800	0.92909300
C	-4.39487900	-0.08380900	-0.16206700
C	-4.45726000	-0.32703200	-1.69007100

H	-5.38367500	0.10212700	-2.08311700
H	-3.61260100	0.13996500	-2.20276900
H	-4.44854800	-1.39602100	-1.92022000
C	-4.37609500	1.42957400	0.13720400
H	-5.31688400	1.87385100	-0.20011500
H	-4.27598600	1.62284400	1.20979600
H	-3.55663100	1.93395400	-0.38244100
C	-5.58821600	-0.75711300	0.53566400
H	-5.59714000	-1.83296000	0.34816200
H	-5.55119900	-0.60421900	1.61784400
H	-6.52002300	-0.32732300	0.15741400

3, E=-1474.81974965 a.u.

Rh	0.33693300	0.90265000	0.16734500
C	-0.89122100	0.80813300	2.38053300
O	0.35362700	0.54524600	2.33390300
O	-1.44165600	1.26441700	1.31993800
C	0.28256200	1.90551600	-1.72361000
C	0.59255600	2.89686900	-0.69874100
C	1.81365700	2.52110900	-0.08019500
C	1.37232800	0.96875300	-1.77423500
C	2.29044200	1.30063000	-0.72516300
C	3.58242000	0.61878500	-0.41157500
H	4.41379800	1.14673500	-0.89574100
H	3.76910100	0.60936100	0.66382300
H	3.58516800	-0.41665400	-0.75104100
C	2.51287400	3.20562500	1.05033800
H	2.84003200	2.47885700	1.79815100
H	3.39945800	3.73887700	0.68708600
H	1.86175600	3.92696900	1.54679500
C	-0.28794800	4.05349400	-0.34996400
H	-1.33005200	3.73372300	-0.27013700
H	-0.00229700	4.50128600	0.60314100
H	-0.22665300	4.82679900	-1.12452300
C	-0.89508100	1.92454400	-2.64380900
H	-1.75621300	2.39947800	-2.16950100
H	-0.66294000	2.47966000	-3.56146100
H	-1.18267800	0.90812700	-2.92007900
C	1.49960800	-0.14090800	-2.76730300
H	0.58363700	-0.73220700	-2.83941900
H	1.71266300	0.28223500	-3.75605000
H	2.30968000	-0.81975500	-2.50357300
C	-1.71090900	0.53667900	3.60316500
H	-2.45814800	1.32130200	3.74188500

H	-2.23270900	-0.41013400	3.43002100
H	-1.07494900	0.44903000	4.48489000
C	0.22818200	-2.07960400	-0.59543600
O	-0.23735100	-2.80032500	-1.48064800
N	-0.42300500	-1.02540500	-0.00983000
C	1.60258600	-2.33188900	-0.03830300
C	1.97730400	-1.96583700	1.26096800
C	2.51817900	-3.00552600	-0.85698200
C	3.26665900	-2.24348500	1.71737800
H	1.26252000	-1.46980200	1.90558000
C	3.80911900	-3.26969200	-0.40289900
H	2.18899900	-3.32202600	-1.84107000
C	4.18775200	-2.88409600	0.88634900
H	3.54875700	-1.96306600	2.72818800
H	4.51599200	-3.78466900	-1.04705800
H	5.19115700	-3.09546300	1.24471100
O	-1.73035100	-0.90008900	-0.58121400
C	-2.72809600	-1.24684000	0.27598200
O	-2.55659800	-1.69604800	1.38569800
C	-4.08681100	-1.00380700	-0.38646900
C	-4.21753700	-1.96526600	-1.58652800
H	-5.17502700	-1.79902600	-2.09182600
H	-3.40658800	-1.81189400	-2.30182000
H	-4.18136000	-3.00802100	-1.25678300
C	-4.16814700	0.45873800	-0.86676000
H	-5.16759200	0.65960800	-1.26730200
H	-3.97584600	1.15155300	-0.04216700
H	-3.43518300	0.65353100	-1.65171400
C	-5.18740800	-1.28308700	0.64451000
H	-5.11659800	-2.30380600	1.02691100
H	-5.10801400	-0.60286500	1.49708900
H	-6.17059700	-1.14778500	0.18235000

TS4, E=-1474.78200594 a.u., Imaginary frequency = 936i

Rh	-0.76192800	-0.54373900	0.12309700
C	0.36426800	-0.25035000	2.82588600
O	-0.28501800	0.83117400	2.88287900
O	0.27901700	-1.08721800	1.86605000
C	-0.46031500	-2.36250700	-1.03791500
C	-1.58745900	-2.58841400	-0.14806000
C	-2.60933800	-1.65542000	-0.46915900
C	-0.82725500	-1.30302300	-1.94065600
C	-2.12762400	-0.82673600	-1.56888400
C	-2.91080500	0.24411600	-2.26104100

H	-3.56440400	-0.18937500	-3.02774600
H	-3.53111600	0.79833800	-1.55472200
H	-2.24945300	0.96355200	-2.74666100
C	-3.97433400	-1.57774100	0.13997600
H	-4.37424700	-0.56474200	0.08098900
H	-4.66698100	-2.24380200	-0.38942400
H	-3.96230200	-1.87401400	1.19134200
C	-1.60711700	-3.61258400	0.94113900
H	-0.71539500	-3.51734900	1.56706100
H	-2.48394100	-3.49831900	1.58083900
H	-1.62253200	-4.62307400	0.51702500
C	0.81140500	-3.14941100	-1.05351600
H	1.08939900	-3.45322100	-0.04152700
H	0.71084800	-4.05478700	-1.66541200
H	1.63132400	-2.55414600	-1.45946400
C	0.03021600	-0.76437000	-3.04112500
H	1.08064500	-0.75357600	-2.74728100
H	-0.07580100	-1.38501300	-3.93885300
H	-0.24970600	0.25828100	-3.29874800
C	1.32721200	-0.57964300	3.93781500
H	1.40928400	-1.65964500	4.07136300
H	2.30160600	-0.18836400	3.62976500
H	1.02381000	-0.09303200	4.86541800
C	0.43333000	2.07922900	-0.55093400
O	1.16224500	2.89159600	-1.11864000
N	0.74413200	0.79911800	-0.20338200
C	-0.97817600	2.36189600	-0.11583200
C	-1.63114000	1.41517700	0.70737300
C	-1.63612500	3.50123500	-0.57100300
C	-2.96963800	1.65583700	1.06131000
H	-0.94868100	0.96802200	1.72616000
C	-2.97065300	3.71054000	-0.21786500
H	-1.09271000	4.19838800	-1.20121500
C	-3.63719400	2.79160100	0.60134900
H	-3.47630400	0.96617900	1.73113900
H	-3.49268500	4.59421900	-0.57357500
H	-4.66869300	2.97299800	0.89067500
O	1.99485800	0.37519700	-0.69677700
C	3.01330400	0.46045000	0.21508600
O	2.86363500	0.73310700	1.38062600
C	4.35558700	0.23732800	-0.48276700
C	4.68848000	1.56760300	-1.19864100
H	5.62197700	1.46037300	-1.76121900
H	3.88529000	1.85489700	-1.88106800

H	4.81377800	2.37519900	-0.47182400
C	4.27417700	-0.90539500	-1.51051000
H	5.25973400	-1.06176300	-1.96106500
H	3.96921000	-1.84442400	-1.03645900
H	3.56712200	-0.67417900	-2.30976200
C	5.41599200	-0.07863400	0.57996500
H	5.45144600	0.70581500	1.33823200
H	5.19797900	-1.02428900	1.08631600
H	6.40067700	-0.16030000	0.10895700

5, E=-1245.74620593 a.u.

Rh	0.82859100	-0.34790100	0.23751000
C	0.81840900	-1.81421500	-1.32256400
C	2.18762500	-1.68469500	-0.85984800
C	2.20354600	-2.04502100	0.51271600
C	0.02593700	-2.41510000	-0.26121800
C	0.85704200	-2.50881200	0.87300500
C	0.46780300	-2.99673900	2.23124700
H	0.80628700	-4.02971400	2.38040100
H	0.92216900	-2.38478100	3.01488500
H	-0.61494100	-2.97184800	2.36768600
C	3.38701100	-2.06343500	1.42768800
H	3.10164700	-1.78696200	2.44567700
H	3.83712500	-3.06352000	1.46659000
H	4.15400300	-1.36018300	1.09719000
C	3.34814500	-1.28462000	-1.71588800
H	3.12289600	-0.39580500	-2.30932400
H	4.23291200	-1.06961400	-1.11447900
H	3.60517200	-2.09779700	-2.40501400
C	0.32425600	-1.51450800	-2.69980500
H	1.01197400	-0.85047300	-3.22656500
H	0.23260500	-2.44213700	-3.27971500
H	-0.65286000	-1.02845600	-2.65801100
C	-1.41269400	-2.81214000	-0.37319800
H	-1.93169500	-2.18645200	-1.10026700
H	-1.50311800	-3.85583600	-0.69828700
H	-1.92943300	-2.71466600	0.58452200
C	-0.52558400	2.24904300	0.43534500
O	-1.45294200	3.04452700	0.43833200
N	-0.65008500	0.87482500	0.64876700
C	0.91368900	2.56714700	0.20406700
C	1.78089500	1.46555800	0.08796700
C	1.36227000	3.88146900	0.12241100
C	3.14107200	1.72794700	-0.09209300

C	2.72535700	4.12345400	-0.06839500
H	0.64287100	4.69057700	0.20808400
C	3.60915000	3.04816600	-0.16643200
H	3.85601100	0.91489500	-0.17164700
H	3.09547300	5.14205700	-0.13603300
H	4.67166300	3.23346700	-0.30358100
O	-1.99859300	0.48785400	0.82845400
C	-2.71218200	0.33920700	-0.32611300
O	-2.21732800	0.33426100	-1.43121700
C	-4.20516500	0.22558100	-0.02203300
C	-4.70969500	1.67923600	0.14215700
H	-5.77484700	1.66977400	0.39606000
H	-4.15500500	2.19726400	0.92724500
H	-4.57808600	2.24144700	-0.78638400
C	-4.46440200	-0.56683400	1.27113000
H	-5.54305800	-0.62900000	1.44766000
H	-4.07816600	-1.58885200	1.19571000
H	-3.99917400	-0.08725800	2.13381200
C	-4.90190100	-0.44861600	-1.21156700
H	-4.68529900	0.08020100	-2.14158600
H	-4.57115700	-1.48609600	-1.32827900
H	-5.98453800	-0.45405200	-1.05167500

6, E=-1993.02643964 a.u.

Rh	-0.68821100	-0.62531600	-0.05061700
C	-0.31587200	-2.68131400	0.52032200
C	-1.74580100	-2.53233900	0.40601400
C	-2.04612000	-2.19728900	-0.94854800
C	0.25035100	-2.59223200	-0.82427500
C	-0.80065300	-2.28627100	-1.70790400
C	-0.70442300	-2.14548500	-3.19577900
H	-1.03321100	-3.07302200	-3.68154200
H	-1.33707300	-1.33616500	-3.56892100
H	0.31864000	-1.93898700	-3.51421700
C	-3.41750500	-2.05054100	-1.54112600
H	-3.39783800	-1.45418000	-2.45741900
H	-3.84343400	-3.02787500	-1.80266100
H	-4.10535100	-1.56624900	-0.84268100
C	-2.73074800	-2.77321400	1.50875700
H	-2.37221200	-2.37872300	2.46093800
H	-3.69591300	-2.30898500	1.30023300
H	-2.89325100	-3.85217100	1.62302300
C	0.44266400	-3.05969000	1.75641500
H	-0.13878500	-2.83520400	2.65338800

H	0.66569400	-4.13425700	1.75541300
H	1.38066600	-2.50362800	1.81810100
C	1.69327600	-2.80559600	-1.17372600
H	2.33428100	-2.61515500	-0.31237100
H	1.86408400	-3.83908900	-1.50090400
H	2.01018900	-2.14117800	-1.98240000
C	0.78752100	0.96335200	2.00945700
O	1.66576300	1.64349000	2.54239700
N	0.93881300	0.17325500	0.90470100
C	-0.65281800	0.93955800	2.41751000
C	-1.55944900	0.34795100	1.51716000
C	-1.08916600	1.60528300	3.56380500
C	-2.92807500	0.47028000	1.78252300
C	-2.45662900	1.69365300	3.83032800
H	-0.34488200	2.06177900	4.21051400
C	-3.37261100	1.13551000	2.93381800
H	-3.66127200	0.04589700	1.09978800
H	-2.80914500	2.20826400	4.71962300
H	-4.43961200	1.21830900	3.12751200
O	2.14335200	0.45436200	0.20402200
C	3.24700800	-0.21323900	0.64269400
O	3.22749400	-1.13664500	1.42433000
C	4.49943000	0.37898000	-0.01039500
C	4.65583500	1.83034500	0.49684000
H	5.57166900	2.26762400	0.08411700
H	3.80290000	2.44267900	0.19691100
H	4.71367600	1.85914000	1.58842400
C	4.33601000	0.36835400	-1.54562900
H	5.23152100	0.79081600	-2.01389500
H	4.20981600	-0.65340200	-1.92084900
H	3.46921500	0.95619500	-1.85682000
C	5.71280800	-0.46592500	0.40244800
H	5.82790000	-0.47904200	1.48893200
H	5.60377300	-1.50204200	0.06891700
H	6.62274000	-0.05061700	-0.04305600
C	-2.21977900	1.49937200	-1.71446100
C	-2.42730500	2.82351400	-2.44609200
C	-0.60797500	3.79494500	-1.34095000
C	-0.32409500	2.51637400	-0.56161900
H	-1.90654800	2.81216700	-3.41628200
H	-3.49593300	2.96665300	-2.63218500
H	-2.80153000	1.49230800	-0.78742100
H	-2.51748800	0.64505200	-2.32318200
H	-0.00149200	3.83890000	-2.25822700

H	-0.34750400	4.65340800	-0.71608500
H	0.73564300	2.38912700	-0.34624100
H	-0.87361700	2.53294200	0.38218900
N	-0.81462700	1.27855400	-1.25478000
O	-1.99206000	3.91553300	-1.65326200
C1	0.23777800	1.06384300	-2.74575200

TS8', E=-1992.96156456 a.u., Imaginary frequency = 261i

Rh	0.61874400	0.43355600	-0.10792000
C	0.55217900	2.66445000	0.37383200
C	1.93077900	2.25201700	0.28050800
C	2.18850400	1.87265200	-1.07994600
C	0.00734100	2.68633200	-0.96003200
C	0.99673100	2.15588800	-1.83638400
C	0.83482800	2.01206100	-3.31562900
H	0.89291500	2.99671700	-3.79721500
H	1.61575300	1.38502200	-3.75223200
H	-0.13711200	1.57598000	-3.55952000
C	3.51984000	1.52916100	-1.68100900
H	3.44974700	0.68711100	-2.37587900
H	3.91746100	2.38231800	-2.24508600
H	4.25366900	1.27186100	-0.91586400
C	2.93399100	2.37383300	1.38426000
H	2.50620300	2.07233500	2.34283300
H	3.81183000	1.75156600	1.20806100
H	3.26090300	3.41765700	1.47070500
C	-0.10789300	3.20640200	1.60320900
H	0.42391000	2.89406100	2.50407600
H	-0.11179700	4.30341000	1.57381500
H	-1.13340100	2.84372900	1.67067900
C	-1.36437100	3.08344100	-1.37452800
H	-1.91793400	3.54539200	-0.55818800
H	-1.32768800	3.76654500	-2.23126800
H	-1.92805700	2.19263100	-1.69277500
C	-0.22243400	-0.78661400	2.49571400
O	-0.90135000	-1.32239800	3.36572500
N	-0.70069600	-0.06849700	1.41821800
C	1.26041900	-0.90198900	2.39649800
C	1.84659200	-0.51329100	1.18711400
C	2.00057900	-1.57449500	3.37189400
C	3.17383500	-0.86595500	0.92683400
C	3.34166300	-1.87321700	3.13411100
H	1.49065500	-1.88336300	4.28001700
C	3.91897400	-1.53503500	1.90473800

H	3.63256600	-0.63137000	-0.02731400
H	3.92843400	-2.39304200	3.88572200
H	4.95401400	-1.79823600	1.70123900
O	-2.02000400	-0.50592800	1.12372500
C	-2.94162600	0.44598600	0.87551100
O	-2.74900100	1.64081600	0.95504000
C	-4.29363600	-0.17492500	0.50167600
C	-5.23116100	0.08124600	1.70340100
H	-6.23582500	-0.29011600	1.47497400
H	-4.86992500	-0.43486500	2.59877600
H	-5.29473700	1.15080900	1.92212000
C	-4.19970500	-1.68187900	0.21190400
H	-5.18943800	-2.06000400	-0.06651800
H	-3.50890400	-1.87677000	-0.61303900
H	-3.85149800	-2.23517700	1.08734100
C	-4.81381000	0.57560300	-0.74043900
H	-4.84837600	1.65159900	-0.55386800
H	-4.16186700	0.39565100	-1.60116800
H	-5.82126200	0.22702800	-0.99063800
C	1.50586700	-1.78455000	-2.24148200
C	0.83417400	-2.75252800	-3.22552100
C	-0.52663300	-3.64163700	-1.54309500
C	0.06474700	-2.69812100	-0.49198200
H	-0.02539100	-2.25306000	-3.69572800
H	1.54342800	-3.05039100	-4.00401500
H	2.45595400	-2.23539700	-1.90072800
H	1.74139100	-0.83795500	-2.73285300
H	-1.42649800	-3.18725300	-1.98098500
H	-0.80041300	-4.59384000	-1.08021200
H	-0.69874700	-2.38165000	0.21987400
H	0.84471900	-3.23588800	0.07553500
N	0.71079100	-1.53060300	-1.06166000
O	0.42620700	-3.93698200	-2.56036700
Cl	-1.21495600	-0.31661400	-1.85412400

7, E=-2241.68976239 a.u.

Rh	-1.18431200	0.34845600	0.80626700
C	-0.94594100	1.73056600	2.42109900
C	-1.98828700	0.80396400	2.82753500
C	-1.39644200	-0.48543100	2.90237000
C	0.31991200	1.00002300	2.44491700
C	0.04051800	-0.36007700	2.67441300
C	1.05525800	-1.45506500	2.81767500
H	1.30316600	-1.60818100	3.87665100

H	0.67581900	-2.40536800	2.43424000
H	1.98002500	-1.20319000	2.29095900
C	-2.06382400	-1.74800900	3.35438400
H	-1.70712400	-2.61345200	2.79067200
H	-1.83070100	-1.93112300	4.41103900
H	-3.15130600	-1.69128800	3.26375300
C	-3.37345400	1.17964000	3.25546200
H	-3.73878300	2.05312900	2.71365600
H	-4.08646900	0.36408200	3.10722900
H	-3.37268700	1.42628100	4.32482800
C	-1.08509200	3.21720900	2.30090300
H	-2.10460300	3.49038500	2.01961400
H	-0.84817700	3.70500400	3.25552600
H	-0.41222400	3.59852800	1.53207900
C	1.67961400	1.61030700	2.36375300
H	1.64793100	2.59876700	1.91142700
H	2.05520000	1.72340500	3.39056200
H	2.39587300	0.97870100	1.82907200
C	-0.83050200	1.65801800	-1.86882400
O	-0.30248300	2.17580800	-2.85198300
N	-0.18006600	0.90512000	-0.90990700
C	-2.28234800	1.73677800	-1.54346700
C	-2.69700800	1.21213300	-0.30496400
C	-3.17425400	2.32149100	-2.44467900
C	-4.06501500	1.28160500	-0.00991100
C	-4.53022200	2.39025700	-2.12461400
H	-2.78035300	2.71601000	-3.37719100
C	-4.97109900	1.86498600	-0.90787800
H	-4.45167400	0.87346600	0.91823300
H	-5.23588000	2.84513200	-2.81359600
H	-6.02692600	1.90711400	-0.65008800
O	1.23739500	1.08469000	-1.01212300
C	1.66489100	2.37433400	-0.79552500
O	0.96818100	3.22292400	-0.28875000
C	3.09260800	2.64501700	-1.28307000
C	2.96163400	3.83924600	-2.25676900
H	3.95139100	4.10991700	-2.63932400
H	2.31242400	3.58138000	-3.09922100
H	2.52900900	4.70338300	-1.74770400
C	3.74412300	1.45341700	-1.99797700
H	4.71054600	1.76545700	-2.40800500
H	3.92896100	0.64924000	-1.28208500
H	3.12150800	1.10507100	-2.82900200
C	3.94865900	3.03369500	-0.05846900

H	3.47434300	3.84349700	0.50275800
H	4.09344900	2.16830800	0.59520900
H	4.93079300	3.37984100	-0.39875400
C	-3.28292400	-2.07193100	-0.02821600
C	-3.85708800	-3.23236200	-0.83866100
C	-2.42109800	-2.76747700	-2.63288100
C	-1.80934100	-1.58837300	-1.88361200
H	-3.34749600	-4.17440800	-0.58365800
H	-4.91948000	-3.34398900	-0.60389400
H	-3.85224900	-1.16188800	-0.23383900
H	-3.31364800	-2.26873200	1.04270300
H	-1.82547500	-3.68160400	-2.48033400
H	-2.43894200	-2.54346900	-3.70324600
H	-0.77677000	-1.38616500	-2.16584500
H	-2.38192400	-0.68312600	-2.10182200
N	-1.88480500	-1.70679800	-0.40099400
O	-3.76815700	-2.97680200	-2.23336300
Cl	-0.81990400	-3.12588000	0.11165600
C	4.59856600	-1.22470700	1.12234000
O	3.69971400	-0.34099900	0.89953900
O	4.66505400	-2.34723000	0.56314000
Cs	2.31679900	-1.84709500	-1.23459200
C	5.66687100	-0.84796700	2.15562200
H	5.18390100	-0.56162400	3.09599500
H	6.36188100	-1.67161500	2.33023400
H	6.21931600	0.02969900	1.80242900

TS8, E=-2241.67769938 a.u., Imaginary frequency = 150i

Rh	-1.24293900	0.15140000	0.72553400
C	-1.11259100	1.43515900	2.49176800
C	-2.09704600	0.40691500	2.78696900
C	-1.41984900	-0.84485200	2.77624200
C	0.18830100	0.79421400	2.47281100
C	-0.00137700	-0.60418800	2.58017600
C	1.08167000	-1.63641800	2.65786000
H	1.32086200	-1.84790000	3.70938000
H	0.76616100	-2.57470600	2.19694700
H	1.99688300	-1.28527900	2.17246600
C	-1.98936900	-2.18189400	3.13879200
H	-1.62278800	-2.96513500	2.47001100
H	-1.67296400	-2.44727600	4.15530300
H	-3.08187300	-2.18235600	3.12610600
C	-3.50347600	0.64388500	3.24377900
H	-3.89769500	1.58683500	2.86349700

H	-4.17959800	-0.16011900	2.93935200
H	-3.52535900	0.69318200	4.33988400
C	-1.35238600	2.91442500	2.48125200
H	-2.37024500	3.14055100	2.15523900
H	-1.20824600	3.33872200	3.48308300
H	-0.66393500	3.40162600	1.78913700
C	1.51496000	1.47698100	2.50064900
H	1.44298900	2.51873300	2.19918400
H	1.87340700	1.44537900	3.53927000
H	2.26762700	0.96101400	1.89580300
C	-0.81966100	1.85283000	-1.71914800
O	-0.27226900	2.48635400	-2.62018400
N	-0.19079200	0.96316100	-0.86799300
C	-2.26678200	1.92707000	-1.39137600
C	-2.71360400	1.23463300	-0.25344300
C	-3.13463500	2.67500800	-2.19070800
C	-4.07834500	1.29280800	0.04777200
C	-4.48874700	2.73775300	-1.86593800
H	-2.72009400	3.19637900	-3.04881400
C	-4.95674500	2.04050600	-0.74976800
H	-4.48544200	0.75359500	0.89551300
H	-5.17429800	3.31813400	-2.47619000
H	-6.01292300	2.07255600	-0.49306800
O	1.22264300	1.14000600	-0.91302700
C	1.63889600	2.41193400	-0.56496100
O	0.92614600	3.19248700	0.02079600
C	3.05672100	2.75443400	-1.02857300
C	2.88918500	4.01384100	-1.91180100
H	3.87007600	4.33480700	-2.27781900
H	2.23937500	3.80280500	-2.76634800
H	2.44071500	4.82790900	-1.33782700
C	3.73688600	1.63752600	-1.83110300
H	4.69924500	2.00072600	-2.20686000
H	3.93077000	0.78290600	-1.17987800
H	3.12675200	1.34403000	-2.69187500
C	3.90069300	3.07705100	0.22303100
H	3.40607000	3.83532800	0.83630400
H	4.05981100	2.17115300	0.81535600
H	4.87548600	3.46767900	-0.08876400
C	-3.22041500	-2.03838400	-0.13750600
C	-3.74747600	-3.16487900	-1.02743600
C	-2.41828300	-2.45465200	-2.81073800
C	-1.85791700	-1.29705500	-1.98803500
H	-3.16568600	-4.08291000	-0.86659500

H	-4.79051600	-3.36217400	-0.76266200
H	-3.89051700	-1.17638500	-0.23604000
H	-3.18817700	-2.33930900	0.90686400
H	-1.75481300	-3.32904600	-2.74639100
H	-2.48594300	-2.14225200	-3.85678900
H	-0.84466300	-1.02025700	-2.27651000
H	-2.48780000	-0.41553600	-2.15578600
N	-1.89036600	-1.50050700	-0.52086600
O	-3.73332300	-2.78925300	-2.39519000
Cl	-0.65129700	-3.22328800	-0.21828000
C	4.65536900	-1.04178900	1.07897900
O	3.64510300	-0.26676400	0.93707500
O	4.85769600	-2.09315300	0.42524100
Cs	2.40880300	-1.79161900	-1.30641900
C	5.68727800	-0.61057300	2.12797500
H	5.18573200	-0.40511700	3.07939300
H	6.45710100	-1.37214400	2.26708200
H	6.15726000	0.32606100	1.80700800

13, E=-1494.90803124 a.u.

Rh	1.79429100	0.19971900	0.25834400
C	0.64621800	1.20430700	2.29512400
O	0.89399500	-0.04442900	2.25325300
O	1.08386100	1.93068600	1.33969300
C	3.19393600	0.77151100	-1.25960700
C	3.89520700	0.77441300	0.02155100
C	3.84661700	-0.54487500	0.55191100
C	2.77855900	-0.58035200	-1.53034300
C	3.13229900	-1.39169100	-0.39960200
C	2.94519000	-2.86978200	-0.26525700
H	3.84515800	-3.39111700	-0.61425100
H	2.77354800	-3.15291000	0.77462500
H	2.09455700	-3.22479000	-0.84805300
C	4.40929100	-1.02369700	1.85316200
H	3.70005800	-1.67855700	2.36550000
H	5.32912600	-1.59375100	1.67762500
H	4.64465100	-0.19409500	2.52129200
C	4.50916500	1.98701100	0.64729100
H	3.83087900	2.84182000	0.58468900
H	4.74640700	1.82192500	1.69917900
H	5.43590100	2.24963100	0.12421100
C	3.03210200	1.95183000	-2.16551900
H	2.92820600	2.87449100	-1.59038300
H	3.90625300	2.05583500	-2.81967600
H	2.14564800	1.84594500	-2.79382300

C	2.07548800	-1.04381000	-2.76689100
H	1.39373700	-0.27942600	-3.14488100
H	2.81281100	-1.26179300	-3.54832500
H	1.49850600	-1.95005600	-2.57963900
C	-0.18119700	1.81107900	3.38809700
H	0.24598600	2.76796000	3.69661000
H	-1.17803800	2.00046600	2.97615800
H	-0.25629200	1.13418200	4.23997300
C	-0.95722600	-0.83921700	-1.01162500
O	-1.96531200	-0.63136900	-1.71788700
N	-0.13292500	0.11543800	-0.54271300
C	-0.63923300	-2.24424800	-0.57216300
C	-0.33560600	-2.56799400	0.75874600
C	-0.77380000	-3.26947400	-1.52131500
C	-0.14883500	-3.90409100	1.12540000
H	-0.23552600	-1.78030000	1.49743400
C	-0.55836900	-4.59831400	-1.15611100
H	-1.05032100	-3.00873400	-2.53819900
C	-0.24768500	-4.91850800	0.17048500
H	0.08085500	-4.14968800	2.15842500
H	-0.64268500	-5.38462200	-1.90035700
H	-0.09039300	-5.95414600	0.45668600
O	-0.49995100	1.41596400	-1.01568000
C	-1.42875100	2.05922500	-0.27715600
O	-2.06181800	1.53288700	0.62425100
C	-1.60175800	3.50026700	-0.75683200
C	-2.28376600	3.45378100	-2.14458500
H	-2.42569900	4.47307400	-2.51652400
H	-1.67678800	2.89948500	-2.86438000
H	-3.26747800	2.97484800	-2.08721400
C	-0.22202000	4.18481100	-0.86578600
H	-0.35781600	5.23290700	-1.14991600
H	0.30921700	4.14236300	0.08885200
H	0.39927000	3.69927400	-1.62161400
C	-2.48816700	4.25085900	0.24869900
H	-3.46344000	3.76832800	0.35710200
H	-2.01971200	4.28773300	1.23638800
H	-2.64712900	5.27689900	-0.09524500
Cs	-4.14207700	-0.72157700	0.37011200

14, E=-1494.89741181 a.u.

