Hypercoordinate β-Carbon in Grubbs and Schrock Olefin Metathesis Metallacycles

Premaja R. Remya and Cherumuttathu H. Suresh

Chemical Sciences and Technology Division, Academy of Scientific & Innovative Research, CSIR-National Institute for Interdisciplinary Science and Technology, Thiruvanathapuram, 695 019, India

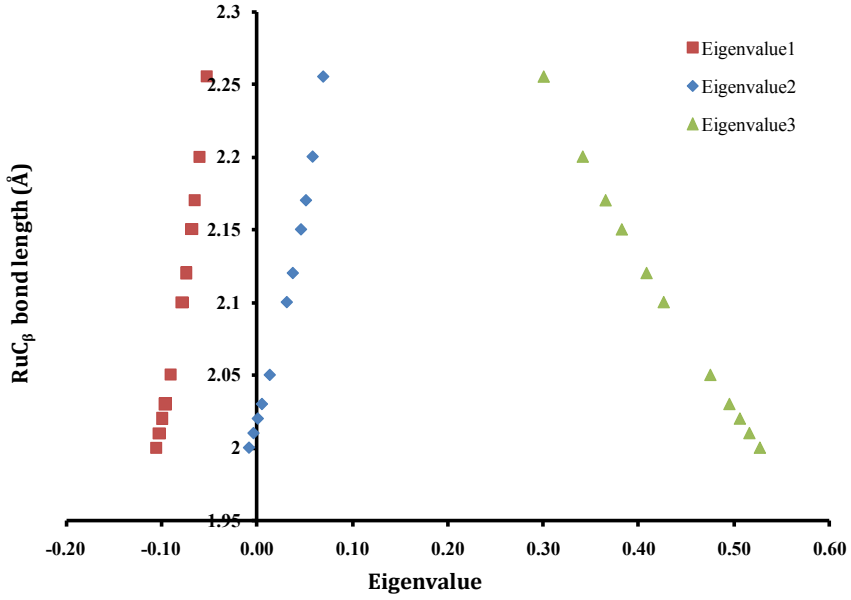
Supporting information

Contents

i) **Constrained geometry of 2**

In order to confirm the catastrophe nature of RCP in **2**, we manually decreased the RuC_{β} distance and optimized the geometry by freezing the Ru and C_{β} coordinates. Table S1 shows the change in RuC_{α} and $C_{\alpha}C_{\beta}$ distance with RuC_{β} distance and their corresponding SCF energy. It is noted that the structure which showed hypercoordianted C_{β} is less stable by 11.02 kcal/mol than the minimum energy structure. Table S1 depicts the eigenvalues at the RCP. With decrease in the RuC_{β} distance, the negative eigenvalue becomes more negative, the positive eigenvalue close to zero becomes smaller and ultimately changes sign and the second positive eigenvalue becomes more positive changing from 0.300 to 0.516 au at the BCP. These changes are graphically represented in Fig. S1.

ii) **Fig. S1** Plot showing correlation between eigenvalues and RuC_β bond length.

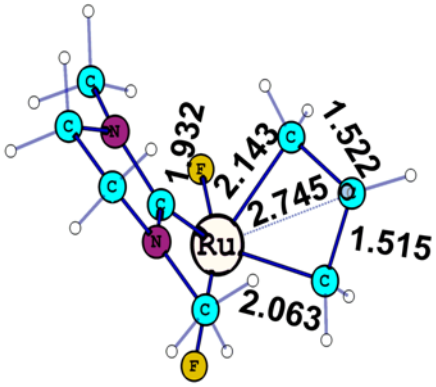


iii) **Table S1**: Distance parameters (Å) SCF energy and eigenvalues at the catastrophe RCP / RuC_β BCP in AIM analysis for **2** with various RuC_β distances.

Distance parameters(Å)			E_{SCF} (au)	Eigenvalues (au) at the RCP /BCP			Nature of critical point
RuC_β	RuC_α	$C_\alpha C_\beta$		Eigenvalue1	Eigenvalue2	Eigenvalue3	
2.255	1.963	1.582	-1439.7588	-0.0526	0.0693	0.3000	(3,+1)
2.200	1.95	1.576	-1439.7580	-0.0600	0.0582	0.3410	(3,+1)
2.170	1.944	1.572	-1439.7569	-0.0647	0.0512	0.3650	(3,+1)
2.150	1.94	1.57	-1439.7558	-0.0682	0.0460	0.3820	(3,+1)
2.120	1.934	1.566	-1439.7538	-0.0739	0.0374	0.4080	(3,+1)
2.100	1.93	1.564	-1439.7521	-0.0781	0.0311	0.4260	(3,+1)
2.050	1.922	1.558	-1439.7465	-0.0901	0.0132	0.4750	(3,+1)
2.030	1.919	1.556	-1439.7437	-0.0957	0.0050	0.4950	(3,+1)
2.020	1.918	1.555	-1439.7422	-0.0986	0.0007	0.5060	(3,+1)
2.010	1.917	1.554	-1439.7406	-0.1020	-0.0039	0.5160	(3,-1)
2.000	1.915	1.553	-1439.7389	-0.1050	-0.0086	0.5270	(3,-1)

iv) **Fig. S2** Optimized geometry of the 14-electron non-agostic complexes **1'**, **3' - 5'**, **7'- 16'**.

<$C_\alpha C_\beta C_\alpha$ =96.4°



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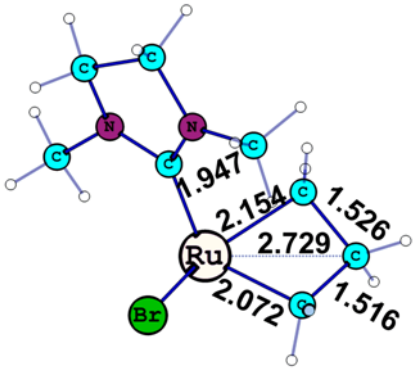
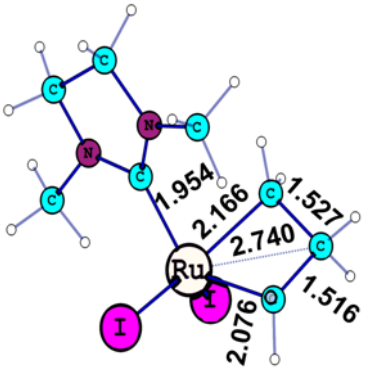
<$C_\alpha C_\beta C_\alpha$ =97.9°



3'

<$C_\alpha C_\beta C_\alpha$ =98.5°



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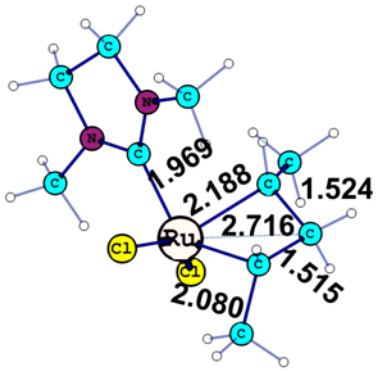
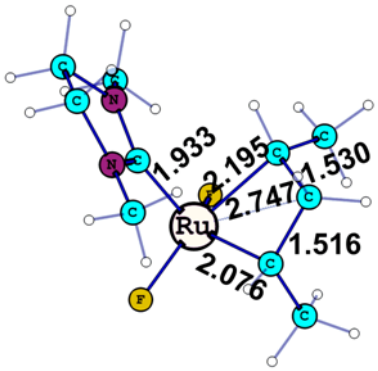


5'

<$C_\alpha C_\beta C_\alpha$ =99.7°



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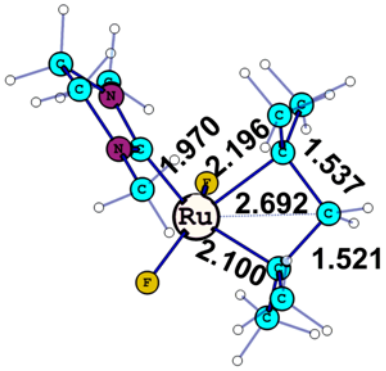
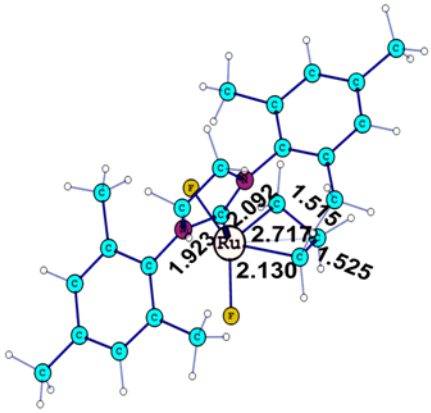


8'

<$C_\alpha C_\beta C_\alpha$ =96.2°



9'

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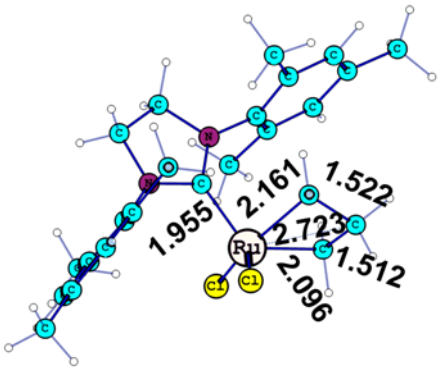
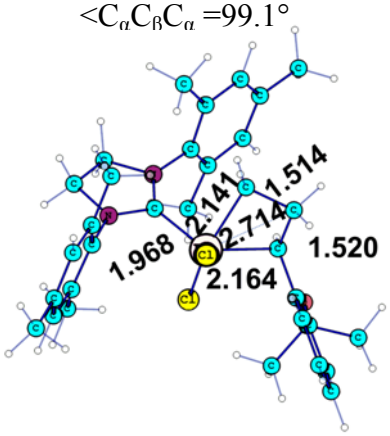


10'

<$C_\alpha C_\beta C_\alpha$ =99.1°



11'

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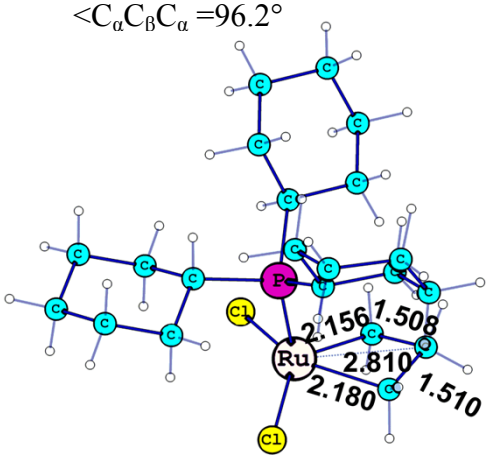
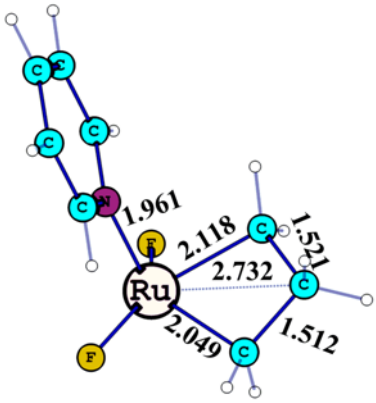


12'

<$C_\alpha C_\beta C_\alpha$ =96.5°



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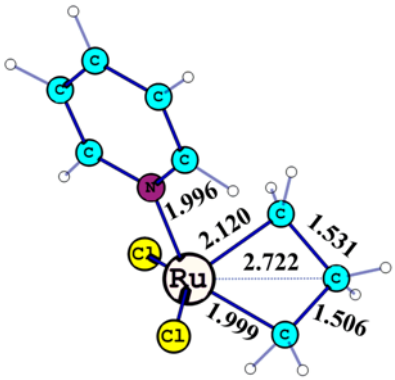
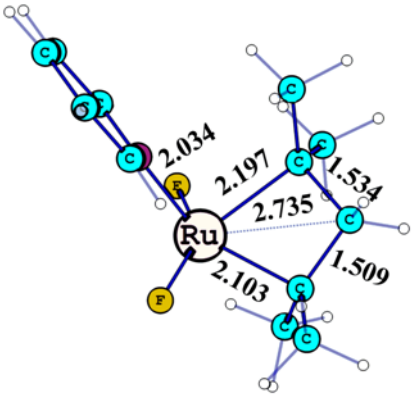
<$C_\alpha C_\beta C_\alpha$ =96.1°



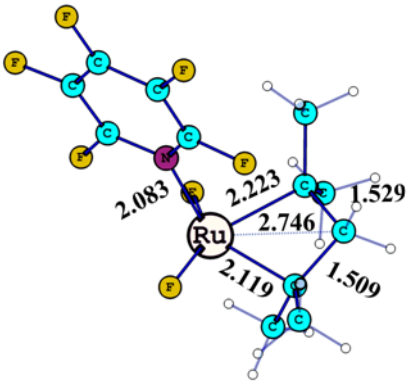
14'

<$C_\alpha C_\beta C_\alpha$ =102.2°



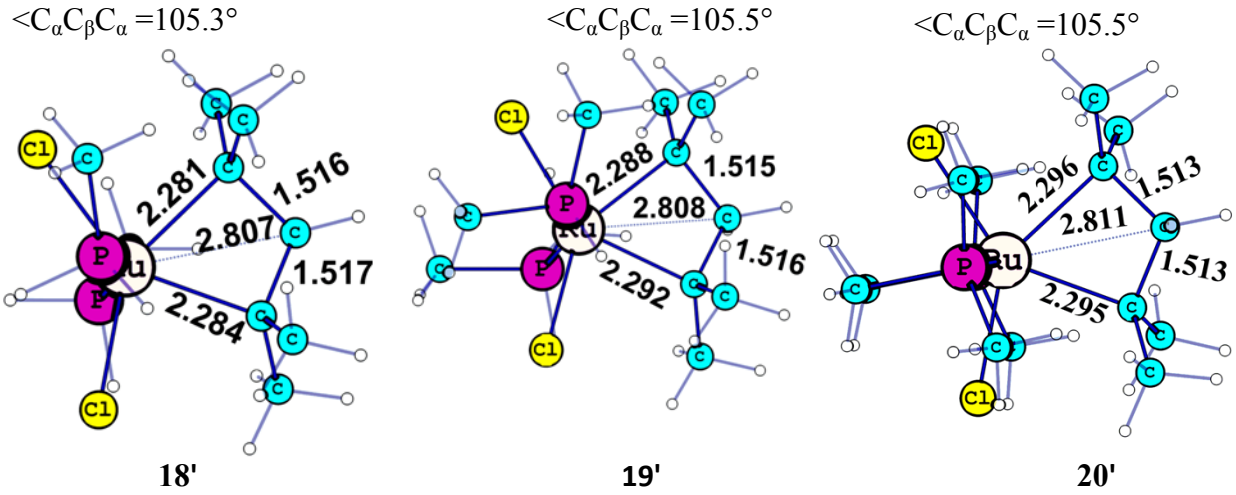
15'

<$C_\alpha C_\beta C_\alpha$ =102.3°



16'

v) **Fig. S3**. Optimized geometries of 16-electron non-agostic complexes **18' - 20'**

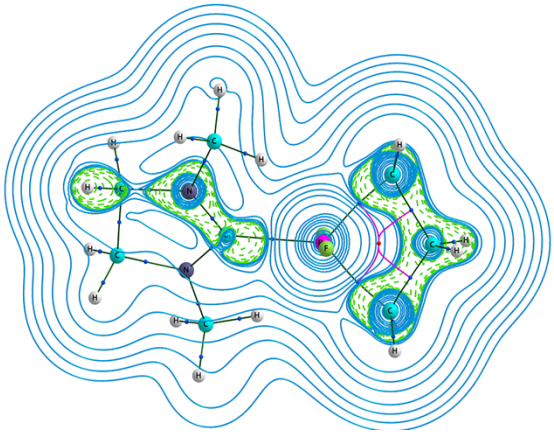


18' **19'** **20'**

vi) **Table S2:** Energy comparison between agostic and non-agostic complexes

MCB	$E_{Agostic}$ (au)	$E_{Non\text{-}agostic}$ (au)	$E_{non\text{-}agostic}$-$E_{agostic}$ (kcal/mol)
1	-718.9606	-718.9657	-3.206
2	-1439.7588	-1439.7463	7.834
3	-5668.1130	-5668.0967	10.246
4	-1114.9415	-1114.9216	12.431
5	-1518.4131	-1518.3993	8.666
6	-1597.0555	-1597.0379	11.051
7	-797.6202	-797.6183	1.194
8	-876.2718	-876.2672	2.862
9	-1338.5435	-1338.5333	6.361
10	-2059.3336	-2059.3083	15.903
11	-2483.6792	-2483.6621	10.695
12	-2181.0565	-2181.0468	6.142
13	-1381.9828	-1381.9617	13.251
14	-661.1905	-661.1808	6.116
15	-818.5049	-818.4986	3.988
16	-1314.8752	-1314.8648	6.551
17	-1977.3055	-1977.3085	-1.875
18	-2055.9799	-2055.9758	2.576
19	-2134.6462	-2134.6489	-1.693
20	-2213.2992	-2213.3156	-10.253
21	-2058.2300	-2058.2398	-6.180

vii) **Fig. S4**. Contour maps of the Laplacian of electron density in the plane of metallacycle, along with the molecular graphs of 14-electron agostic models **1 -16**.



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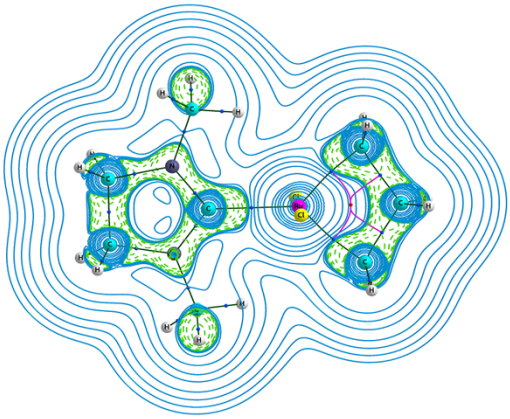

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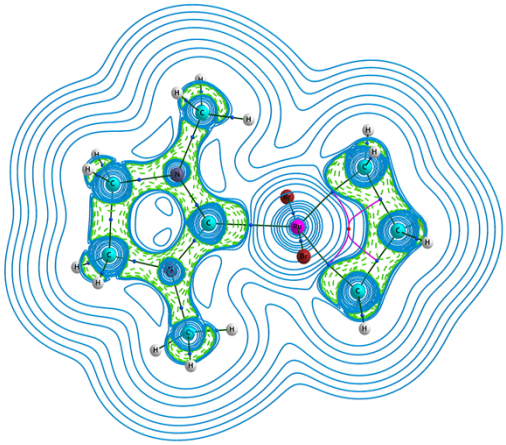

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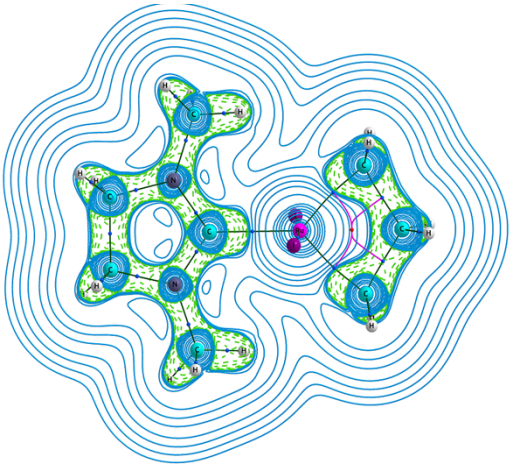

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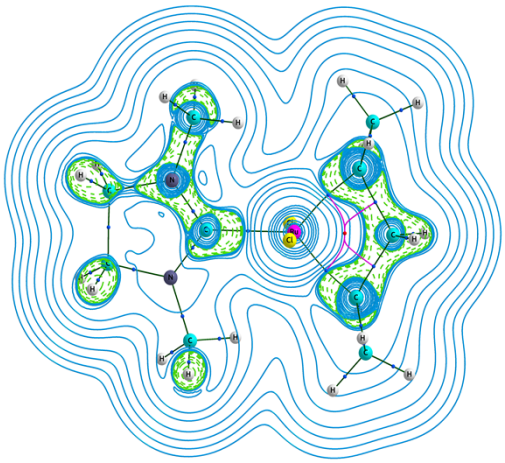

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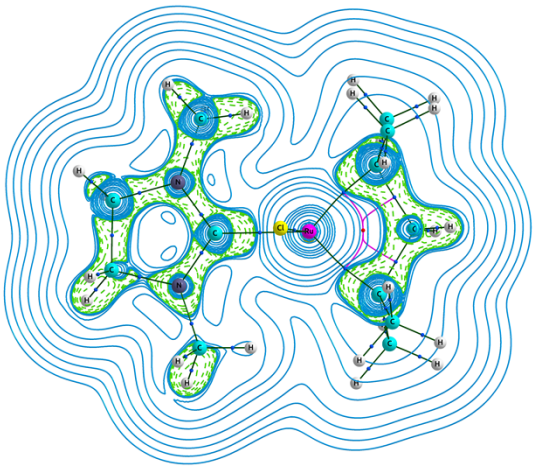

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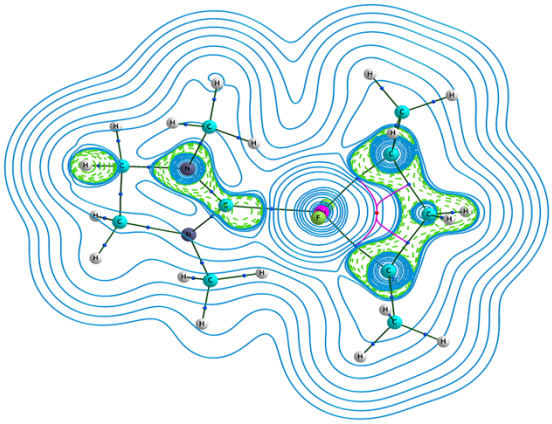

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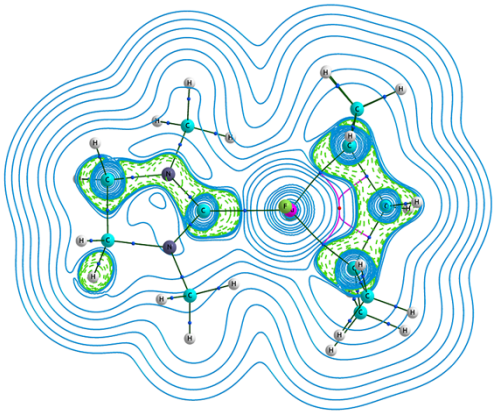

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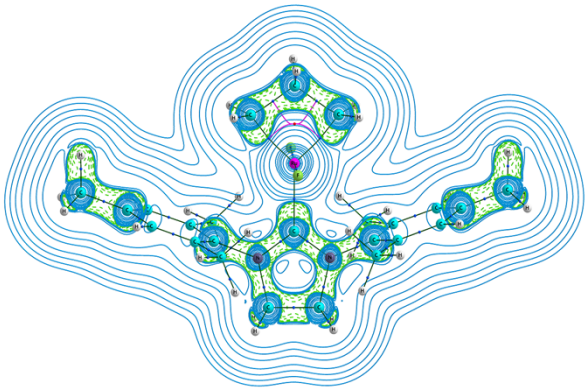