Rh	1.53583600	0.26611000	0.31162500
C	-0.58298700	0.31596200	2.46453000
O	-0.88498900	-0.86982900	2.25001600

O	0.40452400	0.95289200	1.91319900
C	2.70896800	2.00018200	0.06347500
C	3.35397600	1.22531400	1.11929200
C	3.73250200	-0.02188200	0.56310000
C	2.80974000	1.24029000	-1.17563400
C	3.38886600	-0.02215500	-0.86465700
C	3.69811300	-1.12854800	-1.82436300
H	4.74962300	-1.07884900	-2.13098000
H	3.52195900	-2.10635200	-1.37280300
H	3.07988700	-1.06154100	-2.72073600
C	4.42345700	-1.14473600	1.27174200
H	4.13970600	-2.11108500	0.85204300
H	5.50942300	-1.03798000	1.16135300
H	4.19154600	-1.15086200	2.33843400
C	3.48966400	1.68711400	2.53507400
H	2.50685300	1.95542700	2.93496800
H	3.92158500	0.91461100	3.17291500
H	4.13436200	2.57137700	2.58257300
C	2.17924900	3.38844400	0.21659500
H	1.71277200	3.51203500	1.19639000
H	2.99422500	4.11740700	0.12768200
H	1.43347600	3.61205600	-0.54729700
C	2.32804200	1.71587000	-2.50936000
H	1.36527900	2.22252200	-2.41584800
H	3.05146700	2.42242700	-2.93248100
H	2.20685800	0.88946600	-3.21081500
C	-1.41677000	1.16844000	3.40425700
H	-0.81447100	1.94032200	3.88623600
H	-2.18633700	1.65989300	2.79886000
H	-1.90239200	0.54145200	4.15425600
C	-0.70574000	-0.77989300	-1.45913600
O	-1.73641000	-0.82118900	-2.14696500
N	-0.17876400	0.29895600	-0.84675400
C	0.13055400	-2.00447500	-1.18196500
C	0.77072700	-2.17928700	0.06043300
C	0.28387400	-2.96682200	-2.18435800
C	1.57256300	-3.30696100	0.28347800
H	0.46287400	-1.56857700	0.92981900
C	1.09799500	-4.07881000	-1.96109900
H	-0.23128600	-2.82529600	-3.12922400
C	1.74429300	-4.25091500	-0.72938300
H	2.03254200	-3.45313900	1.25633300
H	1.22748000	-4.81806800	-2.74592500
H	2.36052600	-5.12852000	-0.55884000

O	-0.79415300	1.53223300	-1.16650100
C	-1.98056900	1.80860700	-0.55809900
O	-2.51729700	1.06986300	0.24121100
C	-2.54952500	3.13366800	-1.06461000
C	-3.09947700	2.86967200	-2.48774600
H	-3.53336700	3.79173500	-2.88659800
H	-2.30661100	2.53415100	-3.16067300
H	-3.87963400	2.10241200	-2.47250300
C	-1.45520300	4.21921400	-1.11590100
H	-1.89789100	5.16690800	-1.43652500
H	-1.00331900	4.37359900	-0.13056700
H	-0.66608200	3.95681700	-1.82447200
C	-3.68559800	3.56979900	-0.12582100
H	-4.46402400	2.80538400	-0.06696000
H	-3.31473600	3.75270900	0.88737900
H	-4.13506900	4.49473300	-0.49826900
Cs	-3.29676700	-1.83136600	0.59454000

TS15, E=-1494.8721983 a.u., Imaginary frequency = 1199i

Rh	-1.58188800	-0.12321300	0.23041300
C	0.43440000	-0.13960400	2.42298200
O	0.70779300	1.05182000	2.03960200
O	-0.50059600	-0.82995600	1.93083700
C	-2.98502100	-1.79715300	0.08108500
C	-3.53730500	-0.82781400	1.01748600
C	-3.75360700	0.39453400	0.32398800
C	-2.89047800	-1.15800000	-1.20074100
C	-3.30491000	0.21589300	-1.05236400
C	-3.41117400	1.23855700	-2.14238000
H	-4.42332100	1.24916600	-2.56341600
H	-3.18667100	2.23839100	-1.76472700
H	-2.71036900	1.02632900	-2.95177200
C	-4.41432500	1.62167200	0.87277800
H	-4.12850900	2.51307600	0.31372000
H	-5.50353500	1.51580100	0.80164300
H	-4.16335100	1.78138200	1.92393400
C	-3.81742300	-1.11426400	2.45945700
H	-2.95348200	-1.59192000	2.92977900
H	-4.04999600	-0.20392000	3.01447100
H	-4.67119300	-1.79564900	2.54914500
C	-2.66060600	-3.22302400	0.40260000
H	-2.25112400	-3.30933000	1.41187500
H	-3.56115100	-3.84668700	0.34787600
H	-1.92489600	-3.62834100	-0.29428600

C	-2.39484900	-1.80195700	-2.45757200
H	-1.57749500	-2.49414700	-2.24747100
H	-3.20957100	-2.36021800	-2.93318100
H	-2.02837600	-1.06041200	-3.16871300
C	1.30234900	-0.76232800	3.48524300
H	0.73168000	-1.48567500	4.06899100
H	2.10696000	-1.29557000	2.96731900
H	1.73280100	0.00117500	4.13522600
C	0.79669400	0.62784800	-1.45483500
O	1.85388300	0.57519800	-2.10450500
N	0.13709300	-0.39769200	-0.87894200
C	0.09299200	1.91105700	-1.11268700
C	-0.73625900	1.91897000	0.03597100
C	0.28048300	3.05195800	-1.89200500
C	-1.37198700	3.12791800	0.37308400
H	-0.13152900	1.35398200	1.11071300
C	-0.38502100	4.23196800	-1.54678500
H	0.92699300	2.99672700	-2.76343400
C	-1.20518300	4.27150700	-0.41213300
H	-1.97920900	3.17974100	1.27257000
H	-0.26297600	5.12198100	-2.15723100
H	-1.70276600	5.19742800	-0.13760200
O	0.68128800	-1.68234200	-1.10664700
C	1.78807500	-2.00233300	-0.38702600
O	2.32264500	-1.24693700	0.40329900
C	2.26542100	-3.41193300	-0.73296400
C	2.78120100	-3.39052200	-2.19148400
H	3.14986400	-4.38487300	-2.46125200
H	1.98680800	-3.11037500	-2.88701100
H	3.60328600	-2.67753100	-2.30944500
C	1.09246400	-4.40778900	-0.60227300
H	1.45133200	-5.42167200	-0.80269500
H	0.66798300	-4.39144400	0.40707900
H	0.29791900	-4.17945900	-1.31643100
C	3.39915300	-3.79808900	0.22930700
H	4.23393100	-3.09581400	0.15832800
H	3.05321000	-3.80758400	1.26711500
H	3.76745200	-4.79739800	-0.01931100
Cs	3.49498200	1.59066500	0.39034800

16_{Rh}, E=-1265.832566 a.u.

Rh	-1.57749500	-0.07261100	-0.27855500
C	-2.00383400	-0.74487800	1.70127000
C	-3.06628300	0.17162100	1.32512000

C	-3.70633400	-0.38289600	0.18579400
C	-2.11277300	-1.94803600	0.88330200
C	-3.12095600	-1.71152000	-0.06945700
C	-3.56122200	-2.62575900	-1.16820400
H	-4.51563500	-3.09794200	-0.90510000
H	-3.71357200	-2.07702300	-2.10159900
H	-2.83122100	-3.41552900	-1.35320600
C	-4.85789200	0.19544300	-0.57555700
H	-4.77546800	-0.02341700	-1.64293100
H	-5.80304900	-0.23286800	-0.21963500
H	-4.91127100	1.27939800	-0.45899800
C	-3.43544900	1.42067400	2.06554700
H	-2.55537600	2.01449100	2.32368900
H	-4.10746900	2.05079300	1.48064600
H	-3.95334900	1.16162200	2.99625400
C	-1.05780600	-0.57431600	2.84716600
H	-0.97332600	0.47638900	3.13379800
H	-1.41896900	-1.13322400	3.71981700
H	-0.06584300	-0.95207500	2.58573400
C	-1.26928700	-3.17660800	1.03562600
H	-0.28012700	-2.92750200	1.42429800
H	-1.73620700	-3.87787300	1.73714600
H	-1.13857100	-3.69242500	0.08215300
C	0.95390500	0.66397200	-1.57782400
O	2.15171700	0.58369300	-1.86513400
N	0.13417300	-0.39322900	-1.25591700
C	0.20193200	1.94627900	-1.40740700
C	-1.03097700	1.86223500	-0.72775700
C	0.72668000	3.15585900	-1.86551100
C	-1.72654100	3.05706200	-0.51101700
C	0.01103100	4.33562100	-1.63923100
H	1.67227800	3.15661800	-2.40235000
C	-1.21061500	4.28141600	-0.96321000
H	-2.68366000	3.05288300	0.00073300
H	0.39444200	5.28570100	-1.99887500
H	-1.77295500	5.19580400	-0.79359700
O	0.80378800	-1.64488600	-1.31183400
C	1.63665500	-1.91070900	-0.27915600
O	1.73789500	-1.19670500	0.70750600
C	2.47821700	-3.15862300	-0.53423600
C	3.80385200	-2.62177200	-1.13649000
H	4.45629600	-3.46339900	-1.38704000
H	3.61600800	-2.03705500	-2.04095900
H	4.32882000	-1.98641600	-0.41548400

C	1.81196900	-4.12923500	-1.52524500
H	2.45752300	-5.00167600	-1.66261300
H	0.84697900	-4.48203800	-1.14839800
H	1.64919800	-3.66390500	-2.49906200
C	2.75164400	-3.86006100	0.80750900
H	3.18236000	-3.16771900	1.53460800
H	1.83184700	-4.27439500	1.23334500
H	3.45166500	-4.68625600	0.65443700
Cs	2.88280000	1.62050400	1.05416600

17Rh_{Cl}, E=-2013.10947363 a.u.

Rh	1.46266300	0.47292100	0.01985900
C	2.06529300	2.47632200	0.54677600
C	3.27632000	1.68969400	0.49928500
C	3.43263800	1.20353700	-0.82833400
C	1.57670800	2.60441900	-0.82724900
C	2.38485700	1.80961400	-1.65631500
C	2.22791800	1.68413000	-3.14304500
H	2.53073400	2.61488600	-3.63767700
H	2.84727300	0.88640300	-3.55863300
H	1.18773400	1.48678500	-3.41839100
C	4.62593300	0.44366700	-1.32999800
H	4.43583300	-0.04239200	-2.28824100
H	5.47106800	1.12667900	-1.47738600
H	4.94437500	-0.32281100	-0.61828500
C	4.24301400	1.52786300	1.63049300
H	3.73168500	1.36634200	2.58058800
H	4.92954700	0.69518700	1.46721600
H	4.84424100	2.44081400	1.71985200
C	1.58507200	3.25457500	1.73320900
H	1.88185900	2.76356300	2.66239500
H	2.02217900	4.26108500	1.72727800
H	0.49902100	3.34045300	1.73679100
C	0.43607700	3.45983500	-1.28582400
H	-0.11360000	3.87154600	-0.44074600
H	0.81285600	4.29536700	-1.88763000
H	-0.26098500	2.89241000	-1.91004500
C	-0.91805600	-0.16033300	1.73804200
O	-2.09375100	-0.27336500	2.13569600
N	-0.53377500	0.38729300	0.55503000
C	0.27668700	-0.71433100	2.43007900
C	1.51689500	-0.58452800	1.77558200
C	0.14707000	-1.41044400	3.63411600
C	2.62727700	-1.21233200	2.34997900

C	1.27038500	-2.00802100	4.20670600
H	-0.83304400	-1.47138300	4.09894100
C	2.50462400	-1.91608000	3.55702000
H	3.59872900	-1.16476400	1.86615300
H	1.18642400	-2.54621800	5.14575600
H	3.38049900	-2.39221600	3.99015200
O	-1.60962600	0.97062100	-0.18133100
C	-2.08766300	2.15464200	0.32800900
O	-1.61203800	2.71818300	1.28102800
C	-3.32401600	2.64813400	-0.43687700
C	-4.54068200	2.30631800	0.45567000
H	-5.46166400	2.65955500	-0.01838900
H	-4.63158600	1.22720400	0.62123400
H	-4.44483700	2.77862700	1.43597500
C	-3.47683100	2.01067700	-1.82786200
H	-4.34631100	2.44100300	-2.33397400
H	-2.59654600	2.18897700	-2.45134000
H	-3.62385300	0.92791700	-1.77551700
C	-3.21609600	4.17988500	-0.57697100
H	-3.04284600	4.64359800	0.39581900
H	-2.39325800	4.45831100	-1.24227200
H	-4.14225400	4.58045100	-0.99983100
Cs	-3.48961800	-1.73808000	-0.02465100
C	2.24040600	-1.89339200	-1.96882800
C	2.07229500	-3.24304500	-2.66447400
C	0.54744200	-3.96543600	-1.04255600
C	0.67515900	-2.65096400	-0.27952500
H	1.30546000	-3.17722900	-3.45060400
H	3.01872700	-3.52636100	-3.13255700
H	3.06977100	-1.94296900	-1.25708200
H	2.43509300	-1.09599000	-2.68351700
H	-0.30315000	-3.93669700	-1.74307800
H	0.37976200	-4.77765900	-0.32927400
H	-0.22609900	-2.37645400	0.26709700
H	1.47979100	-2.73348000	0.45499200
N	1.06980500	-1.48886000	-1.13022600
O	1.75030700	-4.26267600	-1.73030300
Cl	-0.33571700	-1.16501000	-2.30415600

TS18_{Rh_Cl}, E=-2013.09919956 a.u., Imaginary frequency = 148i

Rh	1.43395100	0.42310100	-0.03041900
C	2.02322200	2.48834900	0.44595800
C	3.23890800	1.71745700	0.39713000
C	3.38657600	1.20150200	-0.92485200

C	1.49933700	2.55601100	-0.91256400
C	2.31494800	1.75874300	-1.74350900
C	2.10772200	1.57132900	-3.21801800
H	2.00366900	2.54364000	-3.71165200
H	2.94860800	1.05566500	-3.68663300
H	1.19474300	1.00108800	-3.42304100
C	4.59698500	0.46625600	-1.42177300
H	4.42383300	-0.01878300	-2.38328000
H	5.42860700	1.16788600	-1.55672600
H	4.92688800	-0.29676000	-0.71137200
C	4.23508500	1.61118600	1.50814100
H	3.75101700	1.47970100	2.47694300
H	4.93198400	0.78474700	1.35828100
H	4.82220600	2.53692100	1.54693500
C	1.55504900	3.28416700	1.62551600
H	1.84146700	2.79459100	2.55893700
H	2.01249600	4.28130900	1.61290600
H	0.47131000	3.39078800	1.62900600
C	0.33420200	3.37031200	-1.38261100
H	-0.17936000	3.84630000	-0.54867400
H	0.68137900	4.15610500	-2.06398300
H	-0.38401400	2.75328600	-1.92986000
C	-0.88947700	-0.10295800	1.79207300
O	-2.05705400	-0.21784300	2.20423800
N	-0.52906600	0.41075500	0.58281800
C	0.32441400	-0.60505400	2.48565100
C	1.54538200	-0.51195200	1.79393100
C	0.23695800	-1.22380200	3.73535800
C	2.68025300	-1.09024000	2.36938000
C	1.38273000	-1.77096700	4.31249100
H	-0.72956400	-1.26489700	4.22960900
C	2.59784000	-1.71236000	3.62332800
H	3.63496000	-1.06956100	1.85221800
H	1.33101900	-2.24756400	5.28637200
H	3.48990900	-2.15288300	4.06061100
O	-1.60974100	0.96068000	-0.15711000
C	-2.11035700	2.14518200	0.33923700
O	-1.63125000	2.73462300	1.27417800
C	-3.36904200	2.59336700	-0.41441400
C	-4.56150200	2.23129600	0.50338000
H	-5.49887000	2.54889000	0.03643100
H	-4.61705900	1.15327300	0.68899100
H	-4.46603900	2.72409600	1.47363300
C	-3.52725900	1.93187200	-1.79344800

H	-4.41698700	2.33222900	-2.28874700
H	-2.66424700	2.12360200	-2.43626000
H	-3.64262800	0.84701100	-1.72505000
C	-3.30349500	4.12539500	-0.57696100
H	-3.12987000	4.60849800	0.38631100
H	-2.49801600	4.41575100	-1.25836800
H	-4.24574600	4.49437200	-0.99271800
Cs	-3.39120500	-1.80098400	-0.00437000
C	2.24550200	-1.84627500	-1.93242200
C	2.02921100	-3.19670900	-2.61719100
C	0.59731700	-3.91230600	-0.92086400
C	0.76093300	-2.59585300	-0.16443300
H	1.21647700	-3.12423000	-3.35233100
H	2.94741600	-3.48002500	-3.13871000
H	3.14073000	-1.90942700	-1.30329000
H	2.38058200	-1.05294100	-2.66434700
H	-0.28475200	-3.87561200	-1.57803000
H	0.46294100	-4.72100700	-0.19632800
H	-0.12924900	-2.31563400	0.39666700
H	1.57217800	-2.70568500	0.56416400
N	1.16318000	-1.43772700	-0.99649200
O	1.76287800	-4.21404200	-1.66475200
Cl	-0.49915600	-1.21249500	-2.31807000

17'_{Rh}_Cl, E=-2013.11431264 a.u.

Rh	1.27068100	0.20098400	-0.63757000
C	0.43512500	0.39667000	-2.61764900
C	1.57047800	1.28164500	-2.56469800
C	2.73125400	0.48476000	-2.33481300
C	0.93636800	-0.97873000	-2.59440400
C	2.32855200	-0.92078900	-2.41321100
C	3.27798500	-2.07736600	-2.37999100
H	3.76124200	-2.18807500	-3.35847900
H	4.06687100	-1.93535600	-1.63779800
H	2.76758500	-3.01271400	-2.14592000
C	4.14619900	0.98503300	-2.31114300
H	4.82269800	0.26264400	-1.84895000
H	4.51132100	1.16076800	-3.33037900
H	4.23196700	1.92637500	-1.76181700
C	1.53464100	2.76009100	-2.79889300
H	0.66540800	3.22536300	-2.33062000
H	2.42610700	3.25484800	-2.41118200
H	1.48844700	2.95369100	-3.87744800
C	-0.98420500	0.79772500	-2.88807100

H	-1.15997400	1.82544000	-2.55793800
H	-1.20435800	0.74605100	-3.96154100
H	-1.67334300	0.13719300	-2.35769100
C	0.09556800	-2.20877900	-2.75777800
H	-0.92879200	-2.03228900	-2.42532600
H	0.05531900	-2.51020500	-3.81164300
H	0.49849900	-3.04659600	-2.18447300
C	-1.08268000	0.63386200	1.16168500
O	-2.11521200	0.44386600	1.83601100
N	-0.46639900	-0.27413600	0.37216300
C	-0.32756700	1.91939700	1.10965500
C	0.88411100	1.92303700	0.38770500
C	-0.75024200	3.03219500	1.84212800
C	1.67619200	3.07466900	0.44647000
C	0.04002000	4.18213900	1.86664900
H	-1.66923000	2.96153400	2.41902200
C	1.25505600	4.19595100	1.17496700
H	2.63018700	3.11224600	-0.07333400
H	-0.27171900	5.05055600	2.43880800
H	1.88468400	5.08123800	1.20757700
O	-0.90237300	-1.61071400	0.58047800
C	-2.08996400	-1.95841300	0.04037200
O	-2.74873000	-1.23328800	-0.68749300
C	-2.48517200	-3.36849900	0.48115300
C	-3.80774500	-3.74938600	-0.20036100
H	-4.09835000	-4.76001000	0.10012400
H	-4.61147000	-3.06403400	0.08487700
H	-3.71576700	-3.72494300	-1.28959200
C	-2.65667200	-3.35508500	2.01848200
H	-3.00259900	-4.33720800	2.35474700
H	-1.71286700	-3.12605500	2.51762800
H	-3.39174600	-2.60569300	2.32892400
C	-1.37254700	-4.36468200	0.08510400
H	-1.24578300	-4.40302200	-1.00145800
H	-0.41625400	-4.09120400	0.53727000
H	-1.64458200	-5.36775100	0.42722400
C	3.78517100	0.03499100	1.18746600
C	4.59553400	-0.35093600	2.42302500
C	2.65410200	-0.75156100	3.66075100
C	1.75665300	-0.37787200	2.48537200
H	4.85981900	-1.41899400	2.39223600
H	5.52147300	0.23067200	2.44010100
H	3.59321000	1.11261000	1.19167000
H	4.29996300	-0.22857000	0.26392600

H	2.83398400	-1.83660300	3.68887100
H	2.15647700	-0.46302800	4.59043000
H	0.82162700	-0.93636100	2.48486700
H	1.53066100	0.68988400	2.52475200
N	2.41683400	-0.57262900	1.14962900
O	3.88299900	-0.03991700	3.60837700
Cl	2.60368300	-2.37888200	0.91950000
Cs	-4.31977800	1.28657600	0.01855200

TS18'_{Rh_Cl}, E=-2013.04203882 a.u., Imaginary frequency = 258i

Rh	1.52156800	-0.01048600	-0.32417500
C	1.85808500	-0.67575600	-2.47619700
C	2.83510700	0.33116200	-2.14097200
C	3.67659600	-0.19869200	-1.10855900
C	2.21406100	-1.88947300	-1.77773300
C	3.29948200	-1.58330200	-0.91536200
C	3.98710000	-2.57097300	-0.03057600
H	4.54435800	-3.28946100	-0.64480200
H	4.69979000	-2.09240100	0.64391600
H	3.26321800	-3.13507200	0.56356900
C	4.93078200	0.42212900	-0.56757000
H	5.01097100	0.30967300	0.51670400
H	5.80988500	-0.06150400	-1.01025400
H	4.98973700	1.48546600	-0.80229000
C	3.01108400	1.61789400	-2.88220900
H	2.04823700	2.07546200	-3.11949300
H	3.59257300	2.34371900	-2.31403200
H	3.53365200	1.42125400	-3.82658200
C	0.85904900	-0.53496600	-3.58151600
H	0.44068000	0.47426600	-3.59921700
H	1.35077500	-0.71165500	-4.54646800
H	0.03612500	-1.23431500	-3.46147900
C	1.55374500	-3.22057100	-1.84921600
H	0.78979700	-3.25885900	-2.62398300
H	2.29671500	-4.00564500	-2.03106800
H	1.07263500	-3.44799900	-0.88718900
C	-1.01765500	1.58631800	-0.57265100
O	-2.21198900	1.94270800	-0.58013200
N	-0.55719900	0.31498200	-0.49679000
C	0.12021300	2.53928400	-0.52732900
C	1.39168700	2.00784600	-0.27143300
C	-0.09492500	3.92071400	-0.52196700
C	2.43441500	2.87127300	0.07077400
C	0.96341600	4.78272800	-0.23885500

H	-1.09970000	4.28927200	-0.70602500
C	2.21946800	4.25452800	0.07824000
H	3.41116200	2.48187100	0.33323600
H	0.80848500	5.85711200	-0.23636800
H	3.03823900	4.92114800	0.33508700
O	-1.56900900	-0.57364500	-0.01674000
C	-1.71381500	-1.73865000	-0.70043900
O	-1.23990100	-1.95393200	-1.79142900
C	-2.59242700	-2.75098200	0.05414500
C	-3.88964000	-2.92451100	-0.76687100
H	-4.51822200	-3.69932300	-0.31810500
H	-4.48088700	-2.00007600	-0.80110600
H	-3.66044200	-3.20946400	-1.79634200
C	-2.90258700	-2.33028900	1.49896800
H	-3.48947100	-3.11159900	1.99183200
H	-1.98114000	-2.17333300	2.06353300
H	-3.47893700	-1.39999800	1.54724900
C	-1.83288000	-4.09656200	0.06184800
H	-1.56059100	-4.38848700	-0.95459100
H	-0.92018600	-4.02163500	0.65769000
H	-2.46693800	-4.87614900	0.49534300
C	2.86328700	0.06515500	2.61358700
C	2.61124400	-0.58724900	3.98109400
C	0.38298200	0.12163100	3.99492300
C	0.53312800	0.79342300	2.62499500
H	2.31149000	-1.63460600	3.83657400
H	3.52317400	-0.55738700	4.58371300
H	3.32756200	1.05396600	2.78122700
H	3.55653300	-0.53433000	2.02185500
H	0.01694100	-0.90655300	3.86371900
H	-0.33280200	0.67759300	4.60747400
H	-0.37813100	0.69721400	2.03265700
H	0.71759200	1.87129600	2.77836000
N	1.65700100	0.30410600	1.85038800
O	1.61684100	0.12777300	4.69697500
Cl	0.88644500	-1.94884600	1.33612000
Cs	-4.83700300	1.00806000	-0.04254200

9Rh, E=-1532.64804025 a.u.