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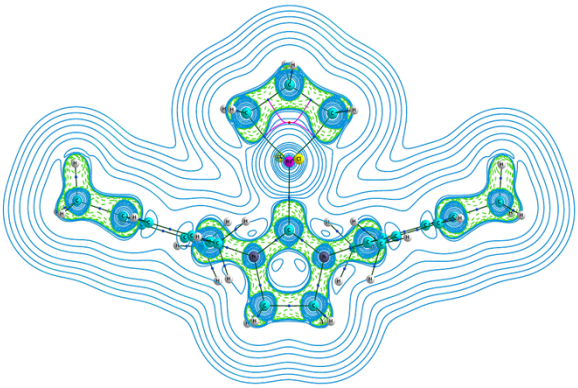

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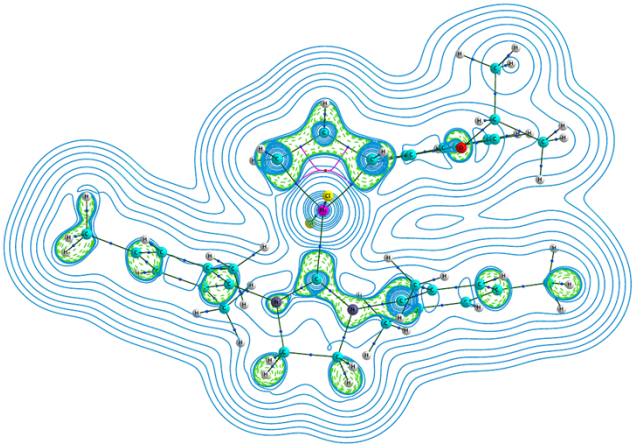

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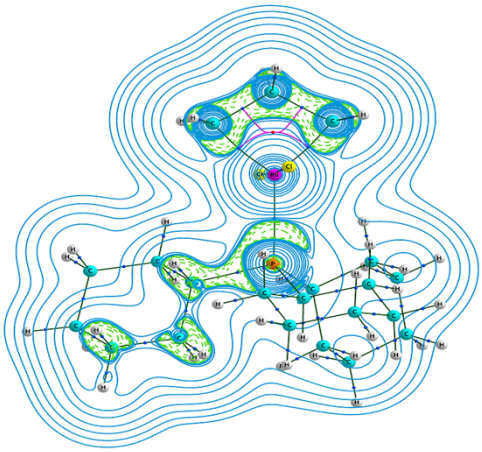

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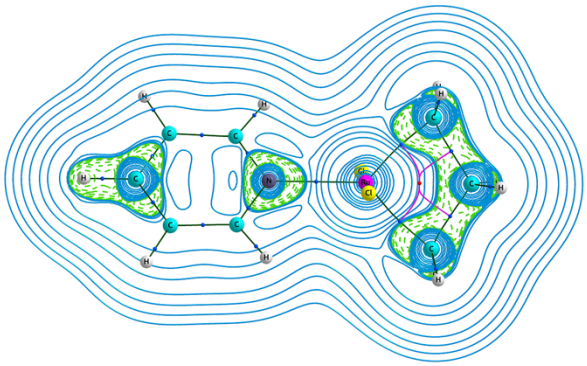

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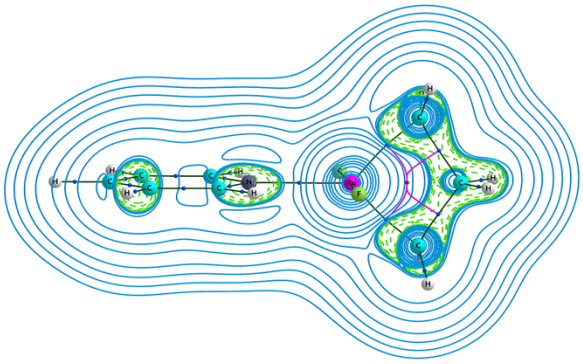

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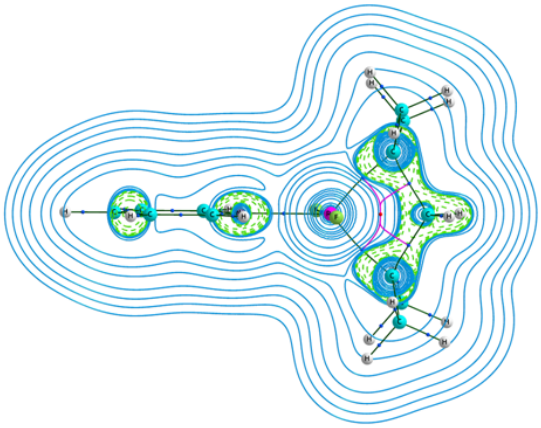

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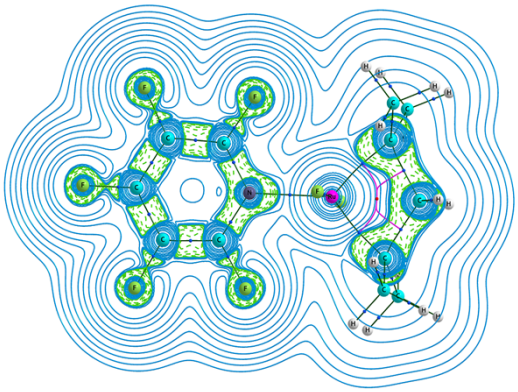
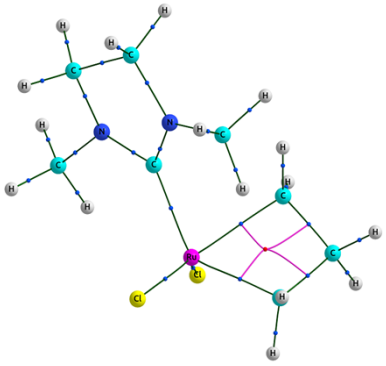


16

viii) **Fig. S5**. Molecular graphs of non-agostic 14-electron models **1' -16'**



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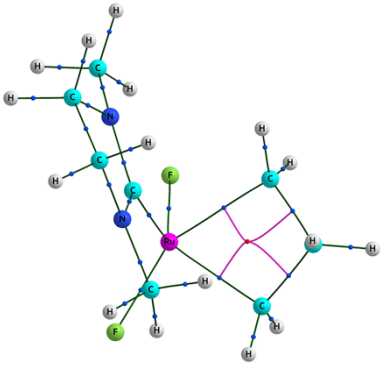

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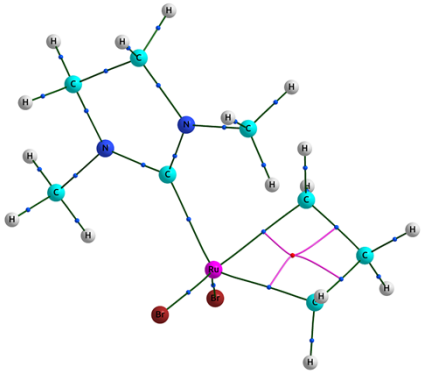

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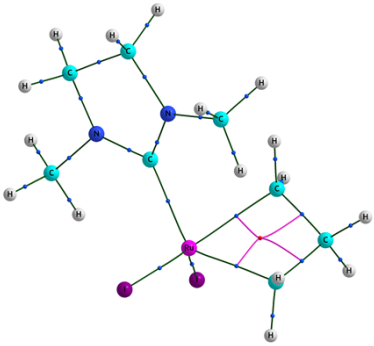

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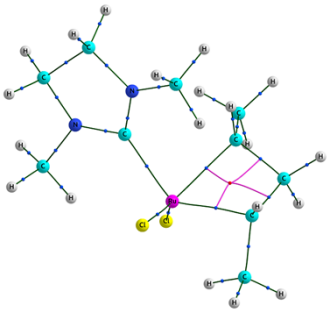

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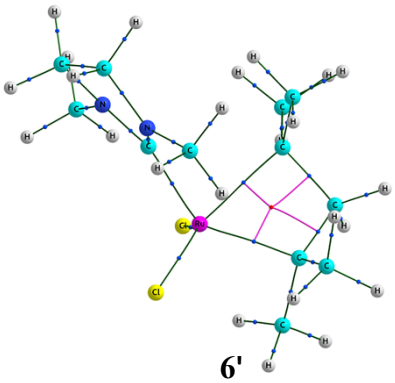

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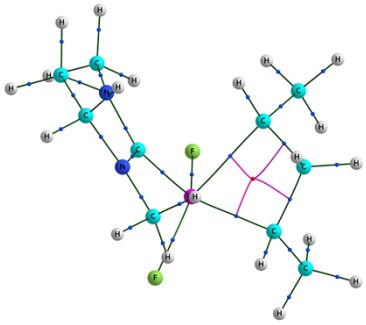

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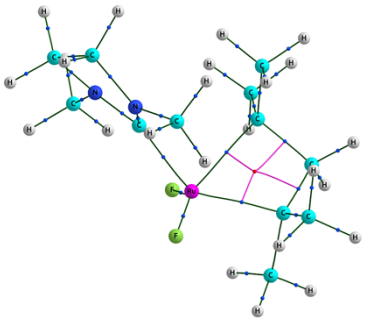

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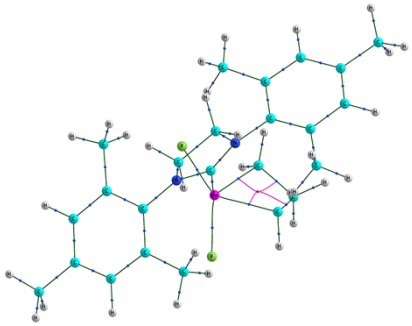

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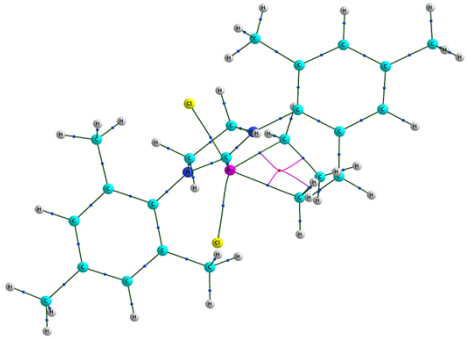

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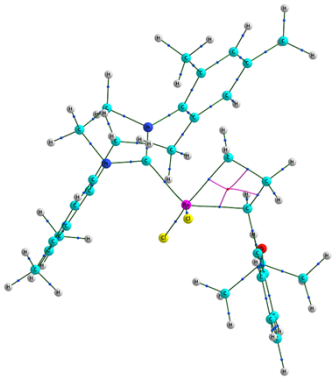

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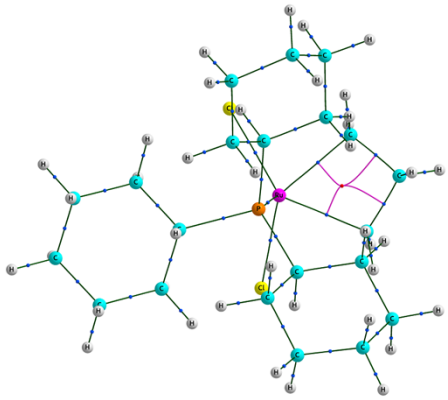

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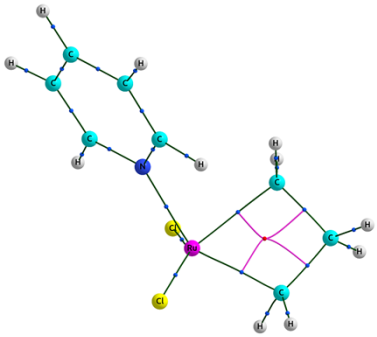

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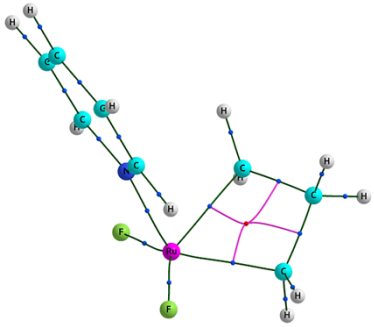
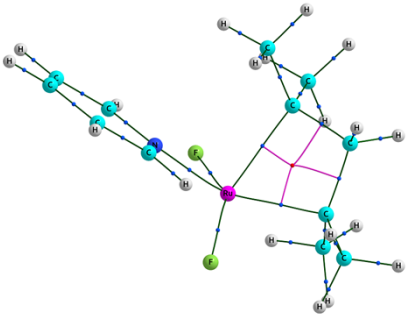
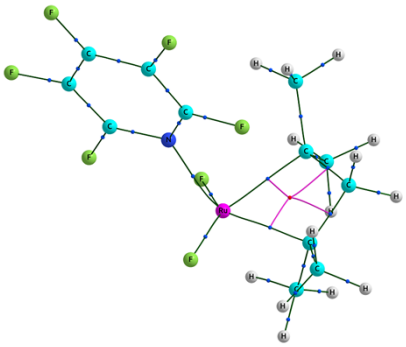


14'

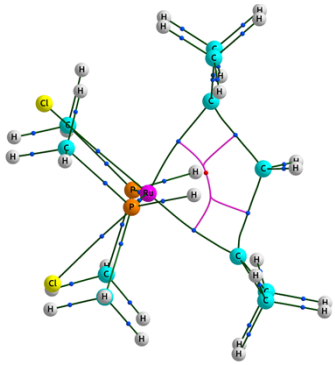


15'

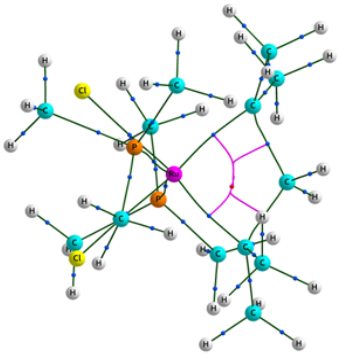


16'

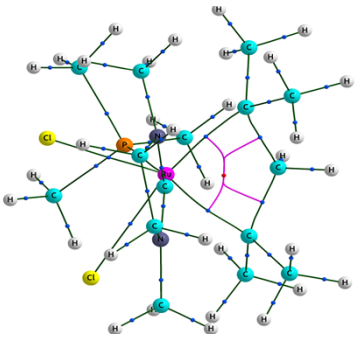
ix) **Fig. S6**. Molecular graphs of 16-electron agostic complexes **19 -21** and non-agostic models **17' -21'**



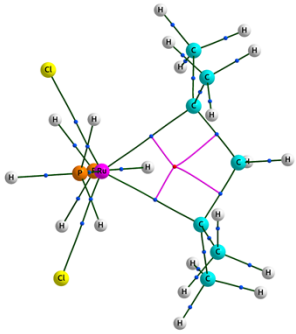
19



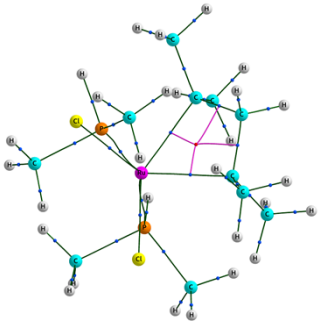
20



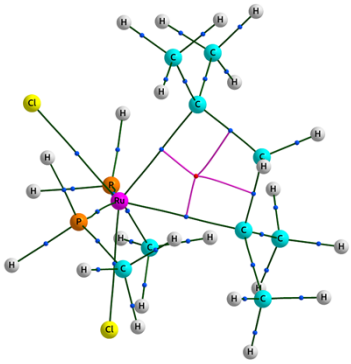
21



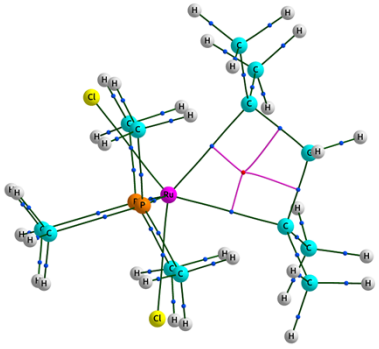
17'



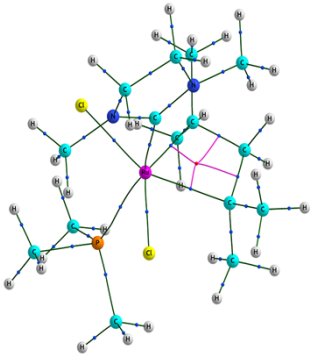
18'



19'

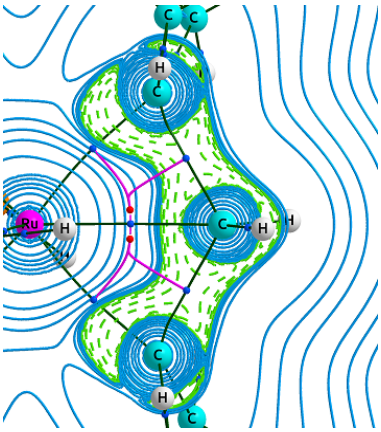


20'

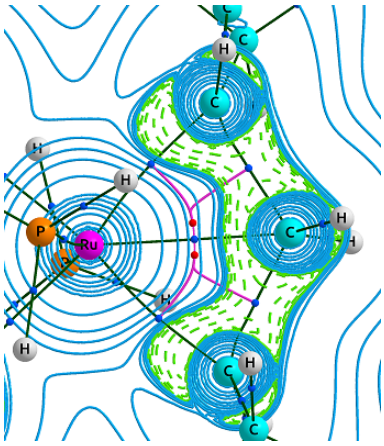


21'

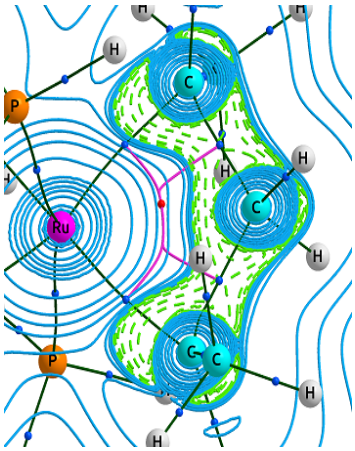
x) **Fig. S7**. Contour map of the Laplacian of electron density in the plane of the metallacycle along with molecular graph of models **17- 21** showing significantly strong RuC_{β} interaction.



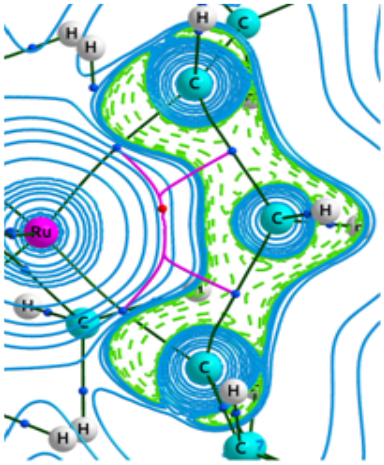
17



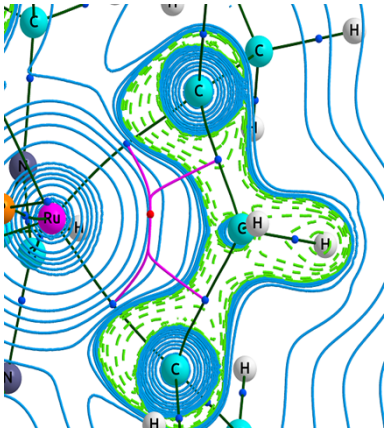
18



19

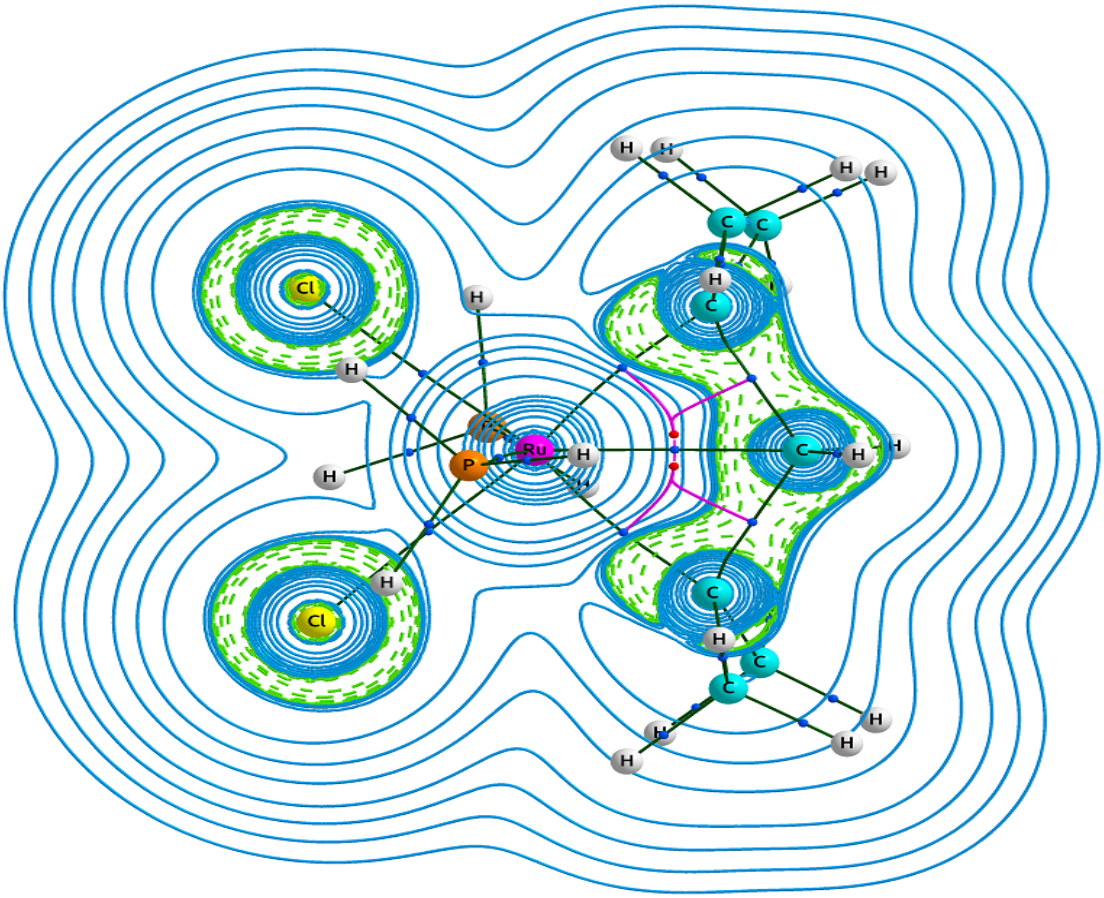


20

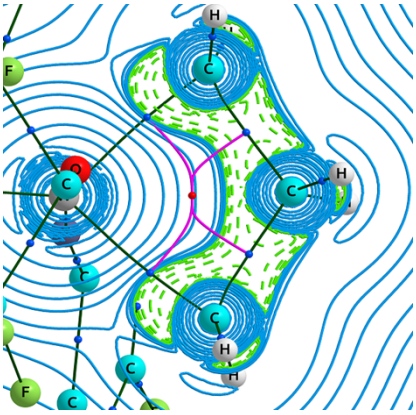


21

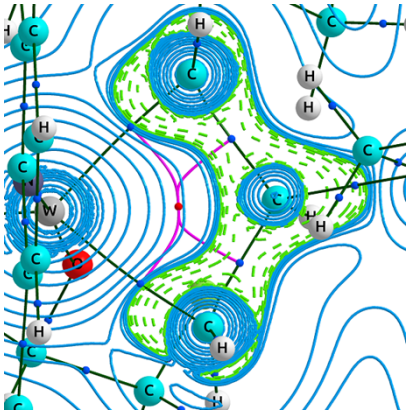
xi) **Fig. S8**. Complete contour map of the Laplacian of electron density in the plane of the metallacycle along with molecular graph of model **17** showing five bond critical points around C_{β}.