Rh	0.92293600	-0.35848900	0.01314200
C	1.09245700	-0.57648600	-2.24681900
C	2.40320600	-0.73089600	-1.69826100
C	2.40551800	-1.90906200	-0.85062300
C	0.29610600	-1.69264400	-1.78735300

C	1. 11259000	-2. 51966400	-0. 94677900
C	0. 68977300	-3. 84944900	-0. 40122200
H	0. 61648200	-4. 57205100	-1. 22295800
H	1. 40589900	-4. 25074000	0. 31792700
H	-0. 29557100	-3. 80130400	0. 07092800
C	3. 59943000	-2. 47018700	-0. 14093900
H	3. 31451200	-3. 03969500	0. 74695400
H	4. 14770100	-3. 14926600	-0. 80515900
H	4. 28917400	-1. 68285900	0. 16956300
C	3. 60169700	0. 07491300	-2. 08109300
H	3. 35869100	1. 13138600	-2. 20084900
H	4. 40957600	-0. 01087300	-1. 35387800
H	3. 97802100	-0. 29736100	-3. 04191500
C	0. 64029400	0. 48458800	-3. 20037700
H	1. 28730200	1. 36208700	-3. 14620400
H	0. 67025300	0. 10445800	-4. 22813200
H	-0. 38103500	0. 79818800	-2. 97384700
C	-1. 09168500	-2. 03075900	-2. 22126400
H	-1. 58354900	-1. 18383000	-2. 69566200
H	-1. 04632000	-2. 85308600	-2. 94684300
H	-1. 70495600	-2. 36811100	-1. 38162500
C	-0. 63692900	2. 18501200	-0. 01818300
O	-1. 60687500	2. 92109400	0. 05720500
N	-0. 70233000	0. 81147600	-0. 19473800
C	0. 79219200	2. 56622300	0. 12434800
C	1. 72004000	1. 52964900	0. 23679600
C	1. 19083100	3. 89668600	0. 28443500
C	3. 05156600	1. 79774700	0. 53876400
C	2. 52800000	4. 17736200	0. 55985900
H	0. 43949500	4. 67693500	0. 20423100
C	3. 44870200	3. 13271700	0. 70118300
H	3. 77555100	1. 00008800	0. 66925600
H	2. 85409400	5. 20516700	0. 68204700
H	4. 48374500	3. 35199000	0. 94731800
O	-1. 96657900	0. 24756900	0. 00021400
C	-2. 88806000	0. 50704800	-1. 02133300
O	-2. 55412300	0. 90824200	-2. 10475400
C	-4. 29953100	0. 20741400	-0. 53249600
C	-4. 65462300	1. 26399500	0. 54139800
H	-5. 68829100	1. 11148200	0. 86622200
H	-3. 99898500	1. 18083700	1. 41146500
H	-4. 55796300	2. 27723300	0. 14363300
C	-4. 36050000	-1. 21022200	0. 07756300
H	-5. 38096200	-1. 41339000	0. 41492400

H	-4.09712200	-1.97427300	-0.66221700
H	-3.69330700	-1.30951500	0.93810200
C	-5.25639900	0.31772500	-1.72956000
H	-5.21188100	1.31335800	-2.17638800
H	-5.00615700	-0.41015800	-2.50683000
H	-6.28101600	0.12906900	-1.39685800
C	0.79969000	-1.90007300	2.55777100
C	-0.66403200	-2.25751300	2.96921400
C	-1.17111700	0.01024300	3.25416400
C	0.28109500	0.40311100	2.83462300
H	-1.27108700	-2.34090600	2.05394000
H	-0.67232500	-3.21052200	3.50400100
H	1.40910700	-1.85217900	3.46890100
H	1.19983300	-2.66384800	1.89406000
H	-1.81592800	0.05465100	2.36768600
H	-1.52804300	0.71201600	4.01086900
H	0.29110600	1.39438700	2.38822300
H	0.90532500	0.40327100	3.73682300
N	0.76618000	-0.60264000	1.90829900
O	-1.17021400	-1.27657100	3.83771700

TS10, E=-1532.63588858 a.u., Imaginary frequency = 251i

Rh	-0.67945700	0.49405600	-0.02139100
C	-0.55856400	1.88767700	-1.79298500
C	-1.93301100	1.56135200	-1.56685100
C	-2.32611700	2.05577100	-0.25205600
C	-0.06631500	2.52392800	-0.60227700
C	-1.18094800	2.65811900	0.33450600
C	-1.11112000	3.36889700	1.64894400
H	-1.26173200	4.44435100	1.49346300
H	-1.88144500	3.02407500	2.34172300
H	-0.13480800	3.23985700	2.12118700
C	-3.72488500	2.07229500	0.28418900
H	-3.74532700	2.20955100	1.36763300
H	-4.28368600	2.90584400	-0.15752800
H	-4.26631600	1.15564400	0.04074400
C	-2.84974100	0.92989600	-2.56452300
H	-2.33442700	0.17115600	-3.15587500
H	-3.71151800	0.46264400	-2.08815700
H	-3.21551200	1.70217200	-3.25231500
C	0.23422200	1.61815400	-3.03177600
H	-0.31790800	0.98515200	-3.72810700
H	0.45583400	2.56451500	-3.53822700
H	1.17932200	1.12775500	-2.78603700

C	1.30453600	3.09067600	-0.41364000
H	2.02530500	2.59790200	-1.06612600
H	1.29482100	4.16133100	-0.65503900
H	1.64339700	2.98860500	0.62063600
C	0.72558600	-1.93235400	-1.04224500
O	1.59919800	-2.76856700	-1.21801600
N	0.92479500	-0.62198100	-0.65887200
C	-0.74165500	-2.21901000	-1.14403600
C	-1.63402300	-1.41409500	-0.43415600
C	-1.24477100	-3.30036600	-1.87022500
C	-2.99440600	-1.68425600	-0.36376300
C	-2.61641000	-3.56433800	-1.85799800
H	-0.54298200	-3.91911500	-2.42185300
C	-3.48654900	-2.76232600	-1.10917800
H	-3.66391400	-1.08632300	0.24505100
H	-3.00915100	-4.40918700	-2.41440400
H	-4.54891800	-2.98568500	-1.08567200
O	2.15350500	-0.47960100	0.03173100
C	3.19105400	0.05904800	-0.69978000
O	3.04655800	0.55699100	-1.78968000
C	4.50347800	-0.09990500	0.06306100
C	4.32418500	0.29961200	1.54287500
H	5.28495900	0.21455100	2.05900900
H	3.98516500	1.33750500	1.63744700
H	3.60587300	-0.34830800	2.05107900
C	5.56700400	0.78500700	-0.60479800
H	6.52934800	0.64160000	-0.10510400
H	5.68046700	0.53299400	-1.66121800
H	5.30094500	1.84463300	-0.53890000
C	4.89930000	-1.59359600	-0.04035900
H	4.12247500	-2.23878900	0.37643900
H	5.05538200	-1.88523600	-1.08277300
H	5.83284000	-1.75860200	0.50639500
C	-2.04382300	-0.50625000	2.44315100
C	-1.41828700	-0.04778400	3.79045800
C	0.50964500	-1.28062900	3.34524700
C	-0.06934000	-1.77073100	1.99276600
H	-0.91495500	0.91996900	3.63806800
H	-2.21132500	0.07088300	4.53331700
H	-2.58549500	-1.44508000	2.60969900
H	-2.73468700	0.25185200	2.07593700
H	1.12482900	-0.38568200	3.16765400
H	1.13526700	-2.07080900	3.76695200
H	0.75546700	-1.96523100	1.31531200

H	-0.64444100	-2.68868100	2.15862300
N	-0.94845700	-0.70688800	1.50133500
O	-0.52628700	-1.02219600	4.26959100

11, E=-1532.71255212 a.u.

Rh	-0.62084500	0.38904500	-0.24269900
C	-0.21733300	1.25121800	-2.19043600
C	-1.66829100	1.23087600	-2.00157300
C	-1.99421000	2.05866000	-0.89277700
C	0.33663700	2.10891000	-1.18761900
C	-0.74748000	2.55882500	-0.33855800
C	-0.59277900	3.53917300	0.77921500
H	-0.49423800	4.55087900	0.36525500
H	-1.45162100	3.53840600	1.45150900
H	0.30646100	3.33187800	1.36374800
C	-3.36670200	2.45397100	-0.44374500
H	-3.41631600	2.62177400	0.63316200
H	-3.64794000	3.39449600	-0.93240100
H	-4.11829500	1.70998400	-0.71498600
C	-2.61450500	0.46955900	-2.87451900
H	-2.28665300	-0.56667300	-3.00156600
H	-3.62541100	0.45548200	-2.46524200
H	-2.65345200	0.92935200	-3.86860900
C	0.52183500	0.56594100	-3.29447000
H	-0.01140200	-0.32746600	-3.62715600
H	0.61213600	1.24193700	-4.15382100
H	1.51833500	0.26658900	-2.96941000
C	1.75651300	2.55046700	-1.04584500
H	2.41956900	1.98533000	-1.69755800
H	1.82526000	3.61346000	-1.30532600
H	2.10345500	2.43512200	-0.01609400
C	0.93258300	-1.88417600	0.26877500
O	1.82873600	-2.71073000	0.32846900
N	0.98054900	-0.56035500	0.58559100
C	-0.44924200	-2.22351600	-0.28355800
C	-1.70162600	-1.76714000	0.23820200
C	-0.45052700	-3.07883000	-1.40027300
C	-2.89657000	-2.20210700	-0.37285900
C	-1.63364300	-3.46074700	-2.01501300
H	0.51078800	-3.43867600	-1.75103500
C	-2.85910100	-3.02289700	-1.49163200
H	-3.85538400	-1.91469400	0.03844600
H	-1.61231800	-4.11758800	-2.87840200
H	-3.79102700	-3.34665600	-1.94441500

O	2.25379700	-0.07582800	0.90768900
C	3.19569600	-0.19022400	-0.10995800
O	2.88247400	-0.41360100	-1.25407200
C	4.60431900	-0.01153800	0.44007900
C	4.90958000	-1.26061200	1.30339800
H	5.93831000	-1.19914900	1.67120900
H	4.23336000	-1.32171800	2.15912100
H	4.80093300	-2.17834000	0.71956000
C	4.69146300	1.26381100	1.30534000
H	5.70785500	1.36317000	1.69736600
H	4.47545600	2.16169500	0.71579500
H	4.00155300	1.22489600	2.15148900
C	5.58047700	0.07426000	-0.74300500
H	5.52052900	-0.81917800	-1.36850400
H	5.36557400	0.94202200	-1.37426600
H	6.60297300	0.16965000	-0.36683900
C	-3.02999600	-0.27790700	1.73982400
C	-2.82143600	0.83086900	2.77219300
C	-0.89415800	-0.19556000	3.58906400
C	-1.04521300	-1.34010900	2.59900500
H	-2.24827200	1.64883800	2.30788500
H	-3.79213000	1.21978800	3.09146600
H	-3.65488500	-1.06846100	2.17574600
H	-3.53072900	0.12013600	0.85756000
H	-0.22801800	0.56975700	3.15927100
H	-0.45215500	-0.56423200	4.51726400
H	-0.07359300	-1.76466900	2.37060400
H	-1.68543100	-2.12640600	3.01780900
N	-1.71092600	-0.83799800	1.34902500
O	-2.15755400	0.36186700	3.92478700

TS12, E=-1761.75202985 a.u., Imaginary frequency = 979i

Rh	0.56610100	-0.53180400	-0.48844200
C	0.08948900	0.42646700	-2.42745500
C	1.49218800	0.11963000	-2.46584700
C	1.66898000	-1.28777400	-2.24560000
C	-0.62366700	-0.83506200	-2.32419200
C	0.34707700	-1.87956400	-2.20167700
C	0.06574900	-3.34058600	-2.08244700
H	0.33253100	-3.84191100	-3.02026200
H	0.65688200	-3.78159600	-1.27661100
H	-0.98960000	-3.53015900	-1.88058600
C	2.95426600	-2.05694600	-2.24552600
H	2.90100600	-2.90001400	-1.55274100

H	3.16211300	-2.45673900	-3.24502200
H	3.80203300	-1.43301100	-1.95542000
C	2.55150600	1.11424400	-2.81069100
H	2.43220200	2.04807500	-2.25810000
H	3.56007400	0.72699500	-2.65907700
H	2.45092900	1.35605700	-3.87602800
C	-0.49927700	1.78031300	-2.67183900
H	0.13333300	2.56238400	-2.24546400
H	-0.58261400	1.96155300	-3.75069700
H	-1.48547500	1.86722300	-2.21958000
C	-2.09442200	-1.05624500	-2.47849300
H	-2.63972200	-0.11609800	-2.51490700
H	-2.27693200	-1.60316300	-3.41051600
H	-2.49461900	-1.65863000	-1.65942100
C	-0.98452300	1.50116500	1.38390800
O	-1.88962100	1.87651400	2.09638400
N	-0.92639100	0.13563000	0.90531100
C	0.08637800	2.42390900	0.89472600
C	1.42572000	2.08141200	0.60496600
C	-0.35835100	3.73254500	0.66492700
C	2.27108600	3.06398000	0.07877000
C	0.48304700	4.69655300	0.11539200
H	-1.38896400	3.96489000	0.90711800
C	1.79812400	4.35429000	-0.18251100
H	3.31109800	2.85356200	-0.12573200
H	0.11501300	5.69967400	-0.07127500
H	2.47730900	5.09037200	-0.60114400
O	-2.26218000	-0.39718300	0.80182400
C	-3.16516000	0.35973400	0.09991400
O	-2.84252500	1.33094000	-0.54574100
C	-4.58774200	-0.14243800	0.32565400
C	-5.07433800	0.60867400	1.59312200
H	-6.10512200	0.31217000	1.80945100
H	-4.44910300	0.36894200	2.45668200
H	-5.04752800	1.69088500	1.44111400
C	-4.65035200	-1.66255600	0.56344000
H	-5.69119200	-1.95448400	0.73038200
H	-4.28671400	-2.22224800	-0.30502800
H	-4.06662600	-1.96023300	1.43678000
C	-5.44314800	0.25431200	-0.88897300
H	-5.37721800	1.32677400	-1.08303400
H	-5.12416400	-0.27764700	-1.79161500
H	-6.48861500	-0.00403000	-0.69909200
C	3.34223200	0.50903400	0.53086000

C	3.86009700	-0.82791500	1.04292800
C	2.59908700	-0.65979900	2.97679900
C	1.88089800	0.58311700	2.44630400
H	3.23794600	-1.65994800	0.68293900
H	4.88392100	-0.97295700	0.68756700
H	3.96946800	1.28236800	0.99036300
H	3.42843600	0.58334500	-0.54876900
H	2.02053800	-1.56177000	2.77666300
H	2.68884600	-0.55208700	4.06098700
H	0.85152000	0.57946200	2.79842900
H	2.37149300	1.47826100	2.84672200
N	1.91310200	0.73334400	0.92798300
O	3.90905500	-0.80060900	2.45758000
C	0.18579000	-2.55637300	1.82076100
O	0.75572800	-2.30731800	0.70979900
C	0.26579600	-3.96169900	2.35598400
H	0.25296900	-3.94927800	3.44681600
H	-0.61853800	-4.51108100	2.01423500
H	1.15596600	-4.46847800	1.98157900
O	-0.44189800	-1.68600600	2.50391300
H	-0.61201900	-0.67430500	1.79985900

P, E=-1032.94298752 a.u.

C	0.00948500	1.26132800	-0.29165400
O	0.74223400	1.94036700	-0.99403100
N	0.47597500	0.24266400	0.51534100
C	-1.46522800	1.53528700	-0.13946800
C	-2.44984700	0.54136700	0.07792500
C	-1.84620900	2.87738000	-0.23066900
C	-3.78177400	0.93914900	0.24667900
C	-3.17354800	3.26179800	-0.05743400
H	-1.06996700	3.60982400	-0.42485900
C	-4.13806200	2.28759300	0.19414300
H	-4.55227600	0.19376200	0.40586200
H	-3.44988700	4.30981000	-0.11259400
H	-5.17754000	2.56977800	0.33373900
O	1.71655300	-0.29219700	0.12982300
C	2.79862200	0.38703300	0.67638700
O	2.69455800	1.21829700	1.53570700
C	4.08093500	-0.06515700	-0.02176600
C	4.02881100	0.48222500	-1.46754300
H	4.94860200	0.20799400	-1.99494900
H	3.17334400	0.07486100	-2.01052200
H	3.93683200	1.57191000	-1.47001600

C	4.17408800	-1.60481700	-0.04150900
H	5.10473300	-1.90720100	-0.53257600
H	4.18036200	-2.01470200	0.97391300
H	3.33805400	-2.04921200	-0.58627800
C	5.27686000	0.53334200	0.73277600
H	5.20927300	1.62293400	0.76995300
H	5.31677600	0.16765900	1.76290800
H	6.20789100	0.25449600	0.22926900
C	-2.93976700	-1.76711600	0.82838600
C	-2.21955200	-3.10719400	0.97202500
C	-1.03646600	-2.75555500	-1.02150500
C	-1.70342200	-1.39668200	-1.21489100
H	-1.31696700	-2.97302700	1.59193800
H	-2.87024800	-3.83980000	1.45762900
H	-3.88927500	-1.93675700	0.29341100
H	-3.16763100	-1.35152100	1.81463800
H	-0.07342900	-2.62114600	-0.50024200
H	-0.84171200	-3.22526300	-1.98947900
H	-1.01792000	-0.71592800	-1.72570700
H	-2.60376800	-1.50733300	-1.84055500
N	-2.06306400	-0.83804400	0.10791800
O	-1.87576300	-3.64565900	-0.29680100
H	-0.18584900	-0.49982700	0.74281700

N-chloromorpholine, E=-747.251265175 a.u.

C	-0.16933700	-1.21057000	0.74883800
C	-1.14731600	-1.17640200	-0.42555600
C	-1.14658700	1.17673900	-0.42539100
C	-0.16899200	1.21031100	0.74918600
H	-0.59591600	-1.22934700	-1.37705200
H	-1.83389900	-2.02677000	-0.37648100
H	-0.73594700	-1.24194100	1.68826500
H	0.48164200	-2.08746300	0.71153800
H	-0.59479800	1.22925300	-1.37672200
H	-1.83274600	2.02745600	-0.37686200
H	0.48233200	2.08700000	0.71263500
H	-0.73571100	1.24140100	1.68857100
N	0.67246200	-0.00031400	0.86883200
O	-1.94955400	0.00041000	-0.37733800
Cl	1.88515500	-0.00006700	-0.48467500

CsCl, E=-480.4479184 a.u.

Cl	0.00000000	0.00000000	-2.37970900
Cs	0.00000000	0.00000000	0.73554600

MeOH, E=-115.697185271 a.u.

C	0.66159600	-0.01939600	0.00000200
H	1.08207800	0.98942000	-0.00066900
H	1.03808600	-0.54236800	0.89211900
H	1.03798100	-0.54349700	-0.89149200
O	-0.74933100	0.12204500	0.00000300
H	-1.13307600	-0.76353700	0.00000900

TS4', E=-1703.36360682 a.u., Imaginary frequency = 1059i

Rh	-0.58112900	-0.13888300	-0.55358100
C	-1.90057000	-2.03227700	2.58986300
O	-1.38476700	-1.60753700	3.62462400
O	-2.41744700	-1.33232300	1.62745200
C	-0.00464100	-0.94518300	-2.49633800
C	-1.06477100	-1.77989000	-1.95556400
C	-2.23332200	-0.98742000	-1.80961400
C	-0.55680400	0.37469100	-2.69742900
C	-1.91308400	0.36834800	-2.25483300
C	-2.87830200	1.51143000	-2.34558800
H	-3.42849700	1.47644700	-3.29538900
H	-3.59769600	1.48935300	-1.52619500
H	-2.35843600	2.47028600	-2.28728900
C	-3.55854600	-1.47489100	-1.29855000
H	-4.30201100	-0.67461000	-1.31353800
H	-3.93233100	-2.29668300	-1.92179200
H	-3.45114900	-1.81783400	-0.26438000
C	-0.91954900	-3.22018300	-1.57094200
H	0.09557500	-3.40977600	-1.21515000
H	-1.61511700	-3.47243500	-0.76786200
H	-1.12118400	-3.87480200	-2.42944300
C	1.33698700	-1.41522400	-2.96169400
H	1.76325100	-2.10992400	-2.23841700
H	1.24911700	-1.89825300	-3.94542500
H	2.02918000	-0.57654200	-3.05431200
C	0.21173000	1.54486100	-3.23403500
H	1.20779400	1.58045200	-2.78637600
H	0.31844800	1.47011300	-4.32363300
H	-0.28690100	2.48748400	-3.00057600
C	-1.93497100	-3.54662900	2.32470700
H	-2.85835600	-3.84652000	1.81813500
H	-1.09526700	-3.77914100	1.65991900
H	-1.81226700	-4.10841000	3.25415800
C	0.44737500	2.31019400	0.86325200

O	1.20978500	3.19305900	1.26548800
N	0.75393000	1.29130600	0.02712300
C	-1.03732900	2.30061100	1.13587500
C	-1.84131400	1.14722200	0.96338700
C	-1.61213900	3.54198300	1.43173300
C	-3.23989700	1.32987400	1.04757200
H	-1.76764400	-0.09653800	1.28734800
C	-2.99414200	3.68506500	1.52236700
H	-0.93940700	4.38396400	1.56672900
C	-3.81346800	2.57102800	1.31509500
H	-3.86903900	0.44937700	0.97215500
H	-3.43062000	4.65528100	1.74872200
H	-4.89505600	2.66430400	1.38902000
O	2.11708400	1.16785200	-0.32867000
C	2.94802500	0.72927500	0.66562600
O	2.61996600	0.56608200	1.81396100
C	4.37582200	0.53841800	0.13518500
C	5.10061300	1.88832900	0.32622500
H	6.14254000	1.80536100	-0.00625400
H	4.61073000	2.67820600	-0.25181200
H	5.09275300	2.18589600	1.37923400
C	4.38930600	0.12089500	-1.34472600
H	5.42303500	-0.05181400	-1.66889500
H	3.81726200	-0.80038200	-1.47158500
H	3.95338500	0.89410800	-1.98278200
C	5.03744900	-0.56046700	0.98487600
H	5.01436100	-0.29573200	2.04449700
H	4.49589600	-1.50183400	0.85338900
H	6.07994400	-0.69769900	0.67372400
C	1.36703200	-1.95640400	0.90716800
O	2.11780700	-2.13103800	-0.06921700
C	1.73985100	-2.49531400	2.28276700
H	0.87548500	-2.51507600	2.94890300
H	2.20468500	-3.48106900	2.18643300
H	2.47618200	-1.79955500	2.69686400
O	0.24714900	-1.31427500	0.92072000

TS15', E=-1723.46026714 a.u., Imaginary frequency = 1085i

Rh	1.09023700	0.81835100	-0.02662000
C	1.22879000	-2.26078000	2.48152500
O	0.24229800	-2.97846000	2.23705000
O	1.98410900	-1.68419300	1.61097800
C	1.39665200	2.95530300	0.35629500
C	2.21545100	2.19447600	1.28222000

C	3.15361100	1.43022300	0.53384200
C	1.85675900	2.64745400	-0.97810000
C	2.92161200	1.70086500	-0.88369000
C	3.73953400	1.18401700	-2.02762500
H	4.56763700	1.87133800	-2.24113200
H	4.15573900	0.20027600	-1.81052100
H	3.13524100	1.08769800	-2.93222800
C	4.22103700	0.55303500	1.11905900
H	4.80330700	0.06453500	0.33552800
H	4.90997100	1.15032900	1.72786600
H	3.77293000	-0.22529800	1.74166600
C	2.07470700	2.19493100	2.77249600
H	1.03621200	2.37926300	3.05362400
H	2.38009800	1.23094700	3.18572200
H	2.70332800	2.97708600	3.21643800
C	0.42559300	4.03545400	0.70848600
H	-0.12253200	3.78625500	1.61450500
H	0.96490600	4.98227100	0.84812700
H	-0.30451500	4.17625000	-0.08945900
C	1.27531600	3.22270300	-2.23334200
H	0.18621000	3.26906100	-2.16338500
H	1.65605100	4.23781100	-2.39837000
H	1.52851800	2.61567000	-3.10425500
C	1.60602700	-1.96596100	3.93079900
H	2.69119800	-1.92706600	4.05739900
H	1.20422000	-0.97682800	4.18092800
H	1.16941400	-2.70323400	4.60700800
C	-0.65846000	-0.56785900	-2.04621500
O	-1.64966200	-0.91580600	-2.70647700
N	-0.52056700	0.53165100	-1.28296600
C	0.62465600	-1.36369100	-2.01600500
C	1.54980800	-1.26853800	-0.94480500
C	0.89979300	-2.13492500	-3.15148900
C	2.77868400	-1.94510900	-1.11499700
H	1.48058100	-1.31202800	0.36853200
C	2.11846500	-2.79807800	-3.27822000
H	0.14544300	-2.17571300	-3.93177600
C	3.06674900	-2.69101900	-2.25608100
H	3.48692500	-1.93118300	-0.29339900
H	2.33152200	-3.38608200	-4.16679900
H	4.02072300	-3.20544000	-2.33983300
O	-1.62561400	1.42023700	-1.25253200
C	-2.72507700	1.02386400	-0.56313300
O	-2.87574400	-0.08345900	-0.08910000

C	-3.78228900	2.12942900	-0.51299200
C	-4.64879200	1.97272900	-1.78361700
H	-5.44390600	2.72602200	-1.78219000
H	-4.04677100	2.10407900	-2.68769000
H	-5.11204000	0.98177200	-1.82232600
C	-3.14270100	3.52786700	-0.46488100
H	-3.93005600	4.28569900	-0.38978600
H	-2.49065700	3.60752100	0.40731000
H	-2.55581400	3.73201800	-1.36390900
C	-4.62870200	1.90749100	0.75334800
H	-5.08953800	0.91669200	0.74829300
H	-3.99754100	1.99298500	1.64270100
H	-5.42008700	2.66238800	0.80554600
Cs	-1.77447000	-2.86167900	0.11397000
C	-1.06120900	0.69630100	2.10174900
O	-1.31017700	1.90386200	1.99816900
C	-1.86223600	-0.17232600	3.06950900
H	-1.39112700	-1.14572600	3.22338700
H	-1.98098700	0.35134500	4.02143300
H	-2.86065700	-0.30377400	2.63807100
O	-0.17364500	0.02543700	1.43672100

TS4_MeOH, E=-1590.47968521 a.u., Imaginary frequency = 1170i

Rh	-0.72463200	-0.46450800	-0.20856900
C	-0.22076400	-1.79079000	-1.89681500
C	-1.41335700	-2.32307500	-1.24361200
C	-2.44659700	-1.35956400	-1.33826300
C	-0.54907100	-0.50030800	-2.41883300
C	-1.90069600	-0.19002700	-2.02531000
C	-2.66877800	1.03014000	-2.43279000
H	-3.12503500	0.88306900	-3.41945600
H	-3.45826400	1.25985600	-1.71643200
H	-2.01685400	1.90443100	-2.48522600
C	-3.87104000	-1.53695900	-0.90506800
H	-4.35906600	-0.57559800	-0.74341400
H	-4.43560800	-2.07445700	-1.67701800
H	-3.94087700	-2.11104900	0.02204400
C	-1.46680100	-3.66393600	-0.58268200
H	-0.64428200	-3.75230000	0.13364700
H	-2.40897500	-3.81653900	-0.05254100
H	-1.36031700	-4.46070700	-1.32814100
C	1.07794800	-2.52402700	-2.00876800
H	1.38568100	-2.87170300	-1.01831000
H	0.98104200	-3.39339300	-2.67040200

H	1. 86580600	-1. 87925400	-2. 39986200
C	0. 36088100	0. 39912100	-3. 19621900
H	1. 39310000	0. 29193300	-2. 86360300
H	0. 30446600	0. 15821800	-4. 26454100
H	0. 08529100	1. 44726900	-3. 06655600
C	0. 34875200	2. 26421700	0. 19362500
O	1. 07948900	3. 23233500	-0. 00824100
N	0. 70673000	0. 94823300	0. 11334400
C	-1. 11009900	2. 35892600	0. 53992300
C	-1. 83896900	1. 18139800	0. 83310700
C	-1. 74099600	3. 59876500	0. 43736500
C	-3. 23199300	1. 31071100	1. 00551800
C	-3. 12139500	3. 69502000	0. 61495600
H	-1. 13032500	4. 46493900	0. 20056200
C	-3. 86911300	2. 54707100	0. 89955900
H	-3. 81582800	0. 43581800	1. 27725900
H	-3. 61478100	4. 65948300	0. 53341700
H	-4. 94252700	2. 62059500	1. 05392100
O	1. 97435000	0. 76509100	-0. 48798300
C	3. 02042500	0. 71740700	0. 39694200
O	2. 89805500	0. 71557200	1. 59584800
C	4. 34807100	0. 71477100	-0. 36851100
C	4. 52845700	2. 12975400	-0. 96553400
H	5. 46600200	2. 17587600	-1. 53056400
H	3. 69714200	2. 38248900	-1. 62763700
H	4. 56268300	2. 88389100	-0. 17401400
C	4. 32859700	-0. 33704000	-1. 49533500
H	5. 30851800	-0. 37135500	-1. 98319700
H	4. 10974600	-1. 33578900	-1. 10270500
H	3. 58122700	-0. 09399800	-2. 25394800
C	5. 47912200	0. 40368700	0. 62291800
H	5. 47161700	1. 10885900	1. 45662500
H	5. 37414300	-0. 60347400	1. 03878400
H	6. 44642600	0. 46598100	0. 11366900
C	1. 14263400	-1. 71723300	2. 15704800
O	0. 77073900	-1. 13338400	3. 20295700
O	0. 51058100	-1. 75955500	1. 04254600
C	2. 46715000	-2. 45703500	2. 20537900
H	2. 56371700	-3. 16043600	1. 37628000
H	3. 25562900	-1. 70173800	2. 13680500
H	2. 57656700	-2. 97106100	3. 16279100
H	-1. 48506400	0. 31164500	1. 77166800
C	-2. 30820600	-1. 41844000	2. 98501100
H	-3. 35286000	-1. 11971300	3. 11299300

H	-2.20262600	-1.99350400	2.05399600
H	-2.02006100	-2.06060300	3.82388400
O	-1.48913600	-0.25305900	2.97111700
H	-0.47173100	-0.57378100	3.08981200

TS15_MeOH, E=-1610.57014632 a.u., Imaginary frequency = 1242i

Rh	1.45150300	0.36116700	0.14355800
C	2.38147700	2.36630300	0.28405500
C	3.16711100	1.42787800	1.08163800
C	3.68444700	0.42723900	0.22096300
C	2.42763900	1.92975300	-1.07394200
C	3.17304000	0.68889900	-1.12216900
C	3.54046600	-0.06283500	-2.36411800
H	4.47298700	0.33213100	-2.78455400
H	3.67810600	-1.12525700	-2.15832700
H	2.76183200	0.02801000	-3.12392400
C	4.67063400	-0.63612800	0.59849700
H	4.70643500	-1.43287100	-0.14411000
H	5.67316300	-0.19719800	0.66542900
H	4.43855300	-1.08029200	1.56964400
C	3.37490000	1.55916300	2.55648000
H	2.41610100	1.72255400	3.05625900
H	3.84401200	0.66926200	2.98027800
H	4.02079600	2.41857200	2.77088600
C	1.70612500	3.57922500	0.83810300
H	1.07026000	3.29492800	1.68093500
H	2.44885100	4.30263700	1.19381900
H	1.08378300	4.06958000	0.08909100
C	1.79129400	2.60736700	-2.24607100
H	0.88213300	3.13292200	-1.95406200
H	2.49168300	3.33170500	-2.67819100
H	1.52345100	1.88861000	-3.02223100
C	-0.70412500	-0.68963600	-1.66663000
O	-1.72079600	-0.75200200	-2.37042600
N	-0.33261600	0.34379300	-0.87225100
C	0.29780000	-1.79993500	-1.53823800
C	1.23493600	-1.76915500	-0.47558900
C	0.33056600	-2.79121700	-2.51937800
C	2.21948900	-2.77791400	-0.46265900
C	1.32312200	-3.77292300	-2.47965300
H	-0.40851600	-2.75915300	-3.31467500
C	2.26924200	-3.76426700	-1.44926800
H	2.92946300	-2.81843200	0.35760600
H	1.36206600	-4.53894900	-3.24827700

H	3.03541300	-4.53344700	-1.40934700
O	-1.02967500	1.55291300	-1.11251700
C	-2.27675000	1.65684800	-0.58049200
O	-2.79031600	0.79763700	0.10644000
C	-2.91850500	2.98860200	-0.97032200
C	-3.04650100	3.03791700	-2.51018000
H	-3.54004300	3.96916900	-2.80458300
H	-2.06625700	2.99476400	-2.99033900
H	-3.64281000	2.19973300	-2.88300400
C	-2.02715700	4.14839600	-0.47415700
H	-2.51167100	5.10308100	-0.69940600
H	-1.86839500	4.09522600	0.60804000
H	-1.05258100	4.13667600	-0.96717900
C	-4.30647000	3.07356000	-0.31672800
H	-4.94555500	2.24757200	-0.63930500
H	-4.23652400	3.03912200	0.77426800
H	-4.78764800	4.01390200	-0.60038800
Cs	-2.95847300	-2.19433900	0.40535500
C	-0.85841000	0.63937700	2.47860500
O	-1.32174700	-0.54194400	2.58182500
O	0.23788200	0.94392900	1.92013400
C	-1.68933200	1.75496900	3.07340500
H	-1.13972300	2.69661500	3.08564900
H	-2.58498900	1.86219200	2.45372200
H	-2.01162400	1.48836400	4.08274400
H	0.79688100	-1.72192600	0.80057300
C	1.36648300	-2.29737400	2.88993800
H	1.99723200	-3.15324000	2.63849500
H	1.97333000	-1.38339300	2.91513900
H	0.92490800	-2.45968000	3.87735300
O	0.32385800	-2.18950400	1.91304800
H	-0.39117500	-1.43680500	2.23253000

N-benzoyloxy morpholine, E=-707.108919731 a.u.

C	-2.45305100	1.17619200	0.48561300
C	-2.79912700	0.04465900	1.45170500
C	-2.94918400	-1.50005700	-0.31434400
C	-2.59094900	-0.41574300	-1.33491800
H	-1.87614400	-0.41761000	1.83542500
H	-3.37423100	0.42414300	2.30131200
H	-3.37058700	1.68116000	0.16406400
H	-1.79254700	1.92091100	0.93363600
H	-2.03856800	-2.03076500	0.00479400
H	-3.63691500	-2.22882000	-0.75385000

H	-2.02473400	-0.82582700	-2.17581500
H	-3.50800300	0.03937100	-1.72445300
N	-1.81777900	0.69856400	-0.76118900
O	-3.61445000	-0.93456400	0.81027800
O	-0.54156500	0.07384000	-0.39538200
C	0.48634700	0.96190200	-0.28010700
O	0.35224400	2.16563500	-0.29061400
C	1.78608600	0.25226000	-0.09429800
C	1.90155800	-1.14469500	-0.13144300
C	2.92482200	1.04055500	0.11997100
C	3.14752400	-1.74293200	0.04628000
H	1.01987700	-1.75188200	-0.29968300
C	4.16761100	0.43822900	0.29621700
H	2.81086600	2.11891600	0.14245800
C	4.28038900	-0.95405300	0.26024800
H	3.23564400	-2.82480500	0.01697300
H	5.04788000	1.05197500	0.46160000
H	5.24991400	-1.42389800	0.39807000

PhCOOCs, E=-440.300651472 a.u.

C	-0.54915000	0.00005700	-0.00036800
O	0.02612300	-1.12956900	-0.00007400
C	-2.07065100	-0.00004700	-0.00027500
C	-2.77931000	1.20720800	-0.00026800
C	-2.77931800	-1.20729500	-0.00018300
C	-4.17459800	1.20922100	-0.00016800
H	-2.20953900	2.13057100	-0.00035400
C	-4.17460500	-1.20924100	-0.00008400
H	-2.20958100	-2.13066700	-0.00020300
C	-4.87603300	-0.00000400	-0.00006900
H	-4.71738200	2.15147900	-0.00016500
H	-4.71740700	-2.15148800	-0.00001500
H	-5.96326900	0.00000300	0.00001600
O	0.02596500	1.12973100	-0.00016800
Cs	2.68768100	-0.00001100	0.00020300

17Rh_O, E=-1972.97183868 a.u.

Rh	1.83996100	-0.29632300	-0.29353100
C	2.63382300	-1.16478900	-2.10805400
C	3.77283900	-0.83417800	-1.28718600
C	3.68504800	-1.59718800	-0.08959600
C	1.94288400	-2.28647200	-1.46624800
C	2.57020600	-2.53611500	-0.23544700
C	2.25939700	-3.65112600	0.71730100
H	2.11631400	-3.30239300	1.74493100

H	1. 35966700	-4. 19067000	0. 41541900
H	3. 08544400	-4. 37193400	0. 73880400
C	4. 73216100	-1. 65406100	0. 98492900
H	4. 35471600	-2. 11460000	1. 90002800
H	5. 58589000	-2. 25534300	0. 64944300
H	5. 11096300	-0. 65955900	1. 23576300
C	4. 89696900	0. 06902600	-1. 68874000
H	4. 53769600	0. 96478400	-2. 19728500
H	5. 49551800	0. 38260300	-0. 83171700
H	5. 55887300	-0. 47055600	-2. 37703200
C	2. 38759000	-0. 65560900	-3. 49548500
H	2. 82878400	0. 33483000	-3. 62663000
H	2. 84212600	-1. 32895900	-4. 23311500
H	1. 32090700	-0. 57371700	-3. 70225200
C	0. 79802000	-3. 05218800	-2. 05530800
H	0. 05567100	-3. 31378600	-1. 29748600
H	0. 30190000	-2. 47407300	-2. 83378200
H	1. 16064600	-3. 98278200	-2. 50883800
C	-0. 13884500	1. 71486600	-1. 30145000
O	-1. 17970500	2. 25324600	-1. 73062200
N	-0. 00673100	0. 42229500	-0. 92755500
C	1. 13057700	2. 44391100	-1. 02785500
C	2. 19235900	1. 70667900	-0. 47377600
C	1. 22169100	3. 82322800	-1. 22858600
C	3. 34148800	2. 40110300	-0. 08172400
C	2. 38380500	4. 49912500	-0. 85453200
H	0. 37790800	4. 34095100	-1. 67688700
C	3. 43600000	3. 78721700	-0. 27092000
H	4. 17450800	1. 87360700	0. 37516500
H	2. 47019000	5. 57007100	-1. 01090000
H	4. 33842800	4. 30965000	0. 03590500
O	-1. 20144100	-0. 33984800	-1. 08484400
C	-1. 56275600	-0. 60663400	-2. 38422200
O	-0. 87005900	-0. 35986200	-3. 34012500
C	-2. 93802600	-1. 28800600	-2. 44573400
C	-3. 96434500	-0. 47838400	-1. 62921600
H	-4. 95074900	-0. 94649400	-1. 70650700
H	-3. 68128100	-0. 44791200	-0. 57414500
H	-4. 04325800	0. 54014500	-2. 02639000
C	-2. 81905000	-2. 71128500	-1. 85922100
H	-3. 79986200	-3. 19702500	-1. 87533300
H	-2. 13372200	-3. 32214600	-2. 45338200
H	-2. 46499800	-2. 69069600	-0. 82785900
C	-3. 37410800	-1. 35732400	-3. 91727600

H	-3.46226600	-0.35743600	-4.35105600
H	-2.64682400	-1.91150700	-4.51444000
H	-4.34384500	-1.85915400	-3.99186500
Cs	-3.20167900	2.71318900	0.26824700
C	2.15774100	-0.40731300	2.82198400
C	1.73682600	-0.19190700	4.27600700
C	0.40017800	1.63046500	3.68669300
C	0.78910200	1.48620000	2.22030400
H	0.86954600	-0.82701800	4.51296400
H	2.56074900	-0.47474600	4.93665000
H	3.06454100	0.15627900	2.59233500
H	2.33645700	-1.46099900	2.61769600
H	-0.53854300	1.09796800	3.89770200
H	0.25163100	2.69013300	3.91434400
H	0.03353900	1.84593300	1.53372400
H	1.71249800	2.03604500	2.03104600
N	1.13897800	0.08005600	1.84300900
O	1.44587100	1.17207400	4.53145100
O	0.03391600	-0.88998800	2.09090100
C	-1.27585200	-0.63627400	1.85661200
O	-1.78517600	0.46864400	1.76452000
C	-2.03813300	-1.91001600	1.79901100
C	-1.40898500	-3.15601700	1.65658900
C	-3.43792300	-1.83900100	1.85442900
C	-2.17707100	-4.31421700	1.55617000
H	-0.32980200	-3.20654400	1.61135400
C	-4.20143400	-2.99864800	1.75597300
H	-3.91087400	-0.87096900	1.97715600
C	-3.57168000	-4.23754200	1.60334400
H	-1.68922000	-5.27668300	1.43807200
H	-5.28439200	-2.94031900	1.79941200
H	-4.16735300	-5.14159300	1.52324900

TS18_{Rh_O}, E=-1972.95593203 a.u., Imaginary frequency = 95i

Rh	1.77195900	-0.47182100	-0.17347400
C	2.47657200	-1.43943000	-2.05030200
C	3.62999800	-1.29308200	-1.20867200
C	3.41415400	-2.05711500	-0.01868200
C	1.59732100	-2.41413700	-1.41958600
C	2.17320800	-2.79375900	-0.18296100
C	1.65796000	-3.84132200	0.75733600
H	1.33893500	-3.41945900	1.71520900
H	0.80252800	-4.36402600	0.32592200
H	2.43656000	-4.58341300	0.96420600

C	4.43720000	-2.28687900	1.05526000
H	4.00396600	-2.76093200	1.93755800
H	5.22755200	-2.94934500	0.68280000
H	4.91513500	-1.35461600	1.36877600
C	4.89181800	-0.58324200	-1.58374200
H	4.69397700	0.36204100	-2.09103800
H	5.52200300	-0.38068800	-0.71634000
H	5.46380300	-1.22133700	-2.26850000
C	2.33492400	-0.87015300	-3.42841700
H	2.92237000	0.04496000	-3.53077000
H	2.69972800	-1.58942000	-4.17201900
H	1.29739400	-0.62575300	-3.65184400
C	0.34690700	-2.98504900	-2.01332800
H	-0.45559400	-3.04545900	-1.27515500
H	0.00030700	-2.38177600	-2.85084200
H	0.54065600	-3.99855200	-2.38513500
C	0.20792600	1.81500000	-1.31683300
O	-0.72444500	2.51308900	-1.75313500
N	0.11484400	0.51537800	-0.93402600
C	1.57730700	2.31854000	-1.03072100
C	2.47851400	1.43597700	-0.41752100
C	1.91952900	3.65320200	-1.26396300
C	3.71739400	1.91974100	0.00767800
C	3.17130000	4.12289600	-0.86615700
H	1.19310300	4.29717400	-1.75172300
C	4.06113100	3.25971800	-0.21907200
H	4.42258700	1.26825300	0.51580000
H	3.45105000	5.15584400	-1.04817400
H	5.02906900	3.62668800	0.11134500
O	-1.17443300	-0.04697300	-1.11270900
C	-1.55318900	-0.23103500	-2.42940900
O	-0.80166500	-0.09304400	-3.36168100
C	-3.01918700	-0.67142300	-2.53897000
C	-3.91744000	0.20520500	-1.64672400
H	-4.95962500	-0.11149900	-1.75147000
H	-3.63550300	0.10719600	-0.59627000
H	-3.85351000	1.25331900	-1.96162900
C	-3.12713500	-2.14498100	-2.08851500
H	-4.16944000	-2.47022100	-2.16025100
H	-2.52817200	-2.79614500	-2.73146400
H	-2.80444800	-2.27307900	-1.05509300
C	-3.44578800	-0.53784300	-4.00982900
H	-3.37181100	0.49863200	-4.35113500
H	-2.81131100	-1.14542500	-4.65835500

H	-4.48228700	-0.87012400	-4.12226100
Cs	-2.65369000	2.98217900	0.45999800
C	2.06623300	-0.69672000	2.80955600
C	1.53867000	-0.45196800	4.22628300
C	0.44555000	1.48625400	3.56820600
C	0.92535900	1.33415500	2.12615400
H	0.58971900	-0.98674400	4.36080200
H	2.26757400	-0.83108400	4.94778700
H	3.07900300	-0.28154800	2.72536900
H	2.10839800	-1.76154300	2.59281900
H	-0.54289800	1.02396000	3.67690200
H	0.36697400	2.55238600	3.80308100
H	0.19389100	1.68790100	1.40713000
H	1.85012700	1.91183300	1.99269700
N	1.29236000	-0.03524600	1.74289900
O	1.38142300	0.93261800	4.47654000
O	-0.31896900	-1.12875900	2.09058500
C	-1.52590900	-0.71051600	1.84642900
O	-1.90209800	0.47259600	1.82107900
C	-2.50856100	-1.82821600	1.61363300
C	-2.08476600	-3.14456300	1.38547800
C	-3.87839900	-1.53414900	1.60923800
C	-3.01887200	-4.14696000	1.12651000
H	-1.02618600	-3.36654500	1.40583100
C	-4.81162700	-2.53705900	1.35386000
H	-4.19360300	-0.51552300	1.80656700
C	-4.38294600	-3.84434300	1.10648100
H	-2.68524100	-5.16359200	0.94126500
H	-5.87189000	-2.30267700	1.34946800
H	-5.10997100	-4.62514900	0.90484700

17'_{Rh_O}, E=-1972.94240314 a.u.

Rh	-2.30960300	-0.52493400	-0.11989700
C	-2.81304000	-2.62153400	0.20704700
C	-4.01007000	-1.82281600	0.30959800
C	-4.30437300	-1.28572000	-1.02228900
C	-2.31296600	-2.45077200	-1.12737800
C	-3.27490300	-1.66236000	-1.90016100
C	-3.13024300	-1.34143500	-3.35704800
H	-3.32097400	-2.22818900	-3.97256500
H	-3.82911600	-0.56311700	-3.67266300
H	-2.11543600	-1.00013100	-3.58294800
C	-5.53657400	-0.49883600	-1.34257300
H	-5.45782500	0.02357900	-2.29813400

H	-6.40019800	-1.17185500	-1.40284400
H	-5.76058000	0.23257800	-0.55976200
C	-4.97219400	-1.81307700	1.45739000
H	-4.47056800	-2.03861800	2.39888900
H	-5.47121300	-0.84519300	1.56066100
H	-5.75059900	-2.56991900	1.29950400
C	-2.20317000	-3.48874400	1.26534900
H	-2.49038800	-3.15362100	2.26318200
H	-2.53835000	-4.52473700	1.13558400
H	-1.11283200	-3.45727600	1.20449200
C	-1.07963000	-3.07293900	-1.69776900
H	-0.35255500	-3.29299900	-0.91711600
H	-1.35115500	-3.99900700	-2.22083300
H	-0.60145500	-2.40448700	-2.41744000
C	0.89164800	-0.80106300	1.02365800
O	1.52168300	0.24877100	0.68888200
N	1.00512900	-2.04051200	0.59625200
C	-0.16265600	-0.66082300	2.09218600
C	-1.50813700	-0.39940200	1.78349700
C	0.26860100	-0.69712800	3.42676300
C	-2.38472600	-0.15943600	2.85728100
C	-0.61747700	-0.46720300	4.47695000
H	1.31082400	-0.93242100	3.63094000
C	-1.95288100	-0.18487500	4.18701300
H	-3.43258100	0.05240000	2.66547600
H	-0.27420800	-0.51363200	5.50634400
H	-2.66259500	0.00124500	4.98897000
O	1.97890000	-2.13311000	-0.50837400
C	3.27318600	-2.07806200	-0.20120700
O	3.73284000	-1.75431800	0.88563000
C	4.17164900	-2.53023900	-1.36718000
C	5.40803700	-1.61295800	-1.40619200
H	6.10899600	-1.95284300	-2.17465300
H	5.12494100	-0.58112100	-1.64910800
H	5.92175300	-1.61882500	-0.44159200
C	3.45566200	-2.51740000	-2.72712000
H	4.13484100	-2.88429700	-3.50370300
H	2.56859200	-3.15355400	-2.71481000
H	3.14055000	-1.50809100	-3.00928400
C	4.60835400	-3.97390400	-1.02252800
H	5.11556800	-4.00470800	-0.05445700
H	3.74258200	-4.64194100	-0.97905400
H	5.29315500	-4.35056300	-1.78940800
Cs	4.08747800	1.23323900	1.43523100

C	-3.10776500	2.18683300	-1.39242700
C	-3.13803000	3.70909600	-1.51675000
C	-2.94617200	3.97501300	0.79910500
C	-2.88550400	2.46596100	1.02932000
H	-2.12392400	4.09890300	-1.69297400
H	-3.76671100	3.99242100	-2.36503700
H	-4.12418100	1.80270900	-1.28819300
H	-2.63952100	1.70560700	-2.25391300
H	-1.93015900	4.38897100	0.71650600
H	-3.44166400	4.44994900	1.64959300
H	-2.24854600	2.19597100	1.87017100
H	-3.88754600	2.06710900	1.20967600
N	-2.39094300	1.72190100	-0.16269600
O	-3.71092300	4.28913600	-0.35689700
O	-0.99814000	2.20636200	-0.31305600
C	-0.20605300	1.34207400	-0.98926900
O	-0.57408600	0.19540600	-1.24548600
C	1.05373800	1.93165200	-1.47009500
C	1.33870400	3.29667100	-1.32812100
C	1.98474400	1.06723300	-2.06940900
C	2.55978200	3.79735000	-1.78389700
H	0.61426600	3.95770200	-0.86538900
C	3.18977300	1.57834900	-2.54217900
H	1.75829100	0.00912700	-2.11376800
C	3.48191300	2.94167100	-2.39520200
H	2.78085700	4.85562700	-1.68400900
H	3.90282400	0.91800800	-3.02600000
H	4.42084400	3.33834200	-2.77130900

TS18'_{Rh_O}, E=-1972.91575212 a.u., Imaginary frequency = 151i

Rh	-2.30544400	-0.40199700	-0.15535600
C	-2.62954600	-2.61724000	-0.07603000
C	-3.90310600	-1.94367900	0.03842400
C	-4.20407300	-1.32849400	-1.25322500
C	-2.10819500	-2.29960700	-1.36536000
C	-3.10292600	-1.52360500	-2.10416600
C	-2.92871900	-1.06272400	-3.51827100
H	-2.99413600	-1.90717500	-4.21431900
H	-3.69265100	-0.33710500	-3.80778100
H	-1.94529800	-0.60276300	-3.65807500
C	-5.51248900	-0.68453600	-1.59218600
H	-5.42636400	0.02002200	-2.42204100
H	-6.23279300	-1.45631000	-1.88976100
H	-5.94365600	-0.16374200	-0.73335900

C	-4.89921300	-2.13720000	1.14026700
H	-4.40883000	-2.38987600	2.08042000
H	-5.50904500	-1.24395300	1.30184400
H	-5.57924300	-2.95900000	0.88319500
C	-1.99665700	-3.52601900	0.93297200
H	-2.35932400	-3.31127400	1.93933800
H	-2.23924600	-4.56803600	0.69215100
H	-0.91126800	-3.39933900	0.93516400
C	-0.80786200	-2.75514900	-1.94190200
H	-0.12863200	-3.10332100	-1.16614100
H	-0.99593800	-3.56354800	-2.65987400
H	-0.31342700	-1.93789300	-2.47246000
C	0.85986600	-0.73818800	1.13093200
O	1.49195900	0.32636800	0.88389700
N	1.01099400	-1.96975200	0.68367400
C	-0.27174400	-0.68995200	2.13704200
C	-1.61276600	-0.46796900	1.79496100
C	0.08162200	-0.83832200	3.48872600
C	-2.56712800	-0.40119000	2.82107100
C	-0.87274000	-0.77305900	4.50028100
H	1.12377800	-1.03238300	3.72952700
C	-2.20850600	-0.54951100	4.16335000
H	-3.61272700	-0.22577600	2.58469400
H	-0.58108900	-0.90340800	5.53816500
H	-2.97209800	-0.49772300	4.93481100
O	2.05381500	-2.05580700	-0.35627000
C	3.32943400	-2.01622500	0.02470700
O	3.73381900	-1.65452900	1.12090300
C	4.28292500	-2.53302000	-1.06915500
C	5.48988200	-1.57902500	-1.14807300
H	6.23152400	-1.96200700	-1.85570200
H	5.18529200	-0.58420100	-1.49562100
H	5.96606000	-1.48308200	-0.16864700
C	3.61360400	-2.66665400	-2.44593500
H	4.33776800	-3.05109600	-3.17175700
H	2.76565300	-3.35348400	-2.40774400
H	3.24521900	-1.70493100	-2.81389200
C	4.75798600	-3.92345400	-0.58519900
H	5.23280100	-3.84974600	0.39662200
H	3.91542900	-4.61787800	-0.50850400
H	5.47992300	-4.33975100	-1.29546400
Cs	4.07207400	1.42418100	1.32121800
C	-3.62431600	2.09214000	-1.01327400
C	-3.56932800	3.62075100	-1.11785800

C	-2.86722500	3.83070500	1.09055700
C	-2.82307400	2.31137100	1.28719200
H	-2.58655300	3.93022000	-1.49678000
H	-4.34143000	3.95697400	-1.81490900
H	-4.64598000	1.80468800	-0.73459700
H	-3.37091600	1.61260100	-1.95980700
H	-1.87519200	4.19272400	0.79507500
H	-3.14539200	4.29836800	2.03831100
H	-1.99478500	2.00641700	1.92278900
H	-3.75417300	1.98101100	1.76944800
N	-2.76631800	1.52841000	0.04543000
O	-3.84734800	4.20731900	0.13727100
O	-0.97353200	2.34380200	-0.49382300
C	-0.23040700	1.44020600	-0.98977200
O	-0.53908400	0.21048600	-1.06215600
C	1.07547600	1.86787500	-1.57876300
C	1.43465800	3.22190200	-1.59526600
C	1.95071100	0.89619300	-2.08527200
C	2.66975300	3.60787800	-2.12001600
H	0.74693100	3.96037000	-1.19803500
C	3.17232400	1.29102700	-2.62990900
H	1.67782600	-0.14901100	-2.00993600
C	3.53678500	2.64360100	-2.64403800
H	2.94417000	4.65843200	-2.14147400
H	3.84198000	0.54596400	-3.04784800
H	4.48696600	2.94525600	-3.07617700

16Ru, E=-1876.94060074 a.u.

Ru	1.79382900	-0.77161600	-0.45551200
C	2.85246600	-1.54969000	1.27013900
C	3.50931600	-2.07727100	0.11860700
H	4.55951900	-1.86275500	-0.04412600
C	2.76528500	-2.72281100	-0.89196100
H	3.25443400	-2.99401700	-1.82241800
C	1.37564500	-3.07122100	-0.70933500
C	0.74252700	-2.64000000	0.46380000
H	-0.31794600	-2.82184700	0.60331200
C	1.44240200	-1.80574200	1.39178600
H	0.89854400	-1.38133900	2.22815500
C	3.63174500	-0.77852300	2.31936200
H	4.52198500	-0.38128000	1.81698500
C	4.08950000	-1.75711700	3.41950300
H	3.22716400	-2.17989200	3.94686400
H	4.71128300	-1.23626000	4.15351800

H	4.67289400	-2.58531100	3.00562500
C	2.86516300	0.41350900	2.90996700
H	2.52428700	1.09031300	2.12194000
H	3.52002000	0.97034400	3.58610700
H	1.99788200	0.09047300	3.49621100
C	0.65144100	-3.84259800	-1.77730000
H	0.93292700	-3.48857100	-2.77305700
H	-0.43071800	-3.75361900	-1.67538900
H	0.92383800	-4.90251700	-1.71286300
C	0.59047600	1.91393600	-0.81797700
O	-0.24079100	2.83423800	-0.92238700
N	0.25672300	0.59583400	-0.58917900
C	-1.07647900	0.28396500	-0.33163200
C	-1.83525600	0.90277600	0.66820400
C	-1.73659500	-0.71690800	-1.06202800
C	-3.17796500	0.61191700	0.88586200
C	-3.05999500	-1.05736800	-0.81168700
C	-3.81956600	-0.39232500	0.15979400
F	-1.26661000	1.85340300	1.45724300
F	-3.81448100	1.34938800	1.81223900
F	-3.61930000	-2.02253500	-1.54482800
F	-1.08113000	-1.35679200	-2.04246100
C	2.05426600	2.10822000	-0.93273900
C	2.85580300	0.96105200	-0.73833100
C	2.59917600	3.36188200	-1.21104600
C	4.24513700	1.12870100	-0.83011900
C	3.98531100	3.50164500	-1.29364700
C	4.80300400	2.38408100	-1.10360100
H	4.91229000	0.28174700	-0.69937100
H	4.42661400	4.46991500	-1.50823400
H	5.88242800	2.48879500	-1.17164600
C	-5.27233300	-0.78012400	0.33222700
F	-5.95584300	-0.54644200	-0.80528100
F	-5.86727600	-0.09290900	1.31997500
F	-5.37883500	-2.09099000	0.61333100
K	-2.03071800	4.26192400	0.18428900
H	1.93541500	4.20758400	-1.36629000

17Ru_Cl, E=-2624.22006402 a.u.