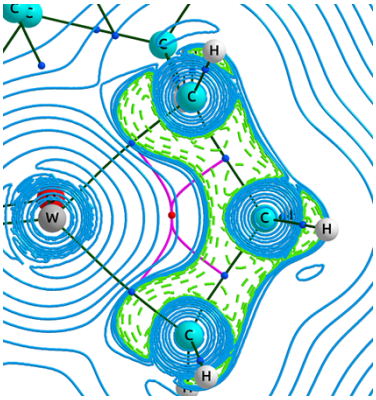
xii) **Fig. S9**. Contour map of the Laplacian of electron density in the plane of the metallacycle along with molecular graph of crystal structures of tungstenacyclobutanes. (Only metallacycle is shown)



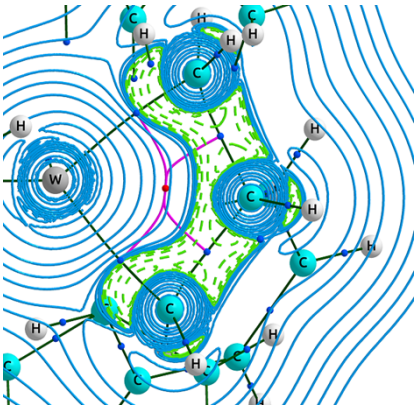
CEQDAF



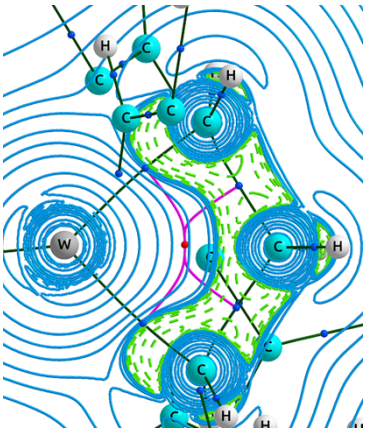
CETCOU



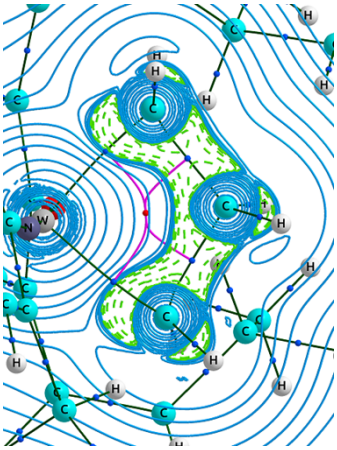
NEZZIC



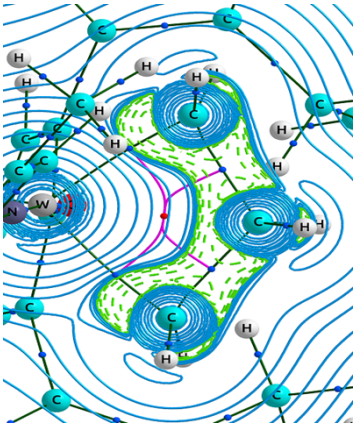
OZAKOO



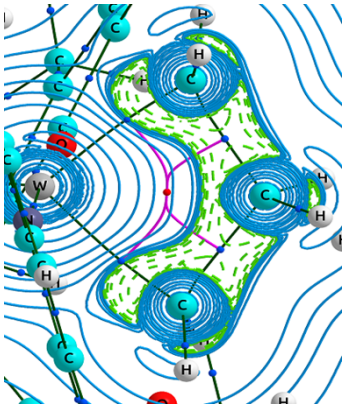
UHOYEW



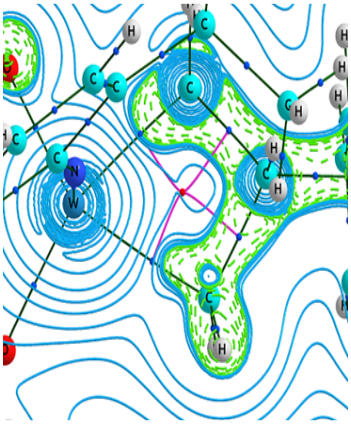
NUHSUF



OZAKIK

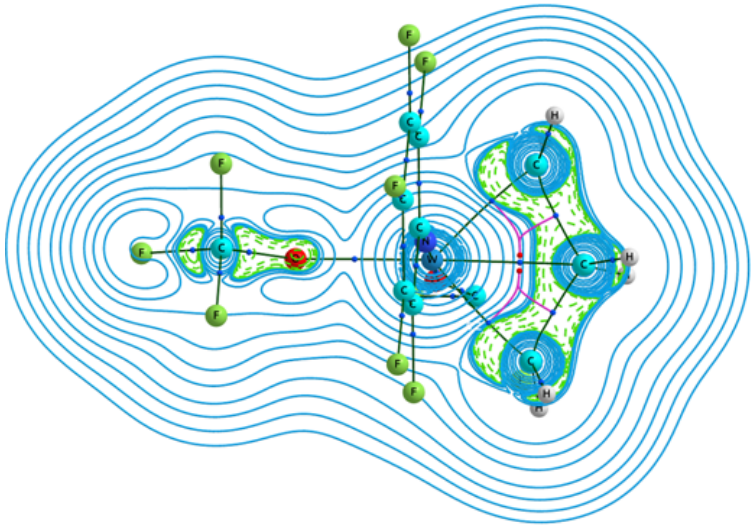


UHOYOG



WUWNOR

xiv) **Fig. S10**. Contour map of the Laplacian of electron density in the plane of the metallacycle along with molecular graph for the constrained geometry of **23** showing fifth BCP for C_β.

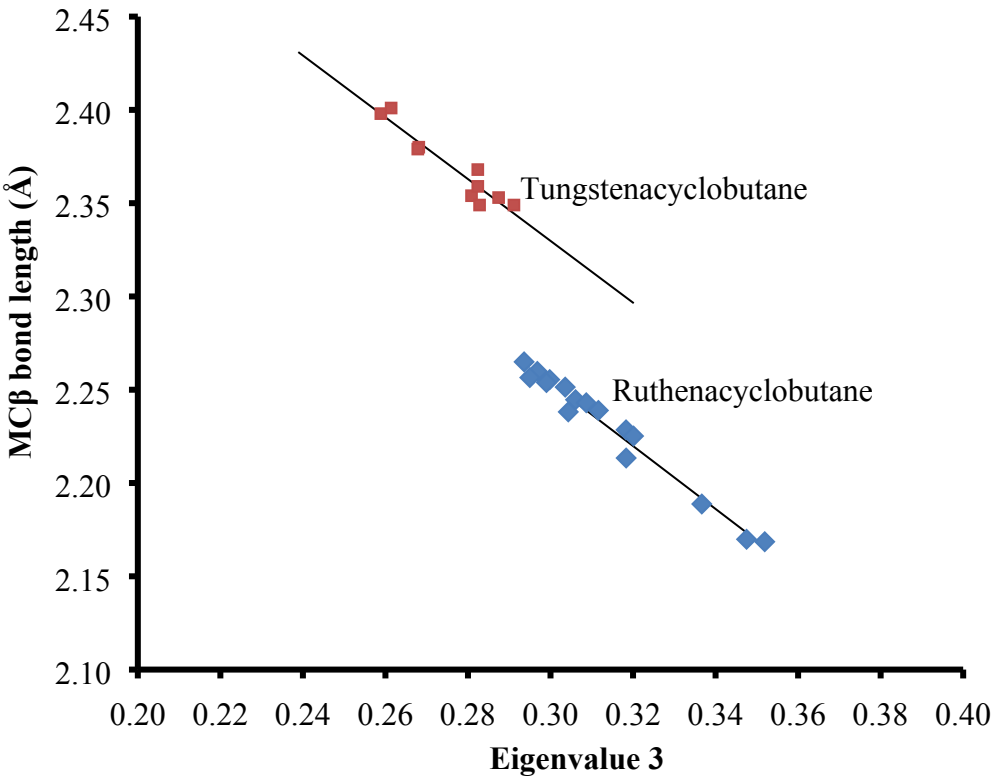


WC_β distance is constrained manually and optimized the other structural parameters. At a WC_β distance of 2.170 Å, the catastrophe RCP separates to one BCP and two RCPs revealing the fifth bond path for C_β.

xiv) Eigenvalues at the RCP

Eigenvalue at the catastrophe RCP is analyzed to understand how it varies with the MC_β interaction. Table S2 depicts the eigenvalues at the catastrophe point for the ruthenium system **1 - 21,** tungsten system **22, 23** and the crystal structures. Among them one is negative and varies from -0.0407 to -0.1087 au. Second and third are positive and they lie in the range 0.0154 – 0.0723 au and 0.2477 – 0.3519 au, respectively. The most positive eigenvalue (eigenvalue 3) shows a linear correlation with the MC_β distance (Fig. S11). These results and the results given in section (ii) suggest that a catastrophe RCP can be identified by its two positive eigenvalues, one should be close to zero and the other should be significantly more positive, typically above 0.24 au. This argument can be further supported by the eigenvalue data given in Table S3 for non-agostic complexes **1' -21'**where the RuC_β distance around 2.8 Å indicates no significant interaction between metal and C_β. In these cases, all three eigenvalues are close to zero.

xv) **Fig. S11** Plot showing correlation between highest eigenvalue (eigenvalue3) and MC_β distance.



xvi) **Table S3**. Eigenvalues at the catastrophe RCP in the metallacycle region of agostic complexes.

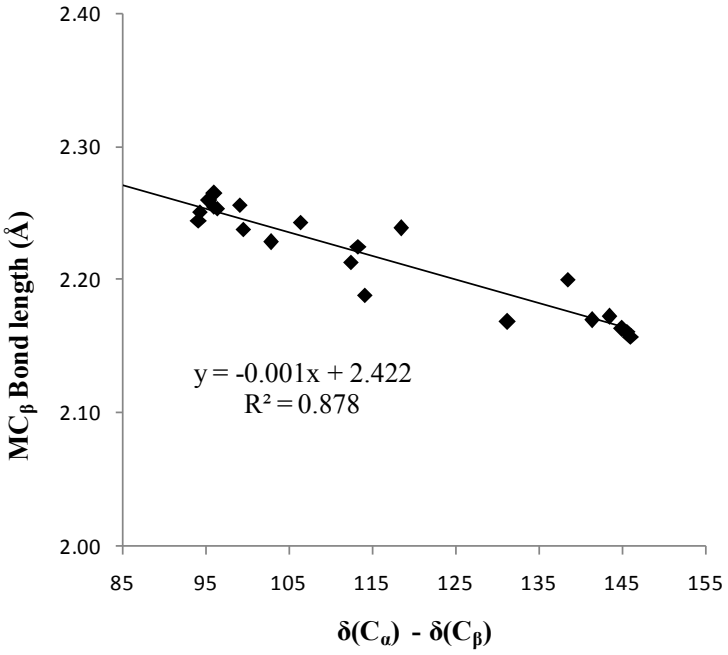
MCB	Eigenvalues at the RCP (au)		
	Eigenvalue1	Eigenvalue2	Eigenvalue3
1	-0.060	0.072	0.306
2	-0.053	0.069	0.300
3	-0.052	0.069	0.297
4	-0.051	0.068	0.294
5	-0.052	0.058	0.309
6	-0.047	0.043	0.312
7	-0.061	0.061	0.318
8	-0.051	0.047	0.320
9	-0.056	0.062	0.304
10	-0.054	0.073	0.304
11	-0.054	0.069	0.299
12	-0.051	0.061	0.295
13	-0.052	0.062	0.318
14	-0.054	0.062	0.337
15	-0.046	0.033	0.352
16	-0.061	0.030	0.348

17	-0.073	0.015	0.335
18	-0.072	0.018	0.335
19	-0.067	0.021	0.337
20	-0.067	0.022	0.337
21	-0.059	0.018	0.327
NUHSUF	-0.100	0.060	0.268
OZAKIK	-0.104	0.053	0.287
UHOYOG	-0.105	0.057	0.291
CETCOU	-0.103	0.050	0.281
UHOYEW	-0.102	0.053	0.282
OZAKOQ	-0.102	0.053	0.282
NEZZIC	-0.101	0.072	0.259
CEQDAF	-0.109	0.051	0.283
22	-0.093	0.055	0.261
23	-0.100	0.053	0.268

xvii) **Table S4**. Eigenvalues at the RCP in the metallacycle region of non-agostic complex **1'** - **21'**.

MCB	Eigenvalues at the RCP (au)		
	Eigenvalue1	Eigenvalue2	Eigenvalue3
1'	-0.058	0.092	0.155
2'	-0.055	0.096	0.145
3'	-0.055	0.096	0.144
4'	-0.053	0.095	0.141
5'	-0.052	0.097	0.135
6'	-0.045	0.101	0.113
7'	-0.053	0.094	0.138
8'	-0.049	0.106	0.122
9'	-0.056	0.092	0.151
10'	-0.055	0.094	0.142
11'	-0.051	0.099	0.129
12'	-0.054	0.077	0.143
13'	-0.061	0.101	0.162
14'	-0.060	0.095	0.162
15'	-0.003	0.005	0.029
16'	-0.060	0.029	0.297
17'	-0.040	0.083	0.095
18'	-0.040	0.082	0.096
19'	-0.039	0.082	0.094
20'	-0.039	0.081	0.093
21'	-0.039	0.077	0.098

xviii) **Fig. S12**. Plot showing correlation between the $\delta(C_\alpha) - \delta(C_\beta)$ and MC_β bond length for various ruthenacyclobutanes.



xix) Cartesian coordinates of the optimized geometries of the models studied. Atom symbol followed by X, Y, Z coordinates in Å unit is given. All geometries are characterized by zero imaginary frequencies in the vibrational frequency analysis.

1 $[NHMeF_2Ru(CH_2CH_2CH_2)]$			
Total SCF energy = -718.96062 Hartree			
C	-3.338007000	-0.719657000	0.324476000
C	-3.360751000	0.724854000	-0.197654000
N	-1.933454000	-1.096455000	0.102891000
C	-1.147924000	-0.000373000	-0.044835000
N	-1.937042000	1.090833000	-0.141659000
C	-1.489403000	2.452736000	-0.374181000
H	-1.544824000	2.721929000	-1.443082000
H	-2.131859000	3.142334000	0.192699000
H	-0.462144000	2.537424000	0.006779000
C	-1.467759000	-2.453256000	0.326058000
H	-2.144796000	-3.155558000	-0.181944000
H	-0.466761000	-2.555206000	-0.114788000
H	-1.443840000	-2.705758000	1.400486000
Ru	0.847682000	-0.032882000	-0.073726000
F	0.781137000	1.495005000	1.302686000

1' $[NHMeF_2Ru(CH_2CH_2CH_2)]$			
Total SCF energy = -718.96573 Hartree			
Ru	0.299187000	-0.227738000	-0.050257000
F	2.241931000	-0.094423000	0.249687000
F	-0.943503000	-1.213471000	-1.161222000
C	0.471467000	1.823302000	-0.194547000
C	-0.847144000	2.217522000	0.439580000
C	-1.514876000	0.856643000	0.302372000
H	-0.709345000	2.504946000	1.492249000
H	-2.084234000	0.502000000	1.171263000
H	1.412863000	2.212145000	0.210789000
H	-1.378941000	3.046086000	-0.063144000
H	0.474046000	1.914632000	-1.299115000
H	-2.099544000	0.722242000	-0.616777000
C	-0.484320000	-2.014116000	3.673765000
C	0.347405000	-0.820679000	4.144726000
N	-0.751519000	-1.665866000	2.273044000

F	0.992573000	-1.540202000	-1.384946000
C	2.169136000	-0.824444000	1.119218000
H	2.191120000	-0.423394000	2.137967000
C	3.084889000	-0.009871000	0.107373000
H	3.626411000	-0.707572000	-0.537292000
C	2.312840000	1.053008000	-0.777335000
H	2.388568000	2.073699000	-0.390263000
H	2.489382000	0.927416000	-1.852447000
H	3.742108000	0.587733000	0.749430000
H	-3.957464000	1.401842000	0.428992000
H	-3.590793000	-0.779424000	1.398759000
H	2.304834000	-1.908513000	1.024144000
H	-3.735987000	0.789050000	-1.234900000
H	-4.009990000	-1.391054000	-0.227613000

C	0.131897000	-0.726205000	1.808689000
N	0.853970000	-0.277404000	2.878611000
C	1.722659000	0.884278000	2.934252000
H	1.179560000	1.773066000	3.302688000
H	2.550137000	0.674668000	3.627971000
H	2.141596000	1.069439000	1.942463000
C	-1.539086000	-2.588374000	1.473733000
H	-2.525288000	-2.721886000	1.943130000
H	-1.667638000	-2.194421000	0.459849000
H	-1.048749000	-3.576573000	1.413427000
H	1.176454000	-1.102485000	4.809122000
H	0.080432000	-2.963281000	3.728496000
H	-0.267808000	-0.062644000	4.664717000
H	-1.422635000	-2.140294000	4.232066000

2 [$NHMeCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1439.75878 Hartree

C	3.436743000	-0.454759000	-0.619384000
C	3.436745000	0.454738000	0.619390000
N	2.018846000	-0.839216000	-0.710174000
C	1.237506000	-0.000006000	0.000005000
N	2.018851000	0.839202000	0.710181000
C	1.548928000	1.786538000	1.703146000
H	1.538629000	1.348935000	2.715447000
H	2.204071000	2.669057000	1.702237000
H	0.537318000	2.111782000	1.429099000
C	1.548919000	-1.786540000	-1.703149000
H	2.204058000	-2.669062000	-1.702249000
H	0.537307000	-2.111783000	-1.429105000
H	1.538620000	-1.348927000	-2.715446000
Ru	-0.758804000	-0.000001000	0.000002000
Cl	-0.752995000	2.038167000	-1.238609000
Cl	-0.753034000	-2.038164000	1.238613000
C	-2.185442000	-0.710353000	-1.145772000
H	-2.294480000	-0.220689000	-2.119066000
C	-3.014231000	0.000001000	-0.000005000
H	-3.607588000	-0.782952000	0.484867000
C	-2.185449000	0.710388000	1.145747000
H	-2.306940000	1.798848000	1.142752000
H	-2.294495000	0.220748000	2.119051000
H	-3.607619000	0.782936000	-0.484870000
H	3.748667000	-0.084089000	1.531567000
H	3.748667000	0.084068000	-1.531560000
H	-2.306936000	-1.798813000	-1.142805000
H	4.072198000	-1.343191000	-0.502761000
H	4.072204000	1.343168000	0.502767000

2' [$NHMeCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1439.74630 Hartree

Ru	-0.033606000	-0.183557000	0.125871000
Cl	2.257169000	-0.544799000	0.468587000
Cl	-1.790749000	-0.737457000	-1.253572000
C	0.558642000	1.754804000	-0.288045000
C	-0.766118000	2.443525000	-0.020014000
C	-1.432775000	1.314981000	0.764868000
H	-0.675280000	3.390553000	0.539178000
H	-1.355455000	1.442176000	1.850380000
H	1.448259000	2.116657000	0.238468000
H	-1.308500000	2.649049000	-0.953648000
H	0.813298000	1.575556000	-1.351156000
H	-2.461590000	1.068621000	0.480822000
C	-0.601052000	-2.389319000	3.656607000
C	-0.224371000	-1.043311000	4.284661000
N	-0.825055000	-2.025947000	2.250426000
C	-0.241451000	-0.824994000	1.948916000
N	0.168512000	-0.256606000	3.108838000
C	0.813056000	1.026766000	3.286054000
H	0.146832000	1.741957000	3.797707000
H	1.724463000	0.902734000	3.890609000
H	1.097476000	1.421087000	2.307555000
C	-1.112733000	-3.092411000	1.305971000
H	-1.995872000	-3.650582000	1.648634000
H	-1.337470000	-2.670219000	0.319843000
H	-0.261797000	-3.790907000	1.221470000
H	0.608686000	-1.117643000	4.997865000
H	0.218599000	-3.127062000	3.732314000
H	-1.078025000	-0.565536000	4.797907000
H	-1.506675000	-2.832871000	4.093306000

3 [$NHMeBr_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -5668.11302 Hartree

3' [$NHMeBr_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -5668.09670 Hartree

C	3.563219000	-0.000300000	-0.768112000
C	3.563244000	-0.010964000	0.768298000
N	2.145794000	-0.260336000	-1.069221000
C	1.365884000	-0.002721000	0.000096000
N	2.146480000	0.252381000	1.069452000
C	1.669579000	0.377481000	2.433903000
H	1.655905000	-0.594490000	2.954367000
H	2.318278000	1.072949000	2.984459000
H	0.655382000	0.796346000	2.417568000
C	1.668600000	-0.382984000	-2.433788000
H	2.314247000	-1.081221000	-2.984438000
H	0.652520000	-0.797260000	-2.417749000
H	1.659353000	0.589175000	-2.954020000
Ru	-0.630627000	0.000859000	-0.000002000
Br	-0.578969000	2.523158000	-0.128810000
Br	-0.588994000	-2.521439000	0.128654000
C	-2.063404000	-0.060783000	-1.347120000
H	-2.178496000	0.836727000	-1.963702000
C	-2.890442000	0.006001000	0.000053000
H	-3.487102000	-0.912278000	0.044089000
C	-2.062995000	0.068558000	1.347196000
H	-2.181313000	1.021712000	1.873561000
H	-2.181874000	-0.828701000	1.963435000
H	-3.482424000	0.927279000	-0.043963000
H	3.864977000	-0.991662000	1.176579000
H	4.202912000	-0.778300000	-1.206220000
H	-2.185939000	-1.013587000	-1.873172000
H	4.204746000	0.765583000	1.206361000
H	3.867097000	0.979747000	-1.176371000