Ru	-1.26925200	0.40774800	-0.66000200
C	-1.68587700	2.53647100	-1.24688600
C	-2.51255100	1.67632700	-2.04267500
H	-3.59075300	1.79069600	-2.01914900
C	-1.92776900	0.66078000	-2.82837800

H	-2.57350600	-0.00221900	-3.39824700
C	-0.50023600	0.52873900	-2.98127600
C	0.29456800	1.33466300	-2.16374400
H	1.37362200	1.21372800	-2.17408500
C	-0.28886100	2.30002100	-1.27784300
H	0.36008500	2.87123100	-0.62887900
C	-2.30551700	3.67110100	-0.45386300
H	-3.29099400	3.32421100	-0.12361700
C	-2.50972200	4.87234100	-1.40083100
H	-1.54705500	5.25197100	-1.76001900
H	-3.01677800	5.68425100	-0.87149000
H	-3.11573800	4.60467100	-2.27235400
C	-1.50872700	4.07174700	0.79355400
H	-1.32224000	3.21200200	1.44102700
H	-2.07443900	4.81303300	1.36439100
H	-0.54852100	4.52967300	0.53327700
C	0.10547700	-0.41038100	-3.99127700
H	-0.58286200	-1.20849100	-4.28098600
H	1.02830400	-0.86322600	-3.61783600
H	0.35253100	0.14270400	-4.90470400
C	-0.31507700	0.18459700	2.16773600
O	0.41985400	-0.02452400	3.15966000
N	0.10502600	0.04013400	0.87694100
C	1.48269100	0.05928900	0.63083100
C	2.23934100	1.22943600	0.77832900
C	2.18165100	-1.06520900	0.17707300
C	3.59046700	1.29321700	0.43721600
C	3.52456600	-1.01953600	-0.16765700
C	4.25929800	0.16501200	-0.05080700
F	1.63780200	2.34218400	1.22430400
F	4.20896800	2.46401200	0.58518700
F	4.11822200	-2.14342300	-0.58837700
F	1.54017200	-2.26686600	0.12262200
C	-1.74479000	0.53718200	2.24903000
C	-2.42212000	0.67439200	1.02090100
C	-2.38532600	0.70424800	3.47929300
C	-3.78973600	0.97860500	1.07606100
C	-3.74277500	1.01957800	3.50932000
C	-4.44071600	1.15162800	2.30492200
H	-4.36618700	1.08886200	0.16074100
H	-4.25392200	1.16253600	4.45606100
H	-5.49993500	1.39520900	2.31908700
C	5.72232700	0.13726800	-0.44170400
F	6.39012300	-0.75119000	0.32230100

F	6.31467000	1.32912100	-0.30751600
F	5.85144400	-0.25263800	-1.72581200
K	1.09112100	-2.51743300	3.14071400
C	-3.45108800	-1.82336400	-0.84063200
C	-3.94976400	-3.24427000	-1.09344700
C	-1.83479600	-3.96870900	-1.77249200
C	-1.23450700	-2.57948100	-1.56682200
H	-3.91526300	-3.84238800	-0.17209000
H	-4.98870500	-3.19708100	-1.43054800
H	-3.60493600	-1.22471400	-1.74125400
H	-3.96846100	-1.34121000	-0.01215000
H	-1.70563500	-4.59257400	-0.87636600
H	-1.31898900	-4.45528700	-2.60518200
H	-0.18683800	-2.60966200	-1.27363600
H	-1.32503100	-2.03226700	-2.50445300
N	-1.97120200	-1.72412200	-0.57623300
O	-3.20360400	-3.86891500	-2.12896800
Cl	-1.74818100	-2.59007200	1.08819500
H	-1.80484400	0.59636600	4.39122800

TS18_{Ru-Cl}, E=-2624.21569122 a.u., Imaginary frequency = 148i

Ru	-1.26637800	0.39956300	-0.64502000
C	-1.67101100	2.56694400	-1.18276700
C	-2.50324900	1.73286300	-2.00060700
H	-3.58102300	1.84785600	-1.96862300
C	-1.92236200	0.75060300	-2.82665500
H	-2.57179200	0.10503100	-3.41219500
C	-0.49613200	0.62841700	-3.00110700
C	0.30289100	1.40309900	-2.16051600
H	1.38268900	1.29228300	-2.18805800
C	-0.27656300	2.33319200	-1.23712900
H	0.37734700	2.88154300	-0.57357600
C	-2.28475700	3.67690300	-0.35123400
H	-3.26815300	3.31997500	-0.02585200
C	-2.49426200	4.90702300	-1.25940900
H	-1.53371100	5.29796000	-1.61197900
H	-2.99835400	5.70161300	-0.70183100
H	-3.10552300	4.66681900	-2.13529100
C	-1.47938800	4.03738500	0.90284200
H	-1.29235700	3.15814900	1.52351200
H	-2.03963700	4.76289300	1.49866600
H	-0.51912800	4.49995100	0.65131300
C	0.09948800	-0.26230800	-4.05978500
H	-0.59543200	-1.03988300	-4.38678500

H	1. 02076000	-0. 73938800	-3. 71390800
H	0. 34690600	0. 33543800	-4. 94458300
C	-0. 32649300	0. 11873900	2. 16941100
O	0. 40608600	-0. 12278500	3. 15327200
N	0. 09997500	0. 02249400	0. 87438200
C	1. 48096300	0. 04446200	0. 63596200
C	2. 23223700	1. 21419700	0. 80847000
C	2. 18572200	-1. 07172400	0. 17197300
C	3. 58585800	1. 28819200	0. 47962500
C	3. 53166300	-1. 01546700	-0. 16039300
C	4. 26154100	0. 16954900	-0. 01986000
F	1. 62375600	2. 31785000	1. 26906000
F	4. 19858800	2. 45892100	0. 65043400
F	4. 13230700	-2. 12969600	-0. 59541100
F	1. 54956000	-2. 27251000	0. 09060700
C	-1. 75593800	0. 46864200	2. 25550700
C	-2. 42910400	0. 63185200	1. 02940000
C	-2. 40014300	0. 61317800	3. 48605000
C	-3. 79465300	0. 94205100	1. 08305700
C	-3. 75653400	0. 93417800	3. 51693100
C	-4. 44896600	1. 09456700	2. 31312900
H	-4. 36757300	1. 07162900	0. 16822400
H	-4. 27084500	1. 05978000	4. 46435700
H	-5. 50695400	1. 34301300	2. 32796900
C	5. 72686600	0. 15355700	-0. 40396800
F	6. 39310900	-0. 75000300	0. 34223200
F	6. 31539800	1. 34375400	-0. 24047500
F	5. 86180900	-0. 20639900	-1. 69638200
K	0. 92946700	-2. 66601700	3. 07429800
C	-3. 42396900	-1. 76606600	-0. 91193300
C	-3. 89675400	-3. 19001000	-1. 20210400
C	-1. 77507800	-3. 86495900	-1. 89577200
C	-1. 19165300	-2. 47182800	-1. 66169500
H	-3. 84847100	-3. 80961300	-0. 29695700
H	-4. 93705400	-3. 14998100	-1. 53620300
H	-3. 62492400	-1. 14495400	-1. 78912500
H	-3. 93604600	-1. 32896600	-0. 05597000
H	-1. 64081400	-4. 50266500	-1. 01158700
H	-1. 24990700	-4. 32617400	-2. 73712900
H	-0. 14944300	-2. 50022400	-1. 35031900
H	-1. 26751600	-1. 92508100	-2. 60168800
N	-1. 94635800	-1. 62610400	-0. 68117600
O	-3. 14302100	-3. 77339800	-2. 25526300
C1	-1. 72179300	-2. 65610100	1. 05631800

H	-1.82369100	0.48436400	4.39777300
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17'_{Ru}_Cl, E=-2624.22421954 a.u.

Ru	-1.40670900	0.23685900	0.74085100
C	-1.59283200	-1.02312700	2.57634700
C	-2.61456700	-0.01394100	2.59598000
H	-3.65772900	-0.30617900	2.64717500
C	-2.26870700	1.35233300	2.50325700
H	-3.05595500	2.09888200	2.46454100
C	-0.89692500	1.79802200	2.55228300
C	0.08864500	0.81433400	2.47274600
H	1.13270000	1.10453300	2.40509100
C	-0.25425100	-0.58097700	2.43039600
H	0.53905100	-1.30930600	2.31541600
C	-1.96474000	-2.48570900	2.72885000
H	-2.93811600	-2.61667300	2.24312400
C	-2.12791300	-2.79970600	4.23007900
H	-1.17585700	-2.67901600	4.75837700
H	-2.46223000	-3.83261000	4.36551500
H	-2.86282000	-2.14084000	4.70309900
C	-0.97965700	-3.45195800	2.05951500
H	-0.83027600	-3.19539400	1.00775400
H	-1.37363900	-4.47079900	2.11226200
H	-0.00769200	-3.45420700	2.56525900
C	-0.54366600	3.25431800	2.68434900
H	-1.37946100	3.89832500	2.40899200
H	0.31364000	3.51532300	2.05871500
H	-0.28240500	3.47008200	3.72692000
C	-0.18462700	-1.41960900	-1.45851500
O	0.63941300	-1.94786500	-2.24086400
C	1.43302000	-0.03985400	-0.43245400
C	2.41263700	-0.98699400	-0.08777400
C	1.88781400	1.28425000	-0.49911600
C	3.74656400	-0.65495500	0.07428600
C	3.21920700	1.63921700	-0.28355800
C	4.18867800	0.66795700	-0.01161300
F	2.06308900	-2.29052700	0.09412400
F	4.61990700	-1.65063700	0.31523600
F	3.53193500	2.93257200	-0.37406800
F	1.01137900	2.26243700	-0.77763600
C	-1.58640700	-1.86527200	-1.33131200
C	-2.35971400	-1.23915000	-0.32882300
C	-2.09641500	-2.88770300	-2.14005500
C	-3.67628000	-1.70118300	-0.16641700

C	-3.40540900	-3.32444900	-1.95916500
C	-4.19037200	-2.72874700	-0.96573000
H	-4.32270300	-1.25612800	0.58586400
H	-3.81510400	-4.11448100	-2.58044500
H	-5.21352600	-3.06287300	-0.81434900
C	5.66371200	0.94578400	0.16566200
F	6.37393600	0.28134600	-0.77453500
F	6.08570200	0.51018100	1.36884600
F	5.96074400	2.24605000	0.06485800
C	-1.82130200	1.45098900	-2.21111600
C	-2.55317500	2.30562500	-3.24156800
C	-4.44552200	2.48431100	-1.88139100
C	-3.79887800	1.63364400	-0.78995000
H	-2.29965600	3.36938200	-3.12253400
H	-2.24423200	1.99143200	-4.24232400
H	-2.03156300	0.39691500	-2.40390500
H	-0.74483200	1.60676900	-2.22745200
H	-4.28168300	3.55626700	-1.69761700
H	-5.52307800	2.29786200	-1.88093900
H	-4.13553800	1.91863700	0.20800400
H	-4.04679700	0.58530200	-0.96195800
N	-2.29620600	1.67030800	-0.80286300
O	-3.95755800	2.11003800	-3.16001700
Cl	-1.82862400	3.38431900	-0.35049700
N	0.09904100	-0.37380000	-0.62863800
K	2.66140000	-3.45083900	-2.42722400
H	-1.45370800	-3.32092500	-2.90137200

TS18'_{Ru-Cl}, E=-2624.15723399 a.u., Imaginary frequency = 238i

Ru	1.56420900	-0.13642800	0.55253200
C	1.93510800	1.65836500	1.82255000
C	3.08133600	0.80556500	1.94693700
H	4.03654600	1.13817400	1.55591700
C	2.95478100	-0.46982400	2.51434000
H	3.82174300	-1.12344900	2.52812000
C	1.80481800	-0.82612400	3.32301800
C	0.70276500	-0.01127000	3.21557600
H	-0.22017700	-0.26323500	3.72861700
C	0.71346700	1.10719400	2.30707600
H	-0.19829800	1.67608600	2.18316500
C	2.11692600	3.09328200	1.35753800
H	2.84232800	3.06920800	0.53503700
C	2.72753400	3.91182100	2.51397800
H	2.03718600	3.95936700	3.36323200

H	2.93545100	4.93527800	2.18709800
H	3.66618700	3.47361900	2.86665500
C	0.83957500	3.76240500	0.83807400
H	0.38702500	3.18792100	0.02932900
H	1.08291400	4.76076600	0.46151200
H	0.09863600	3.88179300	1.63601900
C	1.80666800	-2.10576300	4.10048700
H	1.69505100	-2.95033100	3.40743000
H	0.97621400	-2.14562600	4.80895300
H	2.74331500	-2.24415400	4.64996000
C	0.15415700	1.30823600	-1.66873200
O	-0.73654600	1.93681100	-2.29109800
C	-1.40781300	0.03881000	-0.44520600
C	-2.26217900	0.90102500	0.25343200
C	-1.98553800	-1.15487100	-0.89049200
C	-3.58292700	0.58671900	0.52541500
C	-3.30776800	-1.49997900	-0.59613300
C	-4.13479600	-0.63270200	0.12131600
F	-1.81811700	2.13590300	0.62417900
F	-4.34250000	1.50561600	1.14721100
F	-3.75505200	-2.66538200	-1.06061200
F	-1.28901200	-1.98426600	-1.67475200
C	1.60160100	1.50093300	-1.88824100
C	2.45547700	0.85212700	-0.97332300
C	2.10326400	2.23691600	-2.96132800
C	3.83736700	0.89935300	-1.21128800
C	3.48302900	2.30469500	-3.16345800
C	4.34490300	1.62790300	-2.29257300
H	4.52608500	0.37106200	-0.55821500
H	3.88635800	2.86370200	-4.00191600
H	5.41781300	1.66159400	-2.46061300
C	-5.59428900	-0.89318000	0.42523900
F	-6.36420800	0.00742100	-0.22951400
F	-5.83512300	-0.74739900	1.74131900
F	-5.98938800	-2.11678400	0.06058400
C	1.79130900	-2.03490300	-2.02791700
C	1.55941600	-3.53415700	-2.28167400
C	3.11701100	-4.11149600	-0.62690700
C	3.39397800	-2.62301500	-0.31987100
H	0.70337300	-3.87372200	-1.68479300
H	1.34609000	-3.69949000	-3.34045000
H	2.57642800	-1.69621400	-2.72192400
H	0.89361400	-1.44875700	-2.20478300
H	2.34199300	-4.47756600	0.05925500

H	4.03159700	-4.69199800	-0.48125900
H	3.63868700	-2.48014000	0.73148100
H	4.25486100	-2.31242600	-0.93444700
N	2.29605300	-1.74936800	-0.69334600
O	2.72872500	-4.27567800	-1.97501100
Cl	0.49666800	-2.47229400	0.74028700
N	-0.07174800	0.36058800	-0.72718900
K	-2.66614100	3.51382100	-1.81660100
H	1.40505500	2.72578900	-3.63438400

9Ru, E=-2135.63297199 a.u.

Ru	-1.33414200	0.38617100	0.54268300
C	-1.91181800	-1.70151200	1.71790400
C	-2.53106200	-0.54166900	2.29365600
H	-3.61420400	-0.49726500	2.33581500
C	-1.77023900	0.48617300	2.90250900
H	-2.28597300	1.30061500	3.40248700
C	-0.35328700	0.47176000	2.85892400
C	0.24193700	-0.57673700	2.11660300
H	1.31805700	-0.57972500	1.97719500
C	-0.51496300	-1.67404000	1.61703900
H	0.00551900	-2.45934200	1.08320500
C	-2.76632300	-2.85923500	1.24516300
H	-3.65359500	-2.41765300	0.77584200
C	-3.22605400	-3.66904900	2.47855700
H	-2.37021900	-4.12508100	2.98693100
H	-3.89757400	-4.47139200	2.16154600
H	-3.76197600	-3.04627500	3.20196400
C	-2.07494000	-3.75694100	0.21183700
H	-1.70428200	-3.18500500	-0.64231600
H	-2.78889300	-4.49448900	-0.16265000
H	-1.23881400	-4.31161800	0.65101800
C	0.48972300	1.51833000	3.53207400
H	-0.09780000	2.38904900	3.83137300
H	1.30651100	1.84634100	2.88284200
H	0.93934500	1.09778200	4.43878700
C	-0.76419700	-0.80809800	-2.12069900
O	-0.13142400	-1.26917500	-3.05495700
N	-0.16739300	-0.17117600	-1.01705500
C	1.21960800	-0.26387700	-0.85949900
C	1.88342800	-1.49932700	-0.85999500
C	2.00086200	0.86587800	-0.58486300
C	3.25492600	-1.60212800	-0.63350800
C	3.36131600	0.76994300	-0.32937200

C	4.02158600	-0.46306900	-0.36562600
F	1.17012700	-2.62843100	-0.98991400
F	3.78776600	-2.82262600	-0.63511500
F	4.03607400	1.88634700	-0.04169900
F	1.41250500	2.07875000	-0.51397200
C	-2.23606100	-0.78747400	-1.98344400
C	-2.74669800	-0.21836800	-0.80964700
C	-3.08449300	-1.28370900	-2.97688400
C	-4.12962500	-0.11986800	-0.63812900
C	-4.46383700	-1.19894300	-2.79714600
C	-4.98186500	-0.61060800	-1.63639800
H	-4.55538700	0.34340500	0.24795000
H	-5.13782800	-1.57939800	-3.55776300
H	-6.05730300	-0.52785100	-1.50702800
C	5.50715300	-0.48697300	-0.06178700
F	6.16490200	0.36013800	-0.87120500
F	6.04128300	-1.70482800	-0.20606000
F	5.71643800	-0.08601300	1.21100500
C	-1.89444400	2.61480300	-1.33649000
C	-0.97773400	3.78576800	-1.75957200
C	-0.64705800	4.42571600	0.45012300
C	-1.57948600	3.30146700	0.95661100
H	0.05210900	3.42357000	-1.86506000
H	-1.32169300	4.16896100	-2.72280000
H	-2.93906900	2.95561700	-1.35350700
H	-1.78584000	1.79004900	-2.03483400
H	0.39205600	4.06680000	0.44614400
H	-0.72636800	5.28359700	1.12288800
H	-1.26653400	2.97510000	1.94686000
H	-2.59978400	3.70449400	1.02027100
N	-1.59334300	2.16806000	0.02570400
O	-1.05096000	4.84951300	-0.83043700
H	-2.64396400	-1.72204500	-3.86759800

17Ru_O, E=-2584.07149793 a.u.

Ru	-1.98132100	-0.71068200	0.17822800
C	-3.81928400	-1.13155700	-1.09555900
C	-4.15652200	-1.18493700	0.29842500
H	-4.88552900	-0.48640600	0.69362100
C	-3.52156700	-2.09858200	1.16233100
H	-3.78721000	-2.10014800	2.21588300
C	-2.68550400	-3.15881300	0.64369700
C	-2.31403500	-3.07308100	-0.68770700
H	-1.62669600	-3.79637800	-1.10856000

C	-2.77699500	-1.99032000	-1.51053600
H	-2.39835900	-1.91790200	-2.52293100
C	-4.58187900	-0.20888500	-2.03086200
H	-4.65192500	0.76706200	-1.53711000
C	-6.01403400	-0.75912300	-2.20205600
H	-5.99888500	-1.74161600	-2.68603700
H	-6.60269500	-0.08272300	-2.82875900
H	-6.52965800	-0.86239900	-1.24213700
C	-3.91384800	-0.00909800	-3.39640000
H	-2.88603900	0.35064600	-3.30907800
H	-4.47543900	0.73197500	-3.97165900
H	-3.90950400	-0.93706800	-3.97898900
C	-2.25930300	-4.31327200	1.51056800
H	-2.26221800	-4.05831300	2.57346300
H	-1.26463700	-4.67595800	1.23810100
H	-2.96299700	-5.14416800	1.38249300
C	-0.81469900	1.19622700	-1.75143800
O	-0.24998700	1.69178800	-2.73988300
N	-0.37975200	0.10115500	-1.03001700
C	0.92217400	-0.34457900	-1.20635800
C	1.29437300	-1.69018800	-1.00162700
C	2.03271500	0.49335800	-1.46841400
C	2.59693600	-2.15809100	-1.10130800
C	3.33415000	0.03094400	-1.60436800
C	3.65821100	-1.31670400	-1.44397100
F	0.36176600	-2.60159200	-0.64638800
F	2.80713600	-3.45641100	-0.85369500
F	4.29094000	0.94892100	-1.78635500
F	1.91417400	1.84437600	-1.41912600
C	-2.01313000	1.83156300	-1.13996500
C	-2.53211300	1.23061900	0.01993800
C	-2.54352100	3.02277000	-1.65372300
C	-3.51751400	1.93463400	0.72835200
C	-3.54448500	3.69572200	-0.95110000
C	-4.00468700	3.16052400	0.25870100
H	-3.93759400	1.52163600	1.64222800
H	-3.97482600	4.61187600	-1.34411000
H	-4.77441500	3.68256800	0.82105300
C	5.08039800	-1.81476100	-1.43939200
F	5.89291900	-1.03605900	-2.16881900
F	5.17148700	-3.06724700	-1.91190600
F	5.56757800	-1.83009300	-0.16711300
K	0.35352900	3.95767100	-1.02163300
C	-1.47835300	0.53443800	3.04200600

C	-0.72700200	0.58755500	4.36970700
C	0.27772100	-1.48957200	3.98801100
C	-0.44339000	-1.63622400	2.64836900
H	0.22380600	1.13211700	4.26119200
H	-1.33818200	1.12291300	5.10097500
H	-2.44453600	0.04311000	3.17924600
H	-1.63956600	1.51944500	2.61399000
H	1.27535500	-1.04949300	3.85295000
H	0.39519400	-2.47981500	4.43631200
H	0.13093600	-2.21232800	1.92129800
H	-1.40061000	-2.12153900	2.81875000
N	-0.78302700	-0.31412300	2.01202900
O	-0.50240400	-0.71503600	4.88648400
O	0.60000600	0.19886500	1.82756900
C	0.87451500	1.49326400	1.55003400
O	0.04857600	2.36584000	1.33622100
C	2.34520300	1.71336400	1.57671600
C	3.26672900	0.66313500	1.44639300
C	2.80484400	3.03321300	1.71426600
C	4.63171700	0.93869100	1.40334500
H	2.91376900	-0.35499900	1.33409400
C	4.17108800	3.30081000	1.69785700
H	2.08497400	3.83205700	1.86785200
C	5.08396400	2.25452400	1.52878100
H	5.33443900	0.12779600	1.24859700
H	4.52639700	4.31919600	1.82074000
H	6.14836300	2.46519300	1.49765100
H	-2.18196000	3.38460000	-2.61500500

TS18_{Ru_O}, E=-2584.06019726 a.u., Imaginary frequency = 230i

Ru	-1.94878800	-0.50610000	0.41384400
C	-3.91126800	-1.25588500	-0.59046400
C	-4.18867100	-0.82741000	0.74713600
H	-4.84900800	0.01740800	0.90449700
C	-3.59664400	-1.46527200	1.84921900
H	-3.80387100	-1.09304900	2.84870100
C	-2.87061100	-2.70043700	1.69721600
C	-2.54414200	-3.08284300	0.40650000
H	-1.94648600	-3.96886200	0.23314500
C	-2.96620800	-2.29521600	-0.71421600
H	-2.62252900	-2.58890800	-1.69803100
C	-4.63223800	-0.61307500	-1.76252000
H	-4.64417500	0.46708900	-1.57528100
C	-6.09311000	-1.11022300	-1.78097100

H	-6.13482300	-2.19028200	-1.95822700
H	-6.64818000	-0.61407000	-2.58243800
H	-6.60610100	-0.90125200	-0.83673900
C	-3.95351700	-0.85649200	-3.11547700
H	-2.90342600	-0.55411100	-3.11048700
H	-4.46387800	-0.27841900	-3.89029400
H	-4.00884800	-1.91083100	-3.40817200
C	-2.52266400	-3.54815800	2.89134200
H	-2.47819400	-2.96545900	3.81543800
H	-1.57141900	-4.06912400	2.75504400
H	-3.29947900	-4.30899200	3.03329700
C	-0.87335900	0.82840300	-1.99489000
O	-0.26157200	1.11523900	-3.03705900
N	-0.54170700	-0.18687600	-1.12716300
C	0.71822200	-0.77609500	-1.24031300
C	0.91533000	-2.15180800	-1.04270200
C	1.90898000	-0.05619900	-1.46648700
C	2.17072700	-2.74913600	-0.95935300
C	3.15997200	-0.64892300	-1.44947000
C	3.33282700	-2.00453700	-1.16194500
F	-0.15357000	-2.96151500	-0.89963500
F	2.20916100	-4.05877600	-0.69563800
F	4.23084500	0.13243100	-1.63519100
F	1.89901500	1.28986600	-1.59670200
C	-2.00679800	1.64619200	-1.49643900
C	-2.48035100	1.34678600	-0.20891100
C	-2.50763900	2.72480100	-2.23695000
C	-3.40109500	2.23577300	0.36544100
C	-3.44963100	3.57893300	-1.66388200
C	-3.87215600	3.34315300	-0.34974900
H	-3.77527000	2.06894800	1.37235400
H	-3.85990200	4.40924600	-2.23042900
H	-4.59325600	4.01136900	0.11333500
C	4.73587900	-2.52451500	-0.97109300
F	5.50684800	-2.25792600	-2.03898200
F	4.77244900	-3.84416500	-0.74693700
F	5.30508500	-1.91064600	0.10025900
K	0.56597100	3.60831100	-1.91202500
C	-1.24811300	1.33889700	2.72728000
C	-0.35547400	1.67126300	3.92257800
C	0.59711200	-0.45102000	3.95647900
C	-0.25543200	-0.91391300	2.77117800
H	0.58657700	2.13173900	3.59498700
H	-0.88035800	2.39096100	4.55645500

H	-2.22902600	1.02127300	3.09843900
H	-1.37308400	2.19182400	2.06587300
H	1.56504200	-0.06453700	3.61736400
H	0.76982200	-1.30807800	4.61354600
H	0.28184700	-1.61574600	2.13125400
H	-1.14187200	-1.40027000	3.17613800
N	-0.78028800	0.18818000	1.90314900
O	-0.10453000	0.52121900	4.71334700
O	0.91395100	0.69071100	1.43378800
C	1.21397400	1.90913500	1.05425000
O	0.41016800	2.77779200	0.69642700
C	2.69651100	2.16100200	1.08638900
C	3.62191800	1.11368100	1.19884400
C	3.15382900	3.48199200	0.96702100
C	4.98846800	1.37859100	1.14454500
H	3.27031500	0.09329000	1.29191900
C	4.52190400	3.74689700	0.94098700
H	2.42933600	4.28986500	0.92533600
C	5.43992200	2.69430000	1.01718600
H	5.69324600	0.55470100	1.18438300
H	4.87416100	4.77123800	0.86481900
H	6.50501900	2.90126900	0.97999400
H	-2.16636000	2.85818500	-3.26190600

17'_{Ru}O, E=-2584.05173522 a.u.