Ru	-0.387949000	-0.104366000	0.079326000
Br	1.944463000	-0.934493000	0.323235000
Br	-2.383413000	-0.396929000	-1.302703000
C	0.499743000	1.691786000	-0.449534000
C	-0.686216000	2.595952000	-0.174300000
C	-1.471205000	1.643136000	0.722620000
H	-0.423323000	3.555869000	0.303759000
H	-1.282977000	1.803393000	1.789383000
H	1.449250000	1.930112000	0.041368000
H	-1.244522000	2.811788000	-1.096092000
H	0.692277000	1.436961000	-1.509459000
H	-2.548636000	1.580474000	0.535503000
C	-1.084194000	-2.079373000	3.722447000
C	-0.529600000	-0.765119000	4.281306000
N	-1.315328000	-1.742793000	2.310127000
C	-0.594278000	-0.639127000	1.940406000
N	-0.073591000	-0.085029000	3.062967000
C	0.754956000	1.097155000	3.167874000
H	0.204525000	1.938384000	3.622446000
H	1.631723000	0.875175000	3.795120000
H	1.104852000	1.380664000	2.171761000
C	-1.734993000	-2.809157000	1.415443000
H	-2.659861000	-3.262248000	1.799795000
H	-1.944743000	-2.402903000	0.418887000
H	-0.959766000	-3.590926000	1.335184000
H	0.306288000	-0.911540000	4.979726000
H	-0.352112000	-2.904039000	3.799222000
H	-1.305459000	-0.164830000	4.789179000
H	-2.018274000	-2.396962000	4.205913000

4 [$NHMeI_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1114.94145 Hartree

C	-0.160223000	3.627305000	-0.750641000
C	0.161405000	3.627259000	0.750541000
N	0.030393000	2.209661000	-1.099736000
C	0.000186000	1.429833000	-0.000025000
N	-0.029780000	2.209721000	1.099697000
C	0.173721000	1.739430000	2.457123000
H	1.237624000	1.774864000	2.743813000
H	-0.412798000	2.359173000	3.149810000
H	-0.181001000	0.704706000	2.537887000
C	-0.172615000	1.739302000	-2.457215000
H	0.413591000	2.359497000	-3.149759000
H	0.182865000	0.704830000	-2.537969000
H	-1.236484000	1.774060000	-2.744102000
Ru	-0.000122000	-0.571002000	0.000028000
I	-2.704299000	-0.455051000	0.038486000
I	2.704079000	-0.455707000	-0.038416000
C	-0.032483000	-2.012696000	-1.349677000
H	-0.966563000	-2.141890000	-1.906284000
C	-0.000407000	-2.835939000	-0.000170000
H	0.920105000	-3.431519000	-0.022010000

4' [$NHMeI_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1114.92164 Hartree

Ru	-0.407967000	-0.097598000	0.071926000
I	2.050998000	-1.112316000	0.282261000
I	-2.533154000	-0.383295000	-1.443848000
C	0.498851000	1.694107000	-0.455600000
C	-0.652998000	2.624397000	-0.127848000
C	-1.478960000	1.667023000	0.727649000
H	-0.349549000	3.546757000	0.397684000
H	-1.307162000	1.786774000	1.802271000
H	1.474391000	1.912135000	-0.007333000
H	-1.203002000	2.913708000	-1.035215000
H	0.639587000	1.450680000	-1.526665000
H	-2.555877000	1.657551000	0.527690000
C	-1.089350000	-2.076025000	3.731062000
C	-0.549310000	-0.752306000	4.282627000
N	-1.304547000	-1.759892000	2.311449000
C	-0.605812000	-0.644170000	1.937104000
N	-0.109831000	-0.067185000	3.061234000
C	0.723331000	1.111785000	3.162746000
H	0.183626000	1.949037000	3.636460000
H	1.613229000	0.881977000	3.768960000

C	0.031831000	-2.012950000	1.349506000
H	-0.879221000	-2.138539000	1.944310000
H	0.965820000	-2.142589000	1.906160000
H	-0.920958000	-3.431459000	0.021604000
H	1.204174000	3.930495000	0.951466000
H	0.512558000	4.267468000	-1.337260000
H	0.878489000	-2.138476000	-1.944561000
H	-0.511102000	4.267748000	1.337120000
H	-1.202860000	3.930964000	-0.951590000

H	1.053542000	1.406592000	2.163349000
C	-1.688492000	-2.844962000	1.424468000
H	-2.611130000	-3.311810000	1.797830000
H	-1.888445000	-2.454769000	0.419287000
H	-0.895403000	-3.610456000	1.365287000
H	0.293559000	-0.886241000	4.975442000
H	-0.355856000	-2.896879000	3.828506000
H	-1.328386000	-0.161293000	4.795875000
H	-2.028250000	-2.392313000	4.206252000

5 [$NHMeCl_2Ru(CHMeCH_2CHMe)$]

Total SCF energy = -1518.41306 Hartree

C	-3.663493000	-0.585484000	0.469509000
C	-3.637780000	0.856270000	-0.060170000
N	-2.275302000	-1.016078000	0.238267000
C	-1.456772000	0.037525000	0.042917000
N	-2.199034000	1.162846000	-0.026589000
C	-1.694809000	2.474671000	-0.381255000
H	-1.763072000	2.661965000	-1.466230000
H	-2.272008000	3.243691000	0.151441000
H	-0.649319000	2.550253000	-0.057626000
C	-1.850208000	-2.378467000	0.491334000
H	-2.565774000	-3.075396000	0.032115000
H	-0.871510000	-2.531596000	0.019340000
H	-1.784497000	-2.594329000	1.570993000
Ru	0.536375000	-0.049414000	-0.097391000
Cl	0.694739000	0.934521000	2.081071000
Cl	0.183628000	-1.017318000	-2.270351000
C	1.929281000	-1.436156000	0.174238000
C	2.768108000	-0.171899000	-0.285730000
H	3.395317000	-0.550756000	-1.104309000
C	1.974999000	1.037918000	-0.935823000
H	1.953329000	0.944389000	-2.030029000
H	3.348526000	0.199263000	0.565912000
H	-4.022182000	0.927067000	-1.093200000
H	-4.365319000	-1.233118000	-0.073643000
H	1.905789000	-2.192811000	-0.622527000
C	2.270513000	-2.009395000	1.531665000
H	1.526154000	-2.764338000	1.825048000
H	3.244909000	-2.528524000	1.483539000
H	2.306351000	-1.239106000	2.310358000
C	2.372169000	2.418845000	-0.464985000
H	3.366475000	2.679138000	-0.870651000
H	1.671110000	3.171873000	-0.855195000
H	2.395926000	2.495057000	0.628149000
H	-4.198948000	1.558504000	0.571419000
H	-3.905674000	-0.629827000	1.546119000

5' [$NHMeCl_2Ru(CHMeCH_2CHMe)$]

Total SCF energy = -1518.39926 Hartree

Ru	-0.334213000	-0.052161000	-0.052775000
Cl	1.572976000	-1.441208000	-0.101947000
Cl	-2.437616000	0.415661000	-0.974437000
C	1.052807000	1.464894000	-0.368773000
C	0.230728000	2.590110000	0.225262000
C	-0.669910000	1.758056000	1.129858000
H	0.820466000	3.361681000	0.756141000
H	-0.142510000	1.532958000	2.062660000
H	2.052202000	1.302049000	0.046916000
H	-0.367467000	3.093548000	-0.550475000
C	0.936024000	1.196795000	-1.850788000
H	1.782167000	0.622928000	-2.242966000
H	0.015257000	0.590626000	-2.088450000
H	0.771968000	2.123276000	-2.423228000
C	-2.044148000	2.309456000	1.454781000
H	-2.590484000	2.634902000	0.562131000
H	-2.672406000	1.576814000	1.980887000
H	-1.923754000	3.183549000	2.123306000
C	-0.659547000	-1.722265000	3.869285000
C	-1.644618000	-2.590046000	3.083357000
N	-0.037467000	-0.924831000	2.805619000
C	-0.733633000	-0.975376000	1.639751000
N	-1.763571000	-1.861545000	1.811555000
C	-2.530019000	-2.506544000	0.757104000
H	-2.068735000	-3.469250000	0.473160000
H	-3.551440000	-2.698343000	1.116427000
H	-2.592972000	-1.852001000	-0.117902000
C	1.188871000	-0.208703000	3.089351000
H	1.918413000	-0.903132000	3.534784000
H	1.609019000	0.171527000	2.154623000
H	1.021450000	0.620452000	3.797763000
H	-2.625325000	-2.683916000	3.570186000
H	-1.166113000	-1.064424000	4.597583000
H	-1.251002000	-3.606452000	2.898285000
H	0.099386000	-2.308776000	4.406733000

6 [$NHMeCl_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -1597.05554 Hartree

6' [$NHMeCl_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -1597.03793 Hartree

C	-3.828310000	0.758807000	-0.047699000
C	-3.814653000	-0.777372000	-0.006000000
N	-2.406709000	1.084348000	0.152047000
C	-1.620983000	0.008876000	-0.044069000
N	-2.394290000	-1.075316000	-0.246422000
C	-1.907862000	-2.440397000	-0.278184000
H	-1.910388000	-2.898621000	0.724322000
H	-2.535900000	-3.037022000	-0.955098000
H	-0.882357000	-2.440561000	-0.668287000
C	-1.957940000	2.462482000	0.143442000
H	-2.331743000	2.995615000	1.030352000
H	-0.862316000	2.482443000	0.145742000
H	-2.307750000	2.979408000	-0.765320000
Ru	0.381503000	-0.006909000	0.050261000
Cl	0.058593000	0.522463000	-2.310539000
Cl	0.091398000	-0.534183000	2.380889000
C	1.858418000	1.348993000	0.282082000
C	2.605746000	-0.060998000	0.300212000
C	1.856991000	-1.341804000	-0.291502000
H	-4.447611000	-1.236208000	-0.778297000
H	-4.450491000	1.205390000	0.740150000
C	2.287541000	2.259637000	-0.862066000
H	1.596325000	3.109327000	-0.958280000
H	3.285960000	2.677275000	-0.636204000
H	2.314731000	1.749237000	-1.829393000
C	2.263497000	-1.697093000	-1.716968000
H	3.260953000	-2.173947000	-1.701304000
H	1.563191000	-2.428892000	-2.144953000
H	2.282135000	-0.833144000	-2.387763000
H	3.455897000	0.082645000	-0.379021000
C	1.926671000	2.089213000	1.613807000
H	1.218844000	2.932390000	1.615250000
H	1.695252000	1.445598000	2.467982000
H	2.933982000	2.526429000	1.740596000
C	1.960086000	-2.563908000	0.614030000
H	2.981219000	-2.982278000	0.550139000
H	1.720747000	-2.337650000	1.657209000
H	1.278675000	-3.353953000	0.263329000
H	2.923375000	-0.280826000	1.324900000
H	-4.165145000	1.147099000	-1.025184000
H	-4.121778000	-1.168344000	0.979836000

Ru	-0.396202000	0.283804000	0.033514000
Cl	1.461000000	-1.099259000	-0.394936000
Cl	-2.271964000	0.827272000	-1.253945000
C	0.933042000	1.930205000	0.203262000
C	-0.122537000	2.864953000	0.776618000
C	-1.094947000	1.887813000	1.443280000
H	0.291170000	3.613419000	1.484359000
H	-0.634555000	3.412244000	-0.029489000
C	1.032828000	1.933423000	-1.315916000
H	1.948700000	1.450112000	-1.672582000
H	0.179800000	1.402106000	-1.805596000
H	0.946737000	2.962312000	-1.705014000
C	-2.553050000	2.329838000	1.425317000
H	-2.886184000	2.664109000	0.437885000
H	-3.227043000	1.526150000	1.756024000
H	-2.678036000	3.169046000	2.137315000
C	-0.690893000	1.611591000	2.887177000
H	-1.345897000	0.868684000	3.364760000
H	0.347808000	1.280101000	2.991387000
H	-0.790289000	2.549110000	3.468089000
C	2.270740000	1.922366000	0.910766000
H	2.164309000	1.843531000	2.001406000
H	2.923520000	1.118373000	0.549582000
H	2.776533000	2.887400000	0.716932000
C	-2.052111000	-2.755017000	2.540987000
C	-0.778897000	-2.446326000	3.319762000
N	-2.118974000	-1.630842000	1.596741000
C	-0.909123000	-1.000339000	1.458840000
N	-0.086448000	-1.518431000	2.419941000
C	1.252220000	-1.125242000	2.806199000
H	1.245731000	-0.702130000	3.826457000
H	1.913533000	-2.005190000	2.796929000
H	1.651200000	-0.397114000	2.099836000
C	-3.268751000	-1.610861000	0.711707000
H	-4.183679000	-1.666529000	1.320541000
H	-3.281993000	-0.694016000	0.117918000
H	-3.254881000	-2.477194000	0.026697000
H	-0.159391000	-3.333509000	3.513573000
H	-1.986000000	-3.709040000	1.986762000
H	-0.983757000	-1.952498000	4.288124000
H	-2.953764000	-2.784458000	3.168705000