Ru	2.32831400	-0.41776900	-0.59961700
C	3.01666300	-2.59715200	-0.36595300
C	4.09201700	-1.75082900	-0.78015600
H	4.99999100	-1.71016500	-0.18952400
C	3.98726500	-0.96888400	-1.96621000
H	4.82530400	-0.33417300	-2.24428400
C	2.85037700	-1.04043900	-2.82963900
C	1.74963600	-1.76191800	-2.32538200
H	0.79770600	-1.71904700	-2.84426600
C	1.81844100	-2.52460400	-1.11299400
H	0.92244500	-3.01073400	-0.75632300
C	3.18585200	-3.48929400	0.84781300
H	3.69614600	-2.88944800	1.60978500
C	4.11144800	-4.66279500	0.45818900
H	3.65008900	-5.28185200	-0.31881100
H	4.29070600	-5.29678500	1.33130200
H	5.08132300	-4.31691500	0.08629600
C	1.86690500	-3.99581300	1.44105000
H	1.16800000	-3.17995400	1.63803900

H	2. 06977900	-4. 51889600	2. 37976500
H	1. 37935000	-4. 71144300	0. 76876500
C	2. 80582700	-0. 34403000	-4. 16350600
H	3. 49222400	0. 50594100	-4. 20284600
H	1. 79684200	0. 00971900	-4. 39522100
H	3. 10178700	-1. 03652000	-4. 95966500
C	-0. 22372300	-0. 40610800	1. 77849000
O	-0. 87079800	0. 67202600	1. 96201900
N	-0. 62992000	-1. 48933500	1. 12055200
C	-1. 90233200	-1. 47799900	0. 61697200
C	-3. 05996200	-1. 12837700	1. 34496300
C	-2. 15800400	-1. 82950100	-0. 72510900
C	-4. 29009900	-0. 93756600	0. 74579600
C	-3. 40483400	-1. 68944500	-1. 32652300
C	-4. 51102200	-1. 21744800	-0. 60606500
F	-2. 97524200	-0. 87673700	2. 67933600
F	-5. 27824300	-0. 40850800	1. 50348900
F	-3. 49766500	-1. 97492800	-2. 63049900
F	-1. 13187700	-2. 21710200	-1. 51275300
C	1. 18082200	-0. 43426500	2. 31526900
C	2. 32693600	-0. 37159400	1. 49515700
C	1. 29900500	-0. 45288400	3. 71462100
C	3. 57281200	-0. 34660600	2. 15888000
C	2. 54210600	-0. 44246000	4. 33947600
C	3. 69061300	-0. 38393000	3. 54996800
H	4. 48925300	-0. 29095900	1. 57708500
H	2. 61444000	-0. 47822900	5. 42228800
H	4. 67553100	-0. 37093400	4. 00930400
C	-5. 85168600	-0. 90164000	-1. 20861400
F	-6. 05140600	0. 45258900	-1. 22536300
F	-6. 85612800	-1. 42439600	-0. 48309000
F	-5. 97560000	-1. 33422700	-2. 46819700
C	3. 67249100	2. 33799800	0. 45387300
C	3. 83459200	3. 85225500	0. 33475800
C	3. 12415900	3. 85458100	-1. 88935400
C	2. 95164100	2. 33683200	-1. 88460200
H	2. 92284500	4. 36277200	0. 67878900
H	4. 66473500	4. 17154800	0. 96967800
H	4. 61059800	1. 83197200	0. 21148600
H	3. 36124700	2. 03182900	1. 45047500
H	2. 17495000	4. 35048100	-1. 63638300
H	3. 42433900	4. 17873500	-2. 88932600
H	2. 14577600	2. 00539400	-2. 54222500
H	3. 88072000	1. 86059500	-2. 20226200

N	2.68233300	1.78003000	-0.51700000
O	4.15341900	4.23756500	-0.99481800
O	1.40441600	2.43457900	-0.10269100
C	0.31861600	1.70571700	-0.41427100
O	0.40345000	0.51925000	-0.74096700
C	-0.94854700	2.45605000	-0.39331200
C	-1.00870100	3.79158600	0.03464000
C	-2.11586800	1.79093300	-0.80318100
C	-2.23927400	4.45022300	0.06601100
H	-0.10511000	4.30377200	0.34570000
C	-3.34026700	2.45599500	-0.78397900
H	-2.05100300	0.75835900	-1.12008400
C	-3.40312500	3.78613600	-0.34362400
H	-2.28813400	5.48601000	0.38787000
H	-4.23817000	1.93848900	-1.10530400
H	-4.35488100	4.30997400	-0.33957100
K	-2.97243600	1.84467000	2.75422000
H	0.39162400	-0.49522400	4.31220200

TS18'_{Ru_O}, E=-2584.03648824 a.u., Imaginary frequency = 282i

Ru	2.34350600	-0.30418900	-0.59378800
C	2.94509600	-2.59821600	-0.46372200
C	4.04189600	-1.78574000	-0.88509000
H	4.97131800	-1.80963100	-0.32777700
C	3.94828000	-0.99488500	-2.06488000
H	4.81587400	-0.41299100	-2.36643400
C	2.78274400	-0.97401700	-2.88041900
C	1.65607700	-1.63260900	-2.33823800
H	0.68971100	-1.52778800	-2.81993700
C	1.73242100	-2.44968400	-1.16794300
H	0.82578500	-2.90485300	-0.79659400
C	3.11511200	-3.54558200	0.70628000
H	3.65104800	-2.98922600	1.48352000
C	4.00907400	-4.72126200	0.25140500
H	3.52151900	-5.29731100	-0.54234300
H	4.18695300	-5.39433700	1.09485900
H	4.98096400	-4.38225300	-0.12126800
C	1.79574700	-4.05064600	1.29989000
H	1.11839100	-3.23104500	1.54910700
H	2.00444300	-4.62143900	2.20887800
H	1.28032100	-4.72285500	0.60406100
C	2.73086500	-0.26126000	-4.20472700
H	3.49592200	0.51619800	-4.27730000
H	1.75052500	0.19484900	-4.37197400
H	2.90609800	-0.96923300	-5.02264000

C	-0.23707200	-0.43558800	1.75201100
O	-0.86069400	0.64223700	1.98558600
N	-0.66654700	-1.49172800	1.06225000
C	-1.94763900	-1.45493500	0.58443100
C	-3.09059300	-1.11356300	1.34024100
C	-2.23236500	-1.77475400	-0.75979300
C	-4.33195300	-0.90782500	0.76796100
C	-3.48857100	-1.61834000	-1.33461200
C	-4.58178700	-1.16454000	-0.58341500
F	-2.98097600	-0.88505600	2.67661200
F	-5.30002300	-0.38587000	1.55613200
F	-3.60471900	-1.86755300	-2.64443800
F	-1.22048400	-2.14251600	-1.57794500
C	1.16828500	-0.52735400	2.28619000
C	2.32672800	-0.41479300	1.49144700
C	1.27450800	-0.69553600	3.67708100
C	3.56644100	-0.50644100	2.15806700
C	2.51062700	-0.79050600	4.30830700
C	3.66937500	-0.69468500	3.53765600
H	4.48892000	-0.42989800	1.58768300
H	2.56975800	-0.93826800	5.38232700
H	4.64938900	-0.76774900	4.00154000
C	-5.92602900	-0.82630400	-1.16553700
F	-6.07892200	0.53154600	-1.24042200
F	-6.92914100	-1.28053300	-0.39347500
F	-6.09764200	-1.31125600	-2.40069600
C	3.82473400	2.18279600	0.59572900
C	4.00042600	3.70096900	0.53496100
C	3.38866000	3.79287700	-1.70554000
C	3.21289000	2.27436100	-1.77620800
H	3.07586900	4.19976900	0.85412600
H	4.80248300	3.98593700	1.22039000
H	4.79054100	1.69091300	0.42696500
H	3.43956000	1.85580300	1.55836400
H	2.43125900	4.27485100	-1.46580100
H	3.72598600	4.15301400	-2.68121100
H	2.41444300	1.98725500	-2.46158000
H	4.15119900	1.82945800	-2.12318200
N	2.94984600	1.62180000	-0.46123300
O	4.38465800	4.13170400	-0.76092600
O	1.42936000	2.52838300	0.00947100
C	0.40415800	1.82244200	-0.33418000
O	0.48244100	0.61148900	-0.67084400
C	-0.91068900	2.51318100	-0.37445000

C	-1.04235900	3.83624300	0.07210800
C	-2.03179200	1.81139500	-0.84325100
C	-2.29781200	4.44845400	0.06174800
H	-0.16927600	4.37231700	0.42795400
C	-3.28291700	2.42761100	-0.86154900
H	-1.91231200	0.78844000	-1.17441200
C	-3.41741700	3.74625100	-0.40397400
H	-2.40003700	5.47655000	0.39616800
H	-4.14855300	1.88229500	-1.22279500
H	-4.38928700	4.23117400	-0.42976900
K	-2.97191800	1.85591000	2.69010500
H	0.36039800	-0.77286700	4.26052000

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C	-0.60794600	-0.67330500	0.14643700
C	0.49064400	0.20801300	0.18221400
C	-0.37141900	-2.03037100	0.38068200
C	1.77737700	-0.25835500	0.46509400
C	0.91500400	-2.50831400	0.66053300
C	2.01034900	-1.61207700	0.70737400
H	2.58926200	0.46510300	0.50377600
H	-1.21597900	-2.71306600	0.35873800
C	3.40264800	-2.11012100	1.01827300
H	4.12289400	-1.28660900	1.02122700
H	3.45379700	-2.60046300	1.99972500
H	3.74690800	-2.85043300	0.28367300
C	1.12723600	-3.98079100	0.92712100
H	1.83309900	-4.42626100	0.21381400
H	1.54440600	-4.15547100	1.92786800
H	0.18560500	-4.53230400	0.85604700
C	0.19573500	1.65067400	-0.01716800
O	1.01007200	2.57553200	0.10371300
O	-1.07446600	1.89137200	-0.28498400
Li	-1.53097700	3.60142400	0.26119400
Pd	-2.34453800	0.24666700	-0.04124700
C	-4.52337700	-1.81800200	0.23938300
O	-3.24530000	-1.58690100	0.18185900
C	-4.80817800	-3.31403900	0.44477500
H	-5.88344500	-3.50280200	0.42551700
H	-4.30975500	-3.90295700	-0.33165600
H	-4.39686500	-3.63343300	1.40902200
O	-5.44615200	-1.00969800	0.17022800
C	-1.66745600	0.84973600	3.31801100
C	-2.98862800	1.23234300	2.98808500

C	-4.07215600	0.32486800	3.04481300
C	-3.77048400	-1.01269300	3.30829600
C	-2.46442900	-1.45611300	3.50583800
C	-1.44314800	-0.50800300	3.55912300
H	-4.58503900	-1.73190900	3.30069400
H	-0.42529500	-0.83357900	3.75667800
C	-5.51238100	0.69122800	2.77748700
H	-5.69106400	0.66803700	1.69933200
H	-6.16560300	-0.05391000	3.24009600
H	-5.77147100	1.67693100	3.16592000
C	-0.48157000	1.78191800	3.43564000
H	-0.08963300	2.07571000	2.46092600
H	-0.72999700	2.70166000	3.96876000
H	0.32141600	1.27256400	3.97560900
C	-2.15603300	-2.92751700	3.59531700
H	-2.01248100	-3.31980400	2.58175100
H	-1.23721200	-3.11981200	4.15825700
H	-2.97425900	-3.48880900	4.05843700
S	-3.35516900	2.90308200	2.44969800
O	-2.08918800	3.57470300	2.04923200
O	-4.18553500	3.60862300	3.42607900
O	-4.33113700	2.73184100	1.15590300
N	-3.93925100	1.95206900	-0.04500100
C	-3.66450900	2.78537100	-1.07400700
O	-3.68063300	2.45496600	-2.25053700
O	-3.24027000	4.09880200	-0.71604200
C	-3.11316800	5.00936000	-1.82950600
H	-3.27409800	6.00438600	-1.40209700
H	-3.90462900	4.79301100	-2.55069300
C	-1.74645200	4.89149900	-2.49345100
H	-1.60936600	3.87258800	-2.86081100
H	-1.66885400	5.59056200	-3.33400000
H	-0.93449400	5.12801400	-1.79328200

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C	-0.46888700	-0.37232100	0.27500000
C	0.61051600	0.52497000	0.20191800
C	-0.19563900	-1.72502600	0.48771100
C	1.92652300	0.07592100	0.33817400
C	1.11898200	-2.18679000	0.63348000
C	2.19985000	-1.27517100	0.55544300
H	2.72936100	0.80827600	0.28319500
H	-1.02792600	-2.42154000	0.55122300
C	3.62416400	-1.75505800	0.71132700

H	4.33045500	-0.92421700	0.62468400
H	3.79097000	-2.23361100	1.68562200
H	3.89079300	-2.50012600	-0.05013900
C	1.37899000	-3.65482300	0.88097300
H	2.00248000	-4.09643700	0.09238300
H	1.91177700	-3.81902400	1.82699200
H	0.44225400	-4.21777600	0.92225900
C	0.27922300	1.96936900	0.03641100
O	1.09978100	2.87782500	-0.05706100
O	-1.03101200	2.20224600	0.02087500
Li	-1.98299600	3.60722000	0.76529700
Pd	-2.23820200	0.52975300	0.16905700
C	-4.41739700	-1.41784200	0.00159800
O	-3.15875600	-1.28840600	0.29616800
C	-4.92613900	-2.84067300	0.25407700
H	-5.95396700	-2.94599700	-0.09723900
H	-4.27856900	-3.56258600	-0.25289600
H	-4.88060300	-3.05461100	1.32659200
O	-5.18055000	-0.54966300	-0.42458900
C	-1.71240700	0.61198400	3.54210800
C	-2.96981100	1.19489200	3.27030600
C	-4.15318700	0.42206800	3.21502000
C	-4.03271900	-0.95913800	3.37258900
C	-2.79835000	-1.58214200	3.55140300
C	-1.66539300	-0.78106700	3.66861500
H	-4.93215500	-1.56598400	3.30210100
H	-0.69696200	-1.25019100	3.82052500
C	-5.52034000	0.99098600	2.91484800
H	-5.59923000	1.18341400	1.84081900
H	-6.29174400	0.26819400	3.19558800
H	-5.70362000	1.92701900	3.44501000
C	-0.40805700	1.36503900	3.67012700
H	-0.09560700	1.77411500	2.70848000
H	-0.48256100	2.20843700	4.35887200
H	0.37249500	0.68455500	4.02128900
C	-2.68353200	-3.08441000	3.53177000
H	-2.59409100	-3.42135300	2.49170000
H	-1.79884700	-3.43410000	4.07330400
H	-3.56727200	-3.56779500	3.96204700
S	-3.14052500	2.95986400	2.93915600
O	-1.78492300	3.57104600	2.73530100
O	-3.96204500	3.56902100	3.99513200
O	-3.83531600	3.07901800	1.54973500
N	-4.00934600	1.69270800	0.13244700

C	-3.93864900	2.48373600	-0.98671900
O	-4.39828000	2.09588100	-2.05044200
O	-3.29519000	3.70356100	-0.86060500
C	-3.00073600	4.36492300	-2.11751700
H	-2.83548100	5.40904100	-1.83548500
H	-3.88282500	4.30431200	-2.75969900
C	-1.77840400	3.75622700	-2.79096200
H	-1.98229200	2.71555100	-3.05281300
H	-1.54869000	4.31199900	-3.70756300
H	-0.90882000	3.77764500	-2.12903300

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C	-1.47029100	-0.67208000	-0.48899500
C	-0.24529100	-0.03212300	-0.32027300
C	-1.78552900	-1.82278000	0.22156000
C	0.69544400	-0.57006300	0.55804600
C	-0.84416800	-2.36294600	1.10916800
C	0.41247500	-1.73178800	1.27714700
H	1.64382400	-0.05158000	0.67266200
H	-2.74370100	-2.31191500	0.07455000
C	1.43458800	-2.30649300	2.22728800
H	2.34743300	-1.70493800	2.23084700
H	1.04941300	-2.33180100	3.25198900
H	1.70809300	-3.33424700	1.95634300
C	-1.16945400	-3.62500900	1.87014900
H	-0.47085500	-4.43451800	1.62274200
H	-1.10339000	-3.46130400	2.95071700
H	-2.18132200	-3.97251900	1.64424200
C	-0.03287700	1.22835300	-1.08729800
O	1.01743400	1.83318100	-1.16903300
O	-1.17770000	1.66996200	-1.66116900
Li	-2.04745900	2.60812700	-0.15057900
Pd	-2.52206500	0.14834400	-1.98530400
C	-2.83187700	-2.27922800	-2.92238400
O	-3.69380200	-1.56498000	-2.28279700
C	-3.26880500	-3.67015400	-3.33173600
H	-2.57255700	-4.08656800	-4.06110400
H	-3.28217700	-4.30964800	-2.44240400
H	-4.28241800	-3.64263300	-3.73904200
O	-1.67836800	-1.85846700	-3.16453700
C	-0.36788200	0.94359300	3.87435300
C	-1.59725800	1.09360000	3.18877300
C	-2.57893400	0.08365900	3.23420400
C	-2.31534100	-1.04884200	4.02233100

C	-1.13453800	-1.20793200	4.74139900
C	-0.16577000	-0.20607400	4.63959800
H	-3.07021200	-1.83055700	4.06696100
H	0.77690500	-0.31949300	5.17137100
C	-3.89360400	0.11242900	2.48540100
H	-3.73141000	0.17228600	1.40711800
H	-4.45956500	-0.79906800	2.70099900
H	-4.49853600	0.98078100	2.75070700
C	0.73888700	1.97021200	3.80133500
H	1.07672100	2.09451400	2.76915200
H	0.38522000	2.95004500	4.13264400
H	1.58452300	1.66483900	4.42442100
C	-0.90024700	-2.42052400	5.61211900
H	-1.68942800	-3.16726600	5.48132700
H	0.05782100	-2.90231800	5.38320900
H	-0.87413200	-2.14686100	6.67420900
S	-1.86612300	2.68598500	2.34360800
O	-0.76135000	2.80440100	1.31796800
O	-1.84364500	3.71154200	3.40310000
O	-3.15054200	2.59545000	1.56891100
N	-4.01158200	1.31400100	-2.27721400
C	-4.12916200	2.64764900	-2.24972000
O	-4.82493000	3.23952100	-3.07544400
O	-3.50965000	3.30868600	-1.21002200
C	-3.88526800	4.69257400	-1.00062400
H	-3.73891800	4.84654800	0.07151800
H	-4.94468300	4.80263200	-1.24428100
C	-3.02427000	5.61609400	-1.84824400
H	-3.19745900	5.41180300	-2.90740200
H	-3.27705200	6.66218400	-1.64085100
H	-1.96237400	5.46677900	-1.62833200

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C	2.57035800	-0.64558200	-0.23876000
C	3.32081400	-1.44935800	0.62503100
C	3.03181200	0.60662900	-0.64870700
C	4.57045800	-0.95620600	1.02870600
C	4.26519400	1.09939500	-0.20141500
C	5.05124600	0.29885100	0.65063500
H	5.17260900	-1.60393600	1.66143800
H	2.43198500	1.21179600	-1.32359300
C	6.39319500	0.78686400	1.14552800
H	6.87424400	0.03752200	1.78092100
H	7.07795000	1.01084600	0.31644600

H	6.30154800	1.71159600	1.73148600
C	4.73362500	2.46901400	-0.63442500
H	4.90241000	3.13071000	0.22581100
H	5.68402400	2.42211900	-1.18290700
H	3.99672300	2.94998400	-1.28471300
C	2.89542900	-2.82071800	1.16246900
O	3.75653500	-3.71242800	1.20207700
O	1.67969600	-2.90703400	1.56105600
Li	0.09210500	-3.14690100	0.81562500
Pd	0.87161200	-1.27038100	-1.02527200
C	-3.48568900	-0.55839600	-0.66151500
C	-3.03046200	0.06792000	0.52157700
C	-3.49801700	1.34278600	0.92125800
C	-4.45242900	1.96609200	0.11258300
C	-4.93619800	1.38012200	-1.05717200
C	-4.44566700	0.12608400	-1.41781100
H	-4.81981000	2.94597800	0.40793300
H	-4.80737400	-0.34026400	-2.33069000
C	-3.02775100	2.07686900	2.15741000
H	-1.93861500	2.13152800	2.18965200
H	-3.42635900	3.09521700	2.15188200
H	-3.35770900	1.57168500	3.06764700
C	-3.01718200	-1.89588000	-1.18782200
H	-1.93853200	-1.90723400	-1.35740300
H	-3.22048500	-2.70833700	-0.48817400
H	-3.51623900	-2.11250000	-2.13569700
C	-5.93166300	2.10289800	-1.93206900
H	-5.41499700	2.71593100	-2.68106200
H	-6.57439900	1.40125800	-2.47275200
H	-6.57039800	2.77136300	-1.34621900
S	-1.76007600	-0.68899700	1.55570100
O	-1.54378100	-2.08030400	1.11704000
O	-2.02422000	-0.46813100	2.97304500
O	-0.43619500	0.21260400	1.21731700
N	-0.20671700	0.24592400	-0.22828300
C	-0.21509900	1.52388900	-0.70175800
O	0.07521700	1.78927400	-1.86477100
O	-0.59460100	2.47316600	0.20373300
C	-0.58470000	3.82303300	-0.28424100
H	-1.24422800	4.36471300	0.40105300
H	-1.01078500	3.85174000	-1.29155700
C	0.82505000	4.39987300	-0.27430300
H	1.45475200	3.84044400	-0.96940500
H	0.81070300	5.45270300	-0.57911900

H	1.25997700	4.32937800	0.72711900
C	1.26120700	-4.06248800	-1.36500200
O	1.78222500	-2.96977000	-1.79000700
O	0.13830300	-4.14635200	-0.79576900
C	2.13496900	-5.29028700	-1.49578400
H	1.53720700	-6.20338100	-1.46892700
H	2.74567500	-5.24463700	-2.40027200
H	2.80565200	-5.26405800	-0.62709700

TS18'_{Pd_O}, E=-2157.72076316 a.u., Imaginary frequency = 150i

C	2.38177100	-0.07025300	-0.14425300
C	3.21948000	-0.44468400	0.91700100
C	2.84456200	0.76285500	-1.16515100
C	4.53406800	0.04813800	0.89215300
C	4.15796000	1.24853300	-1.16828700
C	5.01950500	0.88222500	-0.11445500
H	5.17223200	-0.25647700	1.71742800
H	2.16788600	1.07420100	-1.95496500
C	6.44046500	1.39385400	-0.06699600
H	6.96729700	1.00696800	0.80979800
H	7.01066300	1.09946600	-0.95805600
H	6.47684600	2.49070000	-0.02253300
C	4.62686500	2.16357100	-2.27422300
H	4.96011900	3.13272300	-1.88030300
H	5.47902200	1.73777900	-2.82011100
H	3.82670000	2.35409300	-2.99470400
C	2.84092600	-1.34074900	2.11439500
O	3.75380300	-1.69789400	2.86927700
O	1.59640200	-1.63565200	2.24685300
Li	0.38296400	-2.64087800	1.47329100
Pd	0.52115200	-0.76217900	-0.24076800
C	-3.64544400	-1.01961200	-0.92853700
C	-3.37795400	-0.24151900	0.21775700
C	-4.02989800	0.99496700	0.43741800
C	-4.91712100	1.45554100	-0.53742600
C	-5.17618000	0.73562100	-1.70506900
C	-4.54501500	-0.49473300	-1.86897100
H	-5.41852700	2.40738400	-0.37592600
H	-4.75378700	-1.08150200	-2.76047000
C	-3.81969100	1.84841600	1.66942600
H	-2.82947600	2.31002200	1.65871600
H	-4.57988200	2.63365300	1.71331800
H	-3.87687700	1.25381200	2.58456700
C	-3.04826000	-2.37600700	-1.23469300

H	-1.99702300	-2.30253400	-1.52718200
H	-3.09204200	-3.04788000	-0.37616200
H	-3.59456500	-2.83326400	-2.06505100
C	-6.10115900	1.28558900	-2.76438400
H	-5.56319600	1.96420200	-3.43834800
H	-6.52919400	0.48702800	-3.37844500
H	-6.92531700	1.85476100	-2.32125700
S	-2.22520400	-0.77900200	1.50819200
O	-1.39619100	-1.89612000	0.91273900
O	-2.99791100	-1.16830000	2.69842900
O	-1.32786800	0.42549300	1.78665000
N	-0.40367800	0.89522500	0.01812700
C	0.23865900	2.06937500	0.33185000
O	0.55398200	2.77198300	-0.62635900
O	0.45071500	2.35702600	1.61719700
C	1.26873500	3.52251500	1.87172000
H	1.00680800	3.81066300	2.89284900
H	0.98079500	4.32469600	1.18480700
C	2.74442300	3.17820600	1.73970600
H	2.97963000	2.89991100	0.71070000
H	3.35778000	4.04145700	2.02299800
H	3.00070200	2.33289400	2.38277400
C	0.74221400	-3.43803100	-1.42740600
O	1.10871500	-2.79200200	-0.34570000
O	0.15198200	-2.94072000	-2.38383600
C	1.12161700	-4.91504200	-1.39896000
H	2.19508000	-5.01769600	-1.21517700
H	0.60210500	-5.41339000	-0.57271800
H	0.85095900	-5.39518500	-2.34055100

19'_{Pd}O, E=-2157.7971428 a.u.

C	1.87100800	-0.22277500	-0.34511400
C	2.02093200	0.19380200	0.97875600
C	2.83583500	0.07689000	-1.29807800
C	3.15137700	0.93071600	1.34146300
C	3.96829500	0.82048400	-0.93620300
C	4.12749700	1.25850400	0.39940500
H	3.24602700	1.23657400	2.38087500
H	2.70199800	-0.23868100	-2.32738100
C	5.33352000	2.07560200	0.79927100
H	5.30297100	2.32767500	1.86300900
H	6.27148500	1.53845600	0.60899200
H	5.39055600	3.01499300	0.23429300
C	4.99543600	1.17471200	-1.98433000

H	5.08451400	2.26253200	-2.10218600
H	5.99254000	0.80333500	-1.71629500
H	4.72755000	0.75327700	-2.95628600
C	0.98237600	-0.20704400	1.97114400
O	1.03680500	0.04809400	3.16810900
O	-0.02121600	-0.90747000	1.44779300
Li	-0.34956200	-2.78305300	1.59007300
Pd	0.20676200	-1.26096700	-0.62456000
C	-3.50450500	-0.11750200	-0.83890100
C	-3.19231000	-0.75018000	0.39007400
C	-3.13564700	-0.01882700	1.59286900
C	-3.31400400	1.37106400	1.51806300
C	-3.54680000	2.03454500	0.31688700
C	-3.66896400	1.26846000	-0.84296700
H	-3.25326600	1.94651400	2.43931200
H	-3.88406400	1.76195200	-1.78823000
C	-2.88658900	-0.60095200	2.96704300
H	-1.81522700	-0.76243500	3.11418300
H	-3.23151600	0.10578800	3.72873600
H	-3.38952500	-1.55601000	3.11431700
C	-3.65237300	-0.85577000	-2.15048200
H	-2.66749200	-1.13898400	-2.52784300
H	-4.24071600	-1.76800600	-2.03408700
H	-4.13831100	-0.20895400	-2.88718300
C	-3.64387900	3.53972400	0.25827000
H	-2.69684900	3.97122700	-0.08963500
H	-4.42299300	3.86718500	-0.43915100
H	-3.86099100	3.97048600	1.24091400
S	-2.78353400	-2.52041500	0.28358400
O	-1.68016100	-2.56052200	-0.76048600
O	-3.98959100	-3.26108100	-0.11805600
O	-2.21657400	-2.96433500	1.61155700
N	-0.38414400	-0.15697900	-1.99696000
C	0.05707500	1.08195500	-2.32213300
O	0.55055800	1.36845000	-3.41110200
O	-0.18212000	1.99150100	-1.33085300
C	0.22783700	3.34179900	-1.60239400
H	-0.37574800	3.95140000	-0.92329000
H	-0.02414800	3.59957700	-2.63626300
C	1.71638600	3.53114600	-1.34266000
H	2.29320700	2.93878100	-2.05526900
H	1.99059900	4.58714800	-1.45255700
H	1.97492600	3.19851300	-0.33346500
C	1.77264300	-3.81527000	-0.40618100

O	1.02519300	-3.04063900	0.34446500
O	2.14698800	-3.54373000	-1.54025500
C	2.14896800	-5.12811300	0.27617500
H	2.62113200	-4.92742700	1.24341000
H	1.24135800	-5.71179600	0.46472000
H	2.82679400	-5.70210200	-0.35752300

KCl, E=-488.60033036 a.u.

Cl	0.00000000	0.00000000	-1.47308400
K	0.00000000	0.00000000	1.31802200

PhCOOK, E=-448.454542482 a.u.

C	-0.70597100	0.00001400	-0.00015100
O	-1.28907500	-1.12794400	-0.00012400
C	0.81088700	0.00000700	-0.00006500
C	1.51805800	1.20823900	0.00002000
C	1.51804100	-1.20824000	-0.00006000
C	2.91312700	1.20954200	0.00011000
H	0.94966600	2.13226400	0.00001400
C	2.91310300	-1.20956900	0.00003700
H	0.94963700	-2.13226000	-0.00013600
C	3.61387600	-0.00001800	0.00012300
H	3.45595900	2.15149800	0.00017500
H	3.45592300	-2.15153300	0.00004300
H	4.70097800	-0.00003000	0.00019600
O	-1.28904700	1.12801100	-0.00031400
K	-3.59862700	-0.00001700	0.00016500

N-benzoyloxy morpholine_CF₃, E=-813.191485987 a.u.

C	-1.72373400	1.36271500	0.23986400
C	-2.25477100	0.43221200	1.32930400
C	-2.58033200	-1.30288500	-0.22310400
C	-2.04238700	-0.43271400	-1.36254500
H	-1.41875400	-0.09779500	1.81223000
H	-2.78929400	1.00254200	2.09420200
H	-2.54866200	1.94042200	-0.19066000
H	-0.97738900	2.06621800	0.61509200
H	-1.76544700	-1.90643800	0.20470000
H	-3.35458700	-1.98072200	-0.59376100
H	-1.51705000	-1.02796500	-2.11410100
H	-2.86954600	0.09167600	-1.85264400
N	-1.13387900	0.63550300	-0.90618300
O	-3.18622600	-0.49729300	0.78283600
O	0.03071700	-0.11537000	-0.38749000

C	1.14882900	0.61925000	-0.30805100
O	1.28455600	1.79758400	-0.49599400
C	2.29369700	-0.31582600	0.15579100
F	2.41905000	-1.37107000	-0.66824800
F	3.44976400	0.34923900	0.18246000
F	2.03093000	-0.77731800	1.39532600

17Ru_O_CF3, E=-2690.15516012 a.u.

Ru	-1.71279000	-0.73550700	0.47155100
C	-3.28764200	-2.14802300	-0.29534000
C	-3.77306400	-1.48817400	0.88265100
H	-4.66878400	-0.88076100	0.82088500
C	-3.07937700	-1.58969700	2.10410400
H	-3.46270800	-1.06218600	2.97343800
C	-1.96523200	-2.49418100	2.26498800
C	-1.45286200	-3.08228500	1.11479800
H	-0.57543100	-3.71393000	1.17020500
C	-2.06285200	-2.84060600	-0.16402300
H	-1.59759600	-3.26604600	-1.04150400
C	-4.08544700	-2.09327700	-1.58496500
H	-4.48453900	-1.07581000	-1.66749400
C	-5.27517800	-3.06886000	-1.46987000
H	-4.92394200	-4.10229400	-1.37742000
H	-5.90237100	-3.00359900	-2.36379300
H	-5.90195400	-2.84490800	-0.60061700
C	-3.25474500	-2.38003500	-2.84124600
H	-2.38036300	-1.72776200	-2.90344600
H	-3.86648500	-2.20997500	-3.73126300
H	-2.91768000	-3.42189300	-2.87356500
C	-1.40988500	-2.82148800	3.62632500
H	-1.64176600	-2.05523100	4.37006400
H	-0.32711700	-2.97035200	3.59841200
H	-1.86236400	-3.75453300	3.98173800
C	-0.44309600	0.24715800	-2.07078200
O	0.33860600	0.47493100	-3.02147400
N	-0.12542800	-0.47107100	-0.95491900
C	1.20980600	-0.86697400	-0.80886900
C	1.60238700	-2.19657500	-0.60309300
C	2.27817400	0.04473400	-0.84744800
C	2.92261700	-2.57362000	-0.35159800
C	3.59523500	-0.31024100	-0.61990700
C	3.95395600	-1.63402400	-0.35133200
F	0.69496300	-3.18733700	-0.67679900
F	3.15442700	-3.87145500	-0.14253000

F	4.52859600	0.64952600	-0.65366900
F	2.03630000	1.36025500	-1.09826800
C	-1.80816300	0.81922600	-2.00971300
C	-2.50526200	0.65826900	-0.79898800
C	-2.33089000	1.56408700	-3.07230800
C	-3.71923700	1.35008500	-0.66273600
C	-3.55354500	2.21776600	-2.92859800
C	-4.23290900	2.12592900	-1.70943000
H	-4.28777500	1.28901800	0.26188100
H	-3.97662000	2.78704500	-3.75050600
H	-5.17909500	2.64419200	-1.57741200
C	5.40871900	-1.94745300	-0.08354600
F	6.16837600	-1.59083100	-1.13766800
F	5.61866100	-3.24763000	0.16000700
F	5.84533400	-1.24832800	0.98527000
K	1.03258000	2.99552800	-3.13696800
C	-1.90818400	1.99218200	2.08865100
C	-1.43895100	2.97388400	3.16082000
C	0.02276800	1.40496000	4.08862200
C	-0.39906200	0.34529200	3.07033300
H	-0.61703700	3.60628400	2.79323300
H	-2.27217500	3.63145700	3.42170600
H	-2.76854300	1.42619300	2.45266200
H	-2.18885600	2.48086300	1.15907300
H	0.91352700	1.95070700	3.74834500
H	0.26375200	0.90958700	5.03290200
H	0.40364200	-0.35392100	2.83165800
H	-1.24777200	-0.20076500	3.47096300
N	-0.89543500	0.92444000	1.77335300
O	-1.05383100	2.29349000	4.34496300
O	0.38481000	1.60980500	1.35473100
C	0.40641600	2.60064100	0.47113300
O	-0.43337500	2.97262700	-0.30905800
H	-1.78025900	1.59604900	-4.01024900
C	1.73345900	3.38790900	0.66849100
F	2.74677000	2.64810100	1.11062400
F	2.08900800	3.96410100	-0.50396700
F	1.49120000	4.36912900	1.55469000

TS18_{Ru_O_CF3}, E=-2690.14920888 a.u., Imaginary frequency = 301i

Ru	-1.70171700	-0.69191000	0.44827500
C	-3.36228700	-2.00425600	-0.43506700
C	-3.81158200	-1.42409900	0.79708600
H	-4.66895500	-0.76133200	0.79039500

C	-3.13701700	-1.68407300	2.00273400
H	-3.48706100	-1.20844600	2.91507700
C	-2.09954900	-2.68404000	2.08793700
C	-1.61576300	-3.19259600	0.89136700
H	-0.79287100	-3.89620400	0.88777500
C	-2.18750400	-2.77988900	-0.35932000
H	-1.73785300	-3.15037300	-1.26988100
C	-4.14737800	-1.78502100	-1.71546200
H	-4.46482700	-0.73599700	-1.71685200
C	-5.41155500	-2.66894700	-1.67882500
H	-5.14428600	-3.73113900	-1.66943200
H	-6.02545500	-2.48245700	-2.56478800
H	-6.02479100	-2.46557000	-0.79496700
C	-3.33332400	-2.03726400	-2.98983800
H	-2.40831800	-1.45554000	-3.00076300
H	-3.92288300	-1.74838300	-3.86387800
H	-3.08085600	-3.09711700	-3.10454400
C	-1.60168900	-3.18255300	3.41867700
H	-1.77852700	-2.46786700	4.22653700
H	-0.53643000	-3.42599100	3.38849000
H	-2.14251200	-4.09887400	3.68316500
C	-0.52342100	0.44637200	-2.04828600
O	0.22215300	0.73222100	-3.00776400
N	-0.18262900	-0.37415200	-1.00753600
C	1.15016100	-0.79819300	-0.92122900
C	1.50863300	-2.14368300	-0.75916900
C	2.24460000	0.08346600	-0.96368600
C	2.82081800	-2.56900500	-0.55059100
C	3.55454500	-0.32105300	-0.77616600
C	3.87986200	-1.66150700	-0.55231900
F	0.56624500	-3.10290500	-0.82676300
F	3.01496200	-3.87876300	-0.37832000
F	4.51507400	0.61024800	-0.79965300
F	2.04742900	1.41265300	-1.15874500
C	-1.86697800	1.04829800	-1.87899000
C	-2.50114200	0.83206600	-0.64426600
C	-2.42619500	1.87113100	-2.86293200
C	-3.67880300	1.55107300	-0.38947500
C	-3.61726900	2.54879800	-2.60689700
C	-4.22637700	2.40392000	-1.35581300
H	-4.19215300	1.45165700	0.56355500
H	-4.06968500	3.17830700	-3.36687400
H	-5.14470300	2.94184100	-1.13595100
C	5.32978800	-2.02505700	-0.32378700

F	6.08032300	-1.65251400	-1.37824600
F	5.50555100	-3.33920700	-0.13112900
F	5.80492900	-1.37867200	0.76139100
K	0.83801100	3.32619700	-2.78351800
C	-1.74664100	1.76598600	2.30469100
C	-1.14329300	2.58985500	3.44289900
C	0.27751400	0.86197300	4.09218000
C	-0.26332700	-0.06443400	3.00007600
H	-0.30477500	3.20641400	3.09041700
H	-1.91424600	3.26243000	3.82794300
H	-2.65024300	1.26450600	2.66490600
H	-2.00894600	2.37466600	1.44267400
H	1.16779000	1.40323000	3.74944600
H	0.55287400	0.25268600	4.95734500
H	0.49875800	-0.74218400	2.61306600
H	-1.07781700	-0.64277200	3.43083700
N	-0.88170200	0.64074900	1.82830300
O	-0.73611800	1.75841100	4.51670200
O	0.58694300	1.42547500	1.39263800
C	0.60461600	2.50280600	0.66142300
O	-0.24877700	2.99989200	-0.04721900
H	-1.92805400	1.94620900	-3.82743400
C	1.96184100	3.24367500	0.87525000
F	2.98229300	2.43308500	1.15137200
F	2.26866900	3.95956900	-0.23458100
F	1.80442900	4.10738400	1.89389900

17Rh_O_CF3, E=-2079.04871418 a.u.

Rh	-1.80721900	0.24797800	-0.28336800
C	-2.66197900	1.93560500	-1.32245000
C	-3.75277600	1.02690900	-1.06136600
C	-3.88449000	0.89250200	0.34918100
C	-2.23606900	2.48544100	-0.03410800
C	-2.95490800	1.83358800	0.98225800
C	-2.83749700	2.12933100	2.44887000
H	-1.79251900	2.22513400	2.75325800
H	-3.34336800	3.07233300	2.68880000
H	-3.30115100	1.35566100	3.06526600
C	-4.98278300	0.13494600	1.03749200
H	-4.77452400	-0.03146100	2.09555300
H	-5.92000000	0.70128100	0.97998900
H	-5.15854400	-0.83702700	0.56860600
C	-4.64713500	0.43037800	-2.10308700
H	-4.08383200	0.08962800	-2.97317000

H	-5.21930000	-0.41485000	-1.71632200
H	-5.36345600	1.19008700	-2.43860600
C	-2.25936000	2.43723900	-2.67503700
H	-2.47374800	1.69114700	-3.44320600
H	-2.81955600	3.34804800	-2.92159700
H	-1.19314500	2.65609500	-2.71419500
C	-1.23712400	3.58100900	0.16806900
H	-0.56418600	3.35825700	0.99894200
H	-0.64090300	3.74088800	-0.72930800
H	-1.75566900	4.51916600	0.40105900
C	0.68186200	-0.46481300	-1.79781900
O	1.85615700	-0.48885300	-2.21806300
N	0.21193500	0.31678800	-0.79627200
C	-0.39919400	-1.36814800	-2.27939200
C	-1.66398700	-1.24499000	-1.67548700
C	-0.13684800	-2.34531800	-3.24245000
C	-2.65551700	-2.16306600	-2.03730100
C	-1.14299000	-3.23986300	-3.60886900
H	0.85245300	-2.38354700	-3.69034700
C	-2.39680700	-3.15235600	-2.99709000
H	-3.63941000	-2.12134000	-1.57820700
H	-0.95448100	-3.99990600	-4.36089500
H	-3.18159200	-3.85351500	-3.26901900
O	1.19096800	1.22766900	-0.28882400
C	1.54070800	2.23706500	-1.16329400
O	0.95612300	2.45180100	-2.19507400
C	2.74148000	3.04798000	-0.65327000
C	3.89523600	2.09537200	-0.28280400
H	4.76655100	2.67647400	0.03475000
H	3.60478000	1.43590400	0.53796100
H	4.18562200	1.50371600	-1.15824000
C	2.32934200	3.86917300	0.58727100
H	3.18747600	4.45329000	0.93471400
H	1.52659900	4.57070400	0.34472200
H	1.99871500	3.22955700	1.40560700
C	3.18608900	3.99374500	-1.78071700
H	3.47906400	3.43474700	-2.67352600
H	2.37698500	4.66919300	-2.06665900
H	4.03856700	4.59185400	-1.44456400
Cs	3.97026500	-1.62960500	-0.61151300
C	-2.34104900	-1.61446300	2.21850200
C	-1.95688700	-2.60554300	3.31706400
C	-0.25734500	-3.51792000	2.00123300
C	-0.58025300	-2.56819300	0.85337700

H	-1.24391400	-2.13666400	4.01306800
H	-2.85077800	-2.88525500	3.88054800
H	-3.10865800	-2.03440700	1.56492200
H	-2.70369900	-0.67901900	2.63843100
H	0.54529900	-3.11025900	2.63489900
H	0.08768000	-4.47007900	1.58838600
H	0.27555000	-2.33306700	0.23159900
H	-1.35089900	-3.00512000	0.21484100
N	-1.20549800	-1.28727900	1.30518800
O	-1.41676600	-3.79639700	2.76954700
O	-0.31764200	-0.50701600	2.23995700
C	0.99826600	-0.41669700	2.12118400
O	1.78668500	-1.11087100	1.52404500
C	1.45147100	0.75565400	3.03203900
F	0.70069500	1.85390300	2.83366300
F	2.73052500	1.05736800	2.77703100
F	1.34059000	0.39172600	4.31814800

TS18_{Rh_O_CF3}, E=-2079.03886732 a.u., Imaginary frequency = 290i

Rh	1.74645900	-0.22192600	-0.23398000
C	2.56082900	-1.75206200	-1.58199200
C	3.68327900	-0.97712900	-1.12444100
C	3.77522700	-1.12169600	0.29198800
C	2.04937400	-2.49491900	-0.43453600
C	2.77335400	-2.09763000	0.71009200
C	2.59243900	-2.66054900	2.08787200
H	1.53678800	-2.81359400	2.31849600
H	3.10203700	-3.62843300	2.17028600
H	3.01465300	-2.01151300	2.85848400
C	4.90146600	-0.58711800	1.12861700
H	4.69865300	-0.66373300	2.19781800
H	5.81365800	-1.16257400	0.93185400
H	5.12028200	0.45876100	0.89614400
C	4.65699700	-0.26202900	-2.00712100
H	4.15785900	0.25991400	-2.82472900
H	5.25684900	0.46323600	-1.45460900
H	5.34432800	-0.99663600	-2.44423200
C	2.18309800	-1.95652400	-3.01690500
H	2.45261700	-1.08346600	-3.61533100
H	2.71574500	-2.82401200	-3.42615200
H	1.11153600	-2.11488700	-3.12595400
C	0.99342500	-3.55398400	-0.47017100
H	0.29018400	-3.44514600	0.35743500
H	0.43864600	-3.52558300	-1.40650700

H	1.46016300	-4.54271600	-0.38238600
C	-0.58307300	0.84985700	-1.79550300
O	-1.72312800	1.01472900	-2.26903500
N	-0.22971300	-0.09776600	-0.88971700
C	0.57785200	1.73702100	-2.07324300
C	1.78031000	1.46482500	-1.40059700
C	0.44554100	2.84994800	-2.90777300
C	2.84151600	2.36303400	-1.54355700
C	1.52090400	3.72418000	-3.06654900
H	-0.50081700	3.00752500	-3.41760800
C	2.71178000	3.48518800	-2.37440000
H	3.77750900	2.20298100	-1.01572300
H	1.43277900	4.58865600	-3.71722100
H	3.54749500	4.17172700	-2.48082700
O	-1.28858800	-1.00191300	-0.57831000
C	-1.64918500	-1.84129600	-1.61787500
O	-1.01849400	-1.93166200	-2.64053900
C	-2.91409700	-2.65383400	-1.30090700
C	-4.00907700	-1.75017500	-0.70470900
H	-4.90835000	-2.34256400	-0.51033100
H	-3.68202800	-1.30835700	0.23862100
H	-4.27767000	-0.96581200	-1.42144800
C	-2.56425100	-3.77175000	-0.29379200
H	-3.45900500	-4.37163700	-0.09965900
H	-1.79811600	-4.43911200	-0.69743100
H	-2.21413300	-3.36740400	0.65587900
C	-3.41069200	-3.27736900	-2.61653200
H	-3.65597200	-2.50600400	-3.35198900
H	-2.64766900	-3.92221300	-3.05693600
H	-4.30649700	-3.87536100	-2.42362600
Cs	-3.70837800	1.90044900	-0.29271000
C	2.36071500	1.12273100	2.44810000
C	1.95416500	1.91939800	3.68925200
C	0.27529900	3.03005100	2.52140000
C	0.61479400	2.29039400	1.23120100
H	1.23047400	1.34148200	4.28137300
H	2.84053400	2.09955700	4.30318300
H	3.16839800	1.63911000	1.91862400
H	2.69497200	0.12367000	2.71520200
H	-0.52737100	2.50779100	3.06056800
H	-0.07517300	4.03524900	2.26984700
H	-0.24713700	2.12624500	0.59396400
H	1.35388400	2.86698600	0.66342000
N	1.28521400	0.98657900	1.43452600

O	1.42399500	3.18427700	3.33600300
O	0.23144400	-0.01882800	2.41924500
C	-1.05835400	-0.05420600	2.25992900
O	-1.82706900	0.77705600	1.80877000
C	-1.59656600	-1.39640100	2.83810800
F	-0.88671200	-2.44649400	2.37200500
F	-2.88082000	-1.57455700	2.49601200
F	-1.50648900	-1.38993400	4.17545100

13', E=-1494.89188444 a.u.

Rh	2.14452800	0.17798400	0.21132300
C	2.14784800	0.85316400	2.65527100
O	2.32857800	-0.36511700	2.32273800
O	2.07981400	1.72485200	1.72702100
C	2.65122000	0.96213800	-1.73546700
C	3.84432600	0.89698500	-0.90383100
C	4.05818800	-0.47164100	-0.54558000
C	2.17248200	-0.38183200	-1.92409600
C	3.00933600	-1.26970200	-1.16759900
C	2.91626000	-2.76144500	-1.11448800
H	3.58165300	-3.20229000	-1.86714300
H	3.21692900	-3.14042500	-0.13593400
H	1.90106800	-3.11011200	-1.30490900
C	5.15819100	-1.02355700	0.30520500
H	4.77853700	-1.79465800	0.97956500
H	5.93126400	-1.47463200	-0.32802800
H	5.62525800	-0.24690200	0.91258600
C	4.66738900	2.07841900	-0.49776500
H	4.02851700	2.91481100	-0.20455200
H	5.32036900	1.84414200	0.34419200
H	5.29305300	2.40362600	-1.33711700
C	2.09310800	2.19372600	-2.37524900
H	2.29667500	3.07733700	-1.76561700
H	2.55980200	2.35022700	-3.35606400
H	1.01385100	2.11076300	-2.50954900
C	1.00059300	-0.76204500	-2.77192100
H	0.13397000	-0.13645100	-2.54658200
H	1.26070400	-0.61507800	-3.82704800
H	0.72809000	-1.80742600	-2.62883300
C	1.97489100	1.24710000	4.09334800
H	2.34054300	2.26261400	4.25529000
H	0.90579100	1.22573900	4.33121100
H	2.48969800	0.54188400	4.74778700
C	-0.79776300	-0.70709700	0.23348400

O	0.08665700	0.13145300	0.63177200
N	-2.04435900	-0.39680100	-0.06315500
C	-0.50674400	-2.17254500	0.16029800
C	0.31015500	-2.74871400	1.14436000
C	-1.05317000	-2.97926400	-0.84823700
C	0.56369100	-4.12054200	1.12274000
H	0.74598700	-2.11708100	1.91152800
C	-0.78021000	-4.34803100	-0.87654500
H	-1.66520800	-2.52008700	-1.61801700
C	0.02387600	-4.92192800	0.11312000
H	1.18949900	-4.56318700	1.89206300
H	-1.18823700	-4.96552100	-1.67156300
H	0.23292300	-5.98731300	0.09268700
O	-2.26944400	1.03121200	0.14280400
C	-1.65800200	1.88657600	-0.72201900
O	-1.09949000	1.53423000	-1.73842700
C	-1.78246000	3.32837300	-0.22264300
C	-0.97689200	3.44163300	1.09288700
H	-0.99849600	4.47874300	1.44369100
H	-1.40311600	2.79965600	1.86746700
H	0.06431000	3.13899200	0.95361100
C	-3.26733400	3.66554200	0.03559000
H	-3.35711300	4.70284000	0.37197500
H	-3.86490200	3.55932100	-0.87763600
H	-3.68802600	3.02278500	0.81445000
C	-1.20398800	4.27342500	-1.28566800
H	-0.14618700	4.06269800	-1.45905100
H	-1.72635800	4.16937100	-2.24086100
H	-1.29812300	5.31000900	-0.94849200
Cs	-4.99808800	-0.59875500	0.14841900

I, E=-1476.06390419 a.u.

Rh	0.49869900	-0.04614000	-0.23542200
C	2.51844300	0.20312100	0.51659300
C	1.67648200	-0.46701100	1.49988500
C	1.28907700	-1.76236900	0.95988000
C	2.54635800	-0.61349000	-0.64992600
C	1.78101600	-1.83654600	-0.36892600
C	1.60811200	-2.96573300	-1.33183600
H	2.51653800	-3.58051000	-1.34411700
H	0.76907500	-3.60799600	-1.06008100
H	1.44560800	-2.59961600	-2.34841800
C	0.58817900	-2.84296200	1.72138200
H	0.08436200	-3.55112300	1.06089500

H	1.32662000	-3.40577800	2.30454800
H	-0.14252400	-2.44063000	2.42502600
C	1.38453900	0.05112600	2.86689000
H	1.12904900	1.11154100	2.82057700
H	0.56017800	-0.48854500	3.33629500
H	2.27308100	-0.07156700	3.49950800
C	3.20819000	1.51205200	0.72202900
H	2.60011700	2.18023000	1.33258100
H	4.16162400	1.33920200	1.23551900
H	3.42048900	2.00513900	-0.22778600
C	3.26182200	-0.32223000	-1.92953400
H	3.39626300	0.75052100	-2.07540700
H	4.25278300	-0.79232100	-1.91428500
H	2.71898800	-0.71848500	-2.79058500
C	-2.25840200	-1.25703000	0.71818100
C	-3.78068000	-1.36496100	0.63809400
C	-3.97940800	0.85069100	-0.06906300
C	-2.47066000	1.06993000	-0.03332200
H	-4.08256900	-1.75753900	-0.34540300
H	-4.13133500	-2.06009600	1.40562400
H	-1.96519700	-0.92520500	1.72000700
H	-1.77009500	-2.20461000	0.49284200
H	-4.30156400	0.54951900	-1.07772100
H	-4.47943100	1.78912400	0.18278700
H	-2.13631500	1.75612200	-0.80912400
H	-2.14732400	1.45815200	0.93757900
N	-1.69451800	-0.20825100	-0.18692900
O	-4.38126700	-0.11118600	0.89479900
Cl	-1.84824800	-0.78174600	-1.91705400
C	0.19482500	2.81321400	0.00855300
O	0.26006700	1.86457900	-0.90334200
O	0.14666400	2.58956400	1.22015500
C	0.18784400	4.21292100	-0.56901700
H	-0.07962100	4.93336100	0.20383600
H	1.18685800	4.44734200	-0.95143700
H	-0.50340200	4.27949700	-1.41293700

TSII, E=-1476.03825528 a.u. Imaginary frequency = 174i

Rh	0.32333100	-0.06144800	-0.14941600
C	2.50031400	0.06518600	0.19921200
C	1.85718100	-0.45400000	1.38679300
C	1.25701100	-1.73631200	1.04987400
C	2.22553700	-0.83143700	-0.87857500
C	1.47598300	-1.96973000	-0.33441900

C	1.07412100	-3.17347600	-1.12209100
H	1.94113700	-3.83574600	-1.23510100
H	0.27975600	-3.73763100	-0.63127600
H	0.72984200	-2.89707800	-2.12007600
C	0.63331100	-2.67494800	2.03523400
H	0.01078000	-3.42767700	1.54766600
H	1.42190300	-3.20634700	2.58066300
H	0.02942700	-2.14469500	2.77519200
C	1.91872100	0.16284000	2.74386400
H	1.74820800	1.23865000	2.68241300
H	1.17311200	-0.26637900	3.41515000
H	2.91004100	-0.01652500	3.17931500
C	3.29764600	1.32595500	0.12552800
H	2.96320800	2.04430400	0.87433900
H	4.35357100	1.09599700	0.31081600
H	3.21863200	1.78658800	-0.86048900
C	2.69955600	-0.70117600	-2.29197400
H	2.83861900	0.34580900	-2.56613100
H	3.65937300	-1.21727100	-2.41383100
H	1.98743400	-1.14257800	-2.99177900
C	-2.32645100	-1.03035800	1.03624500
C	-3.75272800	-1.27857500	0.49494100
C	-3.89487800	0.91052500	-0.31000300
C	-2.46059200	1.22767400	0.15373400
H	-3.66915900	-1.70497900	-0.51469800
H	-4.26839200	-1.98741200	1.14640000
H	-2.41502400	-0.68924400	2.07983600
H	-1.71814500	-1.93197900	1.00654600
H	-3.85559100	0.59767300	-1.36265300
H	-4.50788000	1.80990000	-0.22604800
H	-1.95162400	1.90583500	-0.52670700
H	-2.49093100	1.69153200	1.15379600
N	-1.62812600	0.05210800	0.36203300
O	-4.49141000	-0.08243000	0.49775500
C1	-1.36435000	-0.68627900	-1.89980900
C	0.38851000	2.80875800	0.08657600
O	0.26127800	1.88211600	-0.84054300
O	0.41343100	2.56724800	1.29502600
C	0.51910400	4.21050200	-0.47307900
H	0.29987600	4.94152700	0.30574200
H	1.54866900	4.35820500	-0.81683000
H	-0.13637700	4.35262200	-1.33507300

III, E= -1476.08398039 a.u.

Rh	0.39828400	0.21369800	-0.09697400
C	2.52451000	0.27841700	0.00184100
C	2.03455600	0.00326900	1.34337700
C	1.34106000	-1.24387100	1.32723500
C	2.16731200	-0.84739900	-0.83089700
C	1.40060600	-1.76241900	-0.03176400
C	0.93763300	-3.11135900	-0.48625300
H	1.74348600	-3.83772200	-0.32315000
H	0.06162000	-3.46322100	0.05942600
H	0.70172900	-3.11629000	-1.55172300
C	0.81447500	-1.94905500	2.54203100
H	0.27116200	-2.85856900	2.28541300
H	1.65132400	-2.23903700	3.18746200
H	0.15500200	-1.30813800	3.13356300
C	2.23226600	0.89335400	2.52699000
H	2.05546200	1.93919200	2.26504200
H	1.56703500	0.62563500	3.34947400
H	3.26640600	0.80642600	2.88077800
C	3.34620300	1.45717500	-0.41374700
H	3.14487700	2.32234700	0.22077900
H	4.41304200	1.21659000	-0.33344000
H	3.12993000	1.73710400	-1.44598700
C	2.56117300	-1.03169200	-2.25940600
H	2.61196700	-0.07540000	-2.78025700
H	3.54939900	-1.50636000	-2.29806200
H	1.85472200	-1.66701600	-2.79511300
C	-2.50082300	-0.51141100	1.22537600
C	-2.40858400	-2.02754500	1.03030100
C	-2.52648900	-1.80548700	-1.29596700
C	-2.66175200	-0.29060500	-1.18820000
H	-1.35406200	-2.32406500	1.01496600
H	-2.89502600	-2.52536700	1.87270900
H	-3.54799900	-0.20806900	1.32845300
H	-1.93904100	-0.19159800	2.10616600
H	-1.47199600	-2.07842500	-1.44582000
H	-3.09877300	-2.15567300	-2.15739800
H	-2.22768900	0.21615400	-2.04880600
H	-3.71572700	-0.01678100	-1.07467000
N	-1.92446100	0.16169600	0.02872200
O	-3.06215100	-2.44841700	-0.14761100
Cl	0.07764600	1.27117200	-2.20441200
C	-1.40927500	2.43475000	0.54142900
O	-0.24247300	2.10572300	0.76029100
O	-2.35627700	1.57417800	0.16422300

C	-1.91164500	3.83782000	0.64184200
H	-2.97094500	3.86732700	0.89937600
H	-1.31195300	4.38474100	1.36995600
H	-1.77563400	4.30249500	-0.34170100

17'Ru_O_C2H4, E= -2273.32270024 a.u.

Ru	-0.82067500	-0.26932800	-0.94547200
C	-0.51868000	-0.05201400	-3.08844300
H	-1.45573700	-0.15446800	-3.62880900
C	0.18584500	-1.16995600	-2.61992800
H	-0.19709700	-2.17704400	-2.79062300
C	0.71183400	2.17258000	-0.38317900
O	1.53318800	2.95783500	0.13910300
N	0.90364700	0.83004600	-0.56058500
C	2.07259900	0.19490600	-0.20199900
C	3.37906200	0.67590600	-0.41703900
C	2.02102500	-1.10027000	0.35121900
C	4.50220900	-0.01464600	0.00962900
C	3.14069800	-1.82014600	0.74498100
C	4.42256600	-1.27611800	0.60470800
F	3.59065500	1.82508000	-1.11225500
F	5.70089200	0.56049900	-0.18762200
F	2.94371000	-3.02942500	1.27378600
F	0.80268300	-1.69766100	0.51608700
C	-0.63138800	2.59661200	-0.84518300
C	-1.53195600	1.59606600	-1.28521600
C	-0.99534600	3.94799300	-0.83200900
C	-2.79332500	2.00691400	-1.72853100
C	-2.25767900	4.33528300	-1.27255900
C	-3.15333400	3.35985500	-1.72136200
H	-3.52119300	1.28089300	-2.07568700
H	-2.54582300	5.38180900	-1.26851300
H	-4.14177700	3.65160400	-2.06667200
C	5.69963700	-1.95043300	1.04540100
F	6.35517600	-1.16969700	1.93366200
F	6.52445000	-2.14262500	-0.00270400
F	5.48049800	-3.13788600	1.62529000
C	-3.44072800	-1.58254200	-2.20085300
C	-4.61981200	-2.53802500	-2.01814100
C	-3.49893000	-3.73208600	-0.34661500
C	-2.26556000	-2.83686500	-0.46181900
H	-5.34539400	-2.11961300	-1.30518000
H	-5.12283600	-2.67830900	-2.97812000
H	-2.76428300	-1.96749300	-2.96902700

H	-3.76120900	-0.58213700	-2.48603100
H	-4.17041200	-3.35599400	0.43973600
H	-3.18670700	-4.74446500	-0.07831800
H	-1.75021500	-2.72005500	0.49469000
H	-1.56467300	-3.25865000	-1.18752900
N	-2.58943500	-1.46288300	-0.98412000
O	-4.17159500	-3.81567800	-1.59148600
O	-3.53993400	-0.88398600	0.05035600
C	-2.91163900	-0.22112700	1.03542600
O	-1.69394900	0.02522900	1.00812300
C	-3.79058400	0.18169600	2.13721700
C	-5.12298900	-0.25998500	2.21962600
C	-3.26159000	1.03327800	3.12265700
C	-5.91663500	0.14940300	3.28618500
H	-5.52559000	-0.91738400	1.45744800
C	-4.06411700	1.43728700	4.18403300
H	-2.23323200	1.36617000	3.03662800
C	-5.38885500	0.99616100	4.26638300
H	-6.94471700	-0.19047500	3.35655100
H	-3.66153400	2.09616700	4.94645600
H	-6.01259200	1.31324000	5.09662200
K	3.75653100	4.08976700	0.41609100
H	-0.27591000	4.67598500	-0.46810000
H	1.26565400	-1.11729700	-2.49372400
H	0.01318000	0.87209200	-3.29636700

TS18'*Ru*_O_C₂H₄, E= -2273.31854399 a.u. Imaginary frequency = 280i

Ru	-0.87538800	-0.25007900	-0.99026400
C	-0.54818600	0.02411900	-3.13847800
H	-1.48456500	-0.05125200	-3.68352100
C	0.13832600	-1.11248200	-2.69749300
H	-0.25429800	-2.10986500	-2.89656200
C	0.68509400	2.16738500	-0.37380200
O	1.50704200	2.93390700	0.17317800
N	0.86986400	0.82808100	-0.58164100
C	2.03668100	0.18295800	-0.23131000
C	3.34302400	0.66822300	-0.43733800
C	1.98501900	-1.12199800	0.29737900
C	4.46620200	-0.02708100	-0.01862500
C	3.10556800	-1.84697000	0.68111300
C	4.38681200	-1.29866600	0.55419000
F	3.55445700	1.83059000	-1.10997500
F	5.66400500	0.55538100	-0.19997500
F	2.90912000	-3.06553200	1.18766400

F	0.76857300	-1.72358300	0.44816200
C	-0.65180300	2.61369500	-0.83329400
C	-1.56704500	1.63534200	-1.29063700
C	-0.99641900	3.96978400	-0.79850000
C	-2.82301800	2.07003100	-1.72230700
C	-2.25233700	4.38320800	-1.23275500
C	-3.16251300	3.42814500	-1.69424900
H	-3.56603400	1.36256300	-2.07274700
H	-2.52477000	5.43367000	-1.21199800
H	-4.14786700	3.73834500	-2.03184900
C	5.66380300	-1.97767800	0.98880200
F	6.31263600	-1.21047300	1.89366500
F	6.49357400	-2.14870700	-0.05882700
F	5.44515000	-3.17546800	1.54659500
C	-3.48437200	-1.45192700	-2.25880500
C	-4.68352200	-2.37703800	-2.04626900
C	-3.53114000	-3.64641100	-0.45727900
C	-2.27505000	-2.78623300	-0.60513200
H	-5.36114600	-1.95433100	-1.29157700
H	-5.23088800	-2.47601300	-2.98697300
H	-2.86586000	-1.83567500	-3.07813800
H	-3.78765500	-0.43582600	-2.50016200
H	-4.15429300	-3.26949100	0.36597900
H	-3.23668400	-4.67380900	-0.22872200
H	-1.72069600	-2.70564800	0.33304700
H	-1.61837500	-3.22903500	-1.36159600
N	-2.55522800	-1.39916800	-1.10424300
O	-4.25704000	-3.67805600	-1.67342800
O	-3.57737700	-0.81706800	0.09525500
C	-2.89069100	-0.23028300	1.05221600
O	-1.66358200	0.02338500	0.96186400
C	-3.65888800	0.11395300	2.26034500
C	-4.98433400	-0.32017400	2.43067700
C	-3.03430200	0.89286400	3.24868300
C	-5.67656000	0.02189500	3.58827100
H	-5.45954700	-0.91946800	1.66219200
C	-3.73528400	1.23078600	4.40184400
H	-2.01256700	1.22152700	3.09511500
C	-5.05353700	0.79593700	4.57229900
H	-6.69940200	-0.31347700	3.72581200
H	-3.25791300	1.83315500	5.16804200
H	-5.59734900	1.06132200	5.47384800
K	3.74447900	4.02636400	0.52150400
H	-0.26627500	4.68030700	-0.42202600

H	1.21514700	-1.07392300	-2.54757700
H	-0.00858500	0.95159200	-3.30437200

17Ru_O_C₂H₄, E= -2273.30182127 a.u.

Ru	-2.02688800	-1.08523900	-0.93211400
C	-3.83435100	-2.52420200	-0.74472100
C	-3.02132300	-2.74459900	-1.85317400
H	-2.31645100	-3.57787900	-1.88185200
C	-1.21116100	1.59659500	-1.70560800
O	-0.61454700	2.57507500	-2.17555200
N	-0.62435000	0.42226300	-1.28252100
C	0.74824900	0.22140000	-1.31903300
C	1.23436200	-1.07927300	-1.55206200
C	1.74290400	1.16841400	-1.01741100
C	2.57829700	-1.41389000	-1.53034100
C	3.09648700	0.85077900	-1.01387400
C	3.55465400	-0.44035600	-1.28577200
F	0.33796700	-2.08444900	-1.77382900
F	2.90933300	-2.69131200	-1.73262500
F	3.94607200	1.80804800	-0.63005100
F	1.41815900	2.39294400	-0.54155300
C	-2.67977800	1.61463400	-1.42105500
C	-3.25358100	0.48668300	-0.78089800
C	-3.42930900	2.77224100	-1.67405900
C	-4.55932600	0.61841300	-0.28299600
C	-4.74109200	2.86127600	-1.21173000
C	-5.28920900	1.79271500	-0.49045000
H	-5.02493100	-0.19664900	0.26149200
H	-5.33432000	3.74888200	-1.40850800
H	-6.30305800	1.86588400	-0.10650800
C	5.01040700	-0.81096600	-1.12451200
F	5.82399100	0.21517100	-1.40892300
F	5.35293600	-1.84352900	-1.90626900
F	5.25238800	-1.17972500	0.16366800
K	-0.78660300	3.81340800	0.30489000
C	-2.62436600	-1.25745400	2.08507100
C	-2.19137500	-1.72166000	3.47344100
C	-0.72429600	-3.32160500	2.60162700
C	-1.06626700	-2.93244400	1.16062000
H	-1.36581500	-1.10504900	3.85993200
H	-3.03888000	-1.61941100	4.15595800
H	-3.47459100	-1.84828600	1.74883400
H	-2.88347300	-0.20337800	2.04564700
H	0.16278700	-2.77494100	2.94973700

H	-0.50692500	-4.39229600	2.63222100
H	-0.20920700	-3.03594500	0.49224800
H	-1.88489900	-3.55371900	0.79887300
N	-1.55492000	-1.50501700	1.04722300
O	-1.83098000	-3.09364300	3.45679800
O	-0.30049400	-0.80734600	1.51327300
C	-0.27021600	0.52407800	1.77078300
O	-1.21481500	1.28901300	1.66063600
C	1.08485700	0.91802600	2.23559600
C	2.23012600	0.16235200	1.94116000
C	1.20291800	2.11022300	2.96973800
C	3.48535400	0.62332600	2.33213500
H	2.14074700	-0.75540800	1.37225600
C	2.45706100	2.55298200	3.38152900
H	0.30470500	2.65703300	3.24278200
C	3.59950300	1.81629000	3.05044700
H	4.36969800	0.06037200	2.05580000
H	2.54691900	3.46452700	3.96407600
H	4.57870800	2.17074800	3.35653900
H	-2.96850000	3.58063900	-2.23753100
H	-3.79077600	-3.19674800	0.10734200
H	-3.31471900	-2.36218500	-2.83490900
H	-4.76166300	-1.97412200	-0.84890900

TS18Ru_O_C₂H₄, E= -2273.29635153 a.u. Imaginary frequency = 262i

Ru	-2.02430200	-1.16337100	-0.81501500
C	-3.89393700	-2.58308900	-0.61244100
C	-2.93100800	-3.02298200	-1.50827500
H	-2.23537200	-3.82322100	-1.25423100
C	-1.22323900	1.45654100	-1.81354700
O	-0.61787200	2.39650600	-2.34338600
N	-0.64414200	0.30431500	-1.31785500
C	0.72922100	0.08416400	-1.33230300
C	1.19536300	-1.24072200	-1.43447700
C	1.74333800	1.03806000	-1.13384700
C	2.53251400	-1.59577800	-1.39603300
C	3.09287200	0.69804700	-1.11679800
C	3.52765400	-0.62000100	-1.26482800
F	0.28051300	-2.25187100	-1.53477500
F	2.83996800	-2.89271600	-1.46953400
F	3.96067500	1.67626500	-0.84636000
F	1.45434700	2.31120800	-0.78389300
C	-2.69339700	1.49516200	-1.54984100
C	-3.28093600	0.40822700	-0.85678600

C	-3.43685200	2.63252300	-1.89103400
C	-4.60568900	0.55642000	-0.42028400
C	-4.76407100	2.74131200	-1.47995800
C	-5.33414000	1.71170800	-0.72212600
H	-5.08843500	-0.22779100	0.15411800
H	-5.35181600	3.61460200	-1.74496800
H	-6.36181500	1.79854300	-0.38034600
C	4.97799600	-1.00528400	-1.08730800
F	5.80871700	-0.01718100	-1.44598100
F	5.29342800	-2.09469800	-1.80140600
F	5.22155700	-1.29199700	0.22002600
K	-0.66313300	3.83960100	0.03797700
C	-2.71070500	-0.88823900	2.10871100
C	-2.31680500	-1.16750900	3.55787500
C	-0.92096700	-2.94324500	2.96808600
C	-1.22143400	-2.76312000	1.47574600
H	-1.46457600	-0.54442700	3.86280900
H	-3.16682400	-0.92164500	4.19971100
H	-3.61521100	-1.45068100	1.86972100
H	-2.87838100	0.16666000	1.91384300
H	-0.01758600	-2.38883800	3.25026300
H	-0.75595100	-4.00649400	3.16117400
H	-0.35247200	-2.98767000	0.85411000
H	-2.04376500	-3.42804700	1.20134300
N	-1.69276500	-1.37847900	1.11953200
O	-2.03252300	-2.54329800	3.74952500
O	-0.24345400	-0.61061300	1.61184000
C	-0.15817700	0.70820800	1.73342400
O	-1.06781900	1.51478500	1.54317200
C	1.21517400	1.12175800	2.15970300
C	2.34037800	0.31988100	1.92055700
C	1.36682000	2.36611200	2.79205900
C	3.61055100	0.78393900	2.25743100
H	2.22067100	-0.64300400	1.43808900
C	2.63543800	2.81457800	3.15312800
H	0.48337000	2.95379500	3.02545000
C	3.75872700	2.02958800	2.87265400
H	4.47932500	0.17914700	2.02267900
H	2.75071100	3.76946900	3.65674600
H	4.74854800	2.38705100	3.13864500
H	-2.95935600	3.40945900	-2.48358000
H	-3.97447100	-3.01436300	0.38107200
H	-3.06510400	-2.85719300	-2.57998200
H	-4.77196900	-2.05796500	-0.96813600

17Ru_Cl_C2H4, E= -2313.44312601 a.u.

Ru	-1.53020700	-0.51419000	-1.15037500
C	-1.58440800	-0.37858400	-3.29014000
H	-1.64513300	-1.38587900	-3.70426600
C	-0.35369000	0.12315500	-2.84085700
H	0.54582500	-0.48966600	-2.89913500
C	-0.52421400	1.69717600	0.46051200
O	0.12824700	2.34730200	1.30485500
C	1.25062000	0.16302100	-0.09903600
C	2.34067500	1.04978300	-0.19301200
C	1.61145500	-1.19543000	-0.08456200
C	3.65538500	0.61789200	-0.12340100
C	2.92751800	-1.64450000	-0.06310900
C	3.99047800	-0.73632000	-0.05334000
F	2.14094400	2.37753300	-0.40155500
F	4.62118900	1.55052600	-0.15135600
F	3.12668000	-2.96220700	-0.03280100
F	0.62888400	-2.13141200	-0.10930500
C	-1.87157800	2.07541700	-0.00662900
C	-2.50338100	1.19088100	-0.91398000
C	-2.49668200	3.25387500	0.41657100
C	-3.76190200	1.54715200	-1.42046000
C	-3.75482000	3.58461400	-0.08057900
C	-4.37780600	2.73321100	-1.00297800
H	-4.27783300	0.89393700	-2.11911700
H	-4.24996500	4.49604500	0.23881400
H	-5.35690500	2.99297500	-1.39669000
C	5.45187200	-1.11727500	0.02181700
F	6.02342900	-0.53951500	1.10132700
F	6.11201500	-0.67901800	-1.06665000
F	5.63272000	-2.44000900	0.11692000
C	-1.90062500	-2.47813500	1.37126300
C	-2.85878200	-3.20394500	2.31256100
C	-4.20988000	-1.30698400	2.53233300
C	-3.32427800	-0.49004600	1.59707600
H	-3.62394700	-3.74131400	1.72954600
H	-2.30421100	-3.93622600	2.90465000
H	-1.09946000	-1.99395500	1.93938000
H	-1.44904000	-3.14844300	0.63967700
H	-5.03286900	-1.76757500	1.96219200
H	-4.64629400	-0.64896300	3.28784900
H	-3.88711200	0.24442600	1.02237800
H	-2.54542000	0.03630800	2.15985800

N	-2.54710500	-1.34322000	0.64763900
O	-3.45851400	-2.29494100	3.21890500
Cl	-3.65764100	-2.00497700	-0.65135100
N	-0.08215700	0.53465900	-0.12905700
K	1.99231900	3.97455200	1.84382700
H	-1.98776100	3.89078400	1.13491700
H	-2.36923100	0.30342900	-3.60954900
H	-0.17721200	1.19482100	-2.80340100

TS18'Ru_Cl_C2H4, E= -2313.43564946 a.u. Imaginary frequency = 260i

Ru	1.55147800	-0.47273100	1.03370500
C	1.53951700	0.06196300	3.15943400
H	2.28813500	-0.59769100	3.59989300
C	0.27822000	-0.42232600	2.82580400
H	0.01552400	-1.46460800	3.01403300
C	0.41659600	1.75669600	-0.47861600
O	-0.29850500	2.40825700	-1.26936800
C	-1.28628400	0.16179800	0.09659100
C	-2.40061500	1.00685600	0.25788300
C	-1.60311800	-1.20256000	-0.00076900
C	-3.70201700	0.53846200	0.17852100
C	-2.90470300	-1.69221300	-0.03124500
C	-3.99528100	-0.81963900	0.03249000
F	-2.23596100	2.32671500	0.53396100
F	-4.69592300	1.43750900	0.27016400
F	-3.06321900	-3.01078700	-0.14494400
F	-0.59022500	-2.10315200	-0.06529300
C	1.77980600	2.15455200	-0.08244700
C	2.46692300	1.28110200	0.78826900
C	2.35721200	3.35746100	-0.50868400
C	3.72470200	1.66898800	1.27044000
C	3.62060800	3.71674200	-0.04878200
C	4.29430400	2.87531700	0.84788200
H	4.27182300	1.02601300	1.95454200
H	4.07960800	4.64562100	-0.37185900
H	5.27523400	3.16054300	1.21860200
C	-5.44520900	-1.24171800	-0.04726900
F	-6.04627000	-0.62734800	-1.09018500
F	-6.10548900	-0.87979700	1.06870200
F	-5.58687200	-2.56264700	-0.20811900
C	2.05730600	-2.43178800	-1.26961200
C	3.08190300	-3.21617700	-2.08895400
C	4.45460100	-1.33937600	-2.32122400
C	3.50655700	-0.46807900	-1.50393800

H	3.79375600	-3.71612200	-1.41434800
H	2.56581900	-3.98112000	-2.67441100
H	1.29676100	-1.99950800	-1.93113200
H	1.55826500	-3.06052900	-0.53190300
H	5.23064200	-1.76134400	-1.66366700
H	4.94504400	-0.72549700	-3.08069900
H	4.02966100	0.29560900	-0.93167900
H	2.78174000	0.03318300	-2.15900700
N	2.63326200	-1.24357700	-0.58296000
O	3.75350400	-2.36748200	-3.00070100
Cl	3.80714500	-1.93437300	0.86573900
N	0.03330200	0.58220500	0.12743500
K	-2.25831200	3.95050800	-1.70791400
H	1.80327700	3.99143700	-1.19545300
H	1.71025200	1.12252000	3.31566400
H	-0.56056400	0.25891400	2.71723900

17Ru_Cl_C2H4, E= -2313.44425519 a.u.

Ru	-1.58398400	-0.48334000	-1.29577000
C	-1.47524800	0.58304400	-3.22046700
H	-2.43680600	0.49694100	-3.72339000
C	-0.57037800	-0.47999800	-3.21622700
H	-0.80657600	-1.41369700	-3.72868400
C	-0.67931100	1.75846500	0.28292600
O	-0.02732100	2.41420400	1.11641600
N	-0.17767400	0.69080900	-0.43558600
C	1.14468400	0.29947500	-0.35585800
C	2.24869300	1.17206100	-0.29233200
C	1.49094600	-1.06265700	-0.41654100
C	3.54492500	0.70960500	-0.12883000
C	2.79128200	-1.53745200	-0.30312300
C	3.85882000	-0.65119900	-0.12553000
F	2.08780100	2.51354700	-0.42618100
F	4.51735300	1.62672500	0.00915300
F	2.97109000	-2.85701500	-0.35107200
F	0.50304700	-1.98363200	-0.61042500
C	-2.09811200	2.01588400	-0.04144300
C	-2.72377400	1.12461800	-0.94221500
C	-2.79798100	3.09750300	0.50796400
C	-4.04376800	1.37870900	-1.33095800
C	-4.12212600	3.31958900	0.13930200
C	-4.73681100	2.46520300	-0.78625200
H	-4.54505600	0.72760400	-2.04439900
H	-4.67466200	4.15518400	0.55672800

H	-5.76585500	2.64681300	-1.08435200
C	5.30049500	-1.06228900	0.06829400
F	5.76268600	-0.57836800	1.24288800
F	6.07450700	-0.55384500	-0.90876000
F	5.45716000	-2.39130000	0.07859800
K	1.91089200	3.77892400	2.01687100
C	-3.63790200	-0.94727300	1.10493200
C	-4.21472300	-1.81005800	2.22303100
C	-2.91826000	-3.65208300	1.59970000
C	-2.27383400	-2.87701700	0.44948900
H	-3.65137400	-1.66527100	3.15632400
H	-5.25206700	-1.51391400	2.39942500
H	-4.26707900	-1.03609600	0.21418300
H	-3.58183400	0.10605100	1.37766800
H	-2.29385700	-3.58324500	2.50245700
H	-2.99992400	-4.70487500	1.31698500
H	-1.24979000	-3.20255700	0.26606700
H	-2.87258000	-3.03489500	-0.45669400
N	-2.27019800	-1.38376700	0.65217300
O	-4.22999900	-3.18001100	1.84925600
Cl	-1.11609100	-1.03741600	2.05914400
H	-2.29077900	3.74767800	1.21487500
H	0.49164100	-0.29736700	-3.06299000
H	-1.13633300	1.60250300	-3.06082600

TS18Ru_Cl_C2H4, E= -2313.43638994 a.u. Imaginary frequency = 114i

Ru	-1.67414200	-0.51415400	-1.25986100
C	-1.71431500	0.58013900	-3.29895600
H	-2.74134600	0.59546200	-3.65288000
C	-0.94342100	-0.56529300	-3.38814800
H	-1.34301600	-1.47275600	-3.84155400
C	-0.81316100	1.78002900	0.23415200
O	-0.16865600	2.41208000	1.08048500
N	-0.28114000	0.74327900	-0.54017100
C	1.06403600	0.41335400	-0.50564500
C	2.12211000	1.34173800	-0.38951400
C	1.48908800	-0.92067000	-0.65103400
C	3.44037200	0.93244000	-0.23727100
C	2.81224900	-1.33243900	-0.55303800
C	3.83010700	-0.40513800	-0.31348500
F	1.89997500	2.67379200	-0.40703600
F	4.35540800	1.88816000	0.00221000
F	3.05920800	-2.63612800	-0.66837400
F	0.56287100	-1.89148100	-0.88943500

C	-2.24320900	2.00042300	-0.05190300
C	-2.87963000	1.04904500	-0.87810100
C	-2.94854800	3.08846300	0.47755600
C	-4.22656000	1.23236700	-1.20492800
C	-4.29420500	3.25123900	0.15986900
C	-4.92533800	2.32797200	-0.68442700
H	-4.74391600	0.52578300	-1.85103800
H	-4.85226300	4.09306100	0.55647000
H	-5.97327000	2.46127200	-0.93870200
C	5.28412100	-0.75298000	-0.09004200
F	5.65591500	-0.36772200	1.15424900
F	6.07111000	-0.10206000	-0.96410000
F	5.52101800	-2.06407700	-0.20395800
K	1.88159100	2.73043500	2.55945100
C	-3.41252000	-0.99109700	1.25230200
C	-3.76305700	-1.85739100	2.46084400
C	-2.46109100	-3.63313000	1.70035400
C	-2.04009800	-2.86622900	0.44178600
H	-3.07457700	-1.65091700	3.29101900
H	-4.77964400	-1.61461200	2.78124400
H	-4.19293000	-1.11135100	0.49151700
H	-3.35319000	0.06407600	1.51376100
H	-1.71773800	-3.48500800	2.49471400
H	-2.51140000	-4.69824400	1.45931500
H	-1.02414100	-3.12514400	0.14473500
H	-2.73737600	-3.14016600	-0.36341600
N	-2.13925100	-1.37264500	0.56413600
O	-3.75053400	-3.23467300	2.12194300
Cl	-0.68152300	-0.94570200	2.06805700
H	-2.42885600	3.79081900	1.12226300
H	0.14153900	-0.51813400	-3.31936200
H	-1.26480900	1.55218300	-3.12214500

9Rh(IV), E= -1532.82886568 a.u.

Rh	0.96724100	-0.35425000	0.03202600
C	1.21454400	-1.00569500	-2.09013600
C	2.50939000	-1.08690600	-1.47972800
C	2.44012100	-2.05108800	-0.41934400
C	0.37954800	-2.02988000	-1.48372400
C	1.12594800	-2.66907100	-0.47094500
C	0.66883100	-3.87286400	0.30064000
H	0.66118100	-4.75558200	-0.35100200
H	1.32999500	-4.09999700	1.13993600
H	-0.34718700	-3.74741400	0.68739500

C	3.57549500	-2.49735700	0.45491200
H	3.22422500	-2.77543300	1.45258700
H	4.08554700	-3.37028000	0.02779600
H	4.31636700	-1.70416200	0.57847400
C	3.73212800	-0.35402500	-1.94097700
H	3.50214500	0.67492900	-2.22279300
H	4.50397400	-0.32240700	-1.16979900
H	4.15542800	-0.86267900	-2.81582900
C	0.81093700	-0.13179500	-3.24056200
H	1.48418500	0.72335500	-3.33442300
H	0.83675100	-0.68974200	-4.18489900
H	-0.20079400	0.25370900	-3.08892500
C	-1.00912100	-2.39890000	-1.90674500
H	-1.47534900	-1.60034800	-2.48237300
H	-0.98424300	-3.30269900	-2.52925300
H	-1.64577600	-2.61080000	-1.04252800
C	-0.62040600	2.15076700	-0.29025500
O	-1.58508900	2.91456700	-0.27328100
N	-0.68107100	0.78406000	-0.34962800
C	0.81456700	2.55298000	-0.19996400
C	1.74547900	1.53296400	0.05443000
C	1.19803000	3.89546700	-0.23390800
C	3.07205800	1.88219100	0.31530300
C	2.53239300	4.23296500	-0.00919600
H	0.43440800	4.64670900	-0.41519800
C	3.46246300	3.22733600	0.27545100
H	3.80528600	1.11899000	0.56025300
H	2.84586100	5.27261200	-0.03511500
H	4.49840600	3.48969900	0.47683300
O	-1.97976500	0.27885600	-0.08905200
C	-2.84640600	0.33020600	-1.14618500
O	-2.51904600	0.55213000	-2.28836200
C	-4.27549600	0.09371800	-0.65218500
C	-4.74151400	1.42360200	-0.01280200
H	-5.76478200	1.31114000	0.36195300
H	-4.08576800	1.71024200	0.81218500
H	-4.72277500	2.23499100	-0.74536700
C	-4.32287400	-1.03755700	0.39530600
H	-5.35968600	-1.20250400	0.70664900
H	-3.94407800	-1.97844800	-0.01985500
H	-3.73436600	-0.79197900	1.28210300
C	-5.15795400	-0.25834400	-1.85877000
H	-5.10214400	0.52103500	-2.62166000
H	-4.83996800	-1.19937300	-2.31937000

H	-6.19921300	-0.36689600	-1.53850700
C	0.51614700	-1.45835100	2.82469700
C	-0.99597100	-1.62658900	3.09333800
C	-1.27284800	0.71272400	3.08562600
C	0.22664300	0.89341800	2.76222600
H	-1.51367700	-1.75610000	2.12933200
H	-1.17951400	-2.50434400	3.72126300
H	1.02519700	-1.35122000	3.79487200
H	0.91527800	-2.33545900	2.31885300
H	-1.84838600	0.73353800	2.15378900
H	-1.61367600	1.52136100	3.73800900
H	0.38106600	1.81079100	2.19707600
H	0.77958700	0.97055200	3.71067900
N	0.71164400	-0.26315500	2.02344800
O	-1.49812100	-0.50434800	3.79443500