7 [$NHMeF_2Ru(CHMeCH_2CHMe)$]

Total SCF energy = -797.62025 Hartree

C	-3.655432000	-0.646325000	0.100034000
C	-3.573188000	0.886110000	0.031390000
N	-2.256985000	-1.036581000	-0.134204000
C	-1.410546000	-0.000161000	0.052360000
N	-2.143281000	1.119993000	0.280068000
C	-1.611805000	2.461123000	0.437330000
H	-1.598125000	3.011651000	-0.519913000
H	-2.239578000	3.017441000	1.148817000
H	-0.597706000	2.386590000	0.852745000

7' [$NHMeF_2Ru(CHMeCH_2CHMe)$]

Total SCF energy = -797.61834 Hartree

Ru	0.329352000	-0.244348000	-0.077964000
F	2.268330000	-0.096418000	0.237814000
F	-0.854912000	-1.312122000	-1.174279000
C	0.514412000	1.816962000	-0.245850000
C	-0.842060000	2.211043000	0.303755000
C	-1.542445000	0.851497000	0.258176000
H	-0.755346000	2.593886000	1.331971000
H	-1.942350000	0.548326000	1.235521000
H	1.391523000	2.175894000	0.306074000

C	-1.877263000	-2.424403000	-0.328020000
H	-2.578322000	-2.892926000	-1.034342000
H	-0.871951000	-2.435912000	-0.771575000
H	-1.906431000	-2.989839000	0.619576000
Ru	0.588202000	-0.059052000	-0.028858000
F	0.858041000	0.995600000	1.668643000
F	0.360214000	-1.125325000	-1.780542000
C	2.011557000	-1.390696000	0.242008000
C	2.794378000	-0.135907000	-0.333938000
H	3.419261000	-0.555662000	-1.132069000
C	1.903891000	0.955174000	-1.078113000
H	1.821266000	0.725574000	-2.149772000
H	3.383542000	0.340473000	0.457682000
H	-3.863298000	1.275472000	-0.961626000
H	-3.996300000	-1.002650000	1.089097000
H	1.972485000	-2.200182000	-0.498772000
C	2.373473000	-1.815691000	1.647453000
H	1.688060000	-2.600184000	2.000234000
H	3.390294000	-2.248019000	1.669183000
H	2.330586000	-0.971080000	2.347032000
C	2.234550000	2.394845000	-0.757019000
H	3.221769000	2.668808000	-1.170479000
H	1.499590000	3.068536000	-1.222040000
H	2.241001000	2.570942000	0.326250000
H	-4.186142000	1.387841000	0.792926000
H	-4.311003000	-1.079344000	-0.668067000
H	-1.360228000	2.985909000	-0.293987000
C	-0.489473000	-2.014274000	3.654618000
C	0.301272000	-0.794056000	4.124287000
N	-0.735597000	-1.693148000	2.243329000
C	0.135716000	-0.738911000	1.780165000
N	0.829297000	-0.265864000	2.861049000
C	1.672068000	0.915188000	2.918805000
H	1.087880000	1.818517000	3.170253000
H	2.427552000	0.765929000	3.703842000
H	2.185869000	1.041489000	1.962575000
C	-1.461215000	-2.666802000	1.445861000
H	-2.454905000	-2.829395000	1.889599000
H	-1.573059000	-2.308077000	0.417473000
H	-0.928944000	-3.635154000	1.428486000
H	1.117989000	-1.043557000	4.816370000
H	0.099099000	-2.947443000	3.734511000
H	-0.345995000	-0.041349000	4.612707000
H	-1.435634000	-2.157684000	4.195287000
C	-2.617803000	0.705041000	-0.804849000
H	-2.249909000	0.933718000	-1.815585000
H	-3.047827000	-0.303167000	-0.834346000
H	-3.434213000	1.419221000	-0.585112000
C	0.724868000	1.955053000	-1.748065000
H	1.724874000	1.611412000	-2.046866000
H	-0.028961000	1.403832000	-2.336155000
H	0.630602000	3.014417000	-2.049854000

8 [$NHMeF_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -2125.11924 Hartree

C	-3.810385000	-0.818524000	0.042258000
C	-3.825352000	0.716932000	0.076227000
N	-2.381934000	-1.109868000	0.236482000
C	-1.612657000	-0.028276000	-0.019478000
N	-2.424252000	1.035509000	-0.236375000
C	-1.986380000	2.400672000	-0.458295000
H	-2.696282000	2.901952000	-1.132169000
H	-1.934515000	2.974790000	0.483595000
H	-1.004150000	2.371725000	-0.947954000
C	-1.902357000	-2.464470000	0.440241000
H	-1.915515000	-3.048142000	-0.496795000
H	-0.887325000	-2.401724000	0.855507000
H	-2.549413000	-2.968735000	1.172785000
Ru	0.390930000	0.015388000	-0.068981000
F	0.304478000	-0.917185000	1.769590000
F	0.379159000	0.927839000	-1.888565000
C	1.872551000	-1.235792000	-0.530194000
C	2.614215000	0.106393000	-0.078483000
C	1.764531000	1.277157000	0.622200000
H	-4.100089000	1.109179000	1.072444000
H	-4.159048000	-1.217895000	-0.927465000
C	2.191222000	-2.438354000	0.343116000
H	1.544523000	-3.285489000	0.069018000
H	3.233154000	-2.761706000	0.166710000

8'[$NHMeF_2Ru(CMe_2CH_{ww}CMe_2)$]

Total SCF energy = -876.26725 Hartree

Ru	-0.124523000	0.028376000	0.156915000
F	1.747244000	-0.639556000	0.247119000
F	-1.834655000	-0.140193000	-0.812101000
C	0.876422000	1.861928000	-0.058881000
C	-0.330400000	2.707923000	0.318601000
C	-1.180366000	1.701321000	1.109840000
H	-0.064373000	3.606176000	0.909518000
H	-0.872738000	3.049310000	-0.577368000
C	0.965235000	1.506430000	-1.536925000
H	1.923214000	1.042244000	-1.795731000
H	0.155971000	0.794036000	-1.853835000
H	0.774503000	2.388777000	-2.170826000
C	-2.677301000	1.805737000	0.853362000
H	-2.928154000	1.756781000	-0.211385000
H	-3.235104000	1.009535000	1.367195000
H	-3.041075000	2.771388000	1.255127000
C	-0.904084000	1.816432000	2.605692000
H	-1.457921000	1.063642000	3.185528000
H	0.162697000	1.726771000	2.847736000
H	-1.237689000	2.810161000	2.962233000
C	2.193723000	2.212217000	0.588770000
H	2.081246000	2.387889000	1.667975000
H	2.945843000	1.430524000	0.425054000
H	2.574446000	3.154625000	0.151666000

H	2.040575000	-2.221810000	1.405730000
C	1.959353000	1.373580000	2.128400000
H	2.968200000	1.765402000	2.355233000
H	1.234748000	2.084819000	2.551841000
H	1.808631000	0.406585000	2.620057000
H	3.328453000	-0.212858000	0.689072000
C	2.001470000	-1.538504000	-2.018070000
H	1.323399000	-2.359520000	-2.296101000
H	1.760807000	-0.663692000	-2.632261000
H	3.027255000	-1.883792000	-2.244478000
C	1.926511000	2.620268000	-0.076399000
H	2.941558000	3.017995000	0.104730000
H	1.749740000	2.540160000	-1.154799000
H	1.222385000	3.352362000	0.347446000
H	3.105640000	0.535996000	-0.958126000
H	-4.410135000	-1.275494000	0.841377000
H	-4.499263000	1.160948000	-0.669356000

9[$NHMesF_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1338.54346 Hartree

N	1.103693000	-1.541086000	-0.005284000
C	0.000009000	-0.769088000	0.001772000
C	0.772944000	-2.983407000	0.029909000
C	-0.772722000	-2.983598000	-0.016258000
N	-1.103604000	-1.541144000	0.012384000
H	-1.166815000	-3.447354000	-0.933593000
H	1.222782000	-3.500706000	-0.830247000
Ru	-0.000082000	1.205911000	-0.001482000
F	-0.010578000	1.253474000	2.036301000
F	0.010409000	1.251554000	-2.038594000
C	1.344469000	2.615428000	0.006108000
H	1.908597000	2.716436000	0.939234000
H	-1.222453000	-3.496992000	0.846285000
H	1.167035000	-3.442973000	0.949348000
C	-1.344757000	2.615343000	-0.005536000
C	-0.000171000	3.457311000	-0.002671000
H	-0.004138000	4.058067000	0.912265000
C	2.451725000	-1.040530000	-0.001133000
C	3.099980000	-0.814830000	-1.233217000
C	3.093296000	-0.802573000	1.232601000
C	4.425218000	-0.361066000	-1.202516000
C	4.418614000	-0.349458000	1.204111000
C	5.101274000	-0.124293000	0.001374000
H	4.940333000	-0.184628000	-2.150401000
H	4.928580000	-0.163568000	2.153012000
C	-2.451649000	-1.040659000	0.003937000
C	-3.102185000	-0.810161000	1.234235000
C	-3.090930000	-0.807510000	-1.231596000
C	-4.427085000	-0.356527000	1.199482000
C	-4.416564000	-0.354256000	-1.207161000
C	-5.101168000	-0.124403000	-0.006740000
H	-4.943751000	-0.176206000	2.145815000

C	-1.305070000	-2.653894000	3.233219000
C	-0.108573000	-1.999776000	3.919565000
N	-1.521015000	-1.767822000	2.082587000
C	-0.413999000	-1.005726000	1.808539000
N	0.466397000	-1.198576000	2.833766000
C	1.697925000	-0.486717000	3.104737000
H	1.565067000	0.221500000	3.942654000
H	2.480819000	-1.208121000	3.384981000
H	2.019120000	0.033082000	2.201363000
C	-2.617335000	-2.093226000	1.187465000
H	-3.561311000	-2.084855000	1.753623000
H	-2.663016000	-1.360239000	0.374963000
H	-2.482746000	-3.103035000	0.759150000
H	0.624993000	-2.723035000	4.303282000
H	-1.078892000	-3.678968000	2.884706000
H	-0.412140000	-1.341692000	4.755676000
H	-2.203470000	-2.697215000	3.865134000

9' [$NHMesF_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1338.53332398Hartree

Ru	0.329116000	1.401344000	-0.210186000
F	1.492759000	2.073498000	1.177570000
F	0.301634000	1.017981000	-2.149531000
C	-1.038901000	1.889044000	1.347375000
C	-1.751481000	2.974714000	0.548342000
C	-1.382567000	2.439084000	-0.819661000
H	-2.837204000	3.049581000	0.736269000
H	-2.117556000	1.780061000	-1.291793000
H	-1.690563000	1.043912000	1.573560000
H	-1.308712000	3.964173000	0.730484000
H	-0.462930000	2.206477000	2.224693000
H	-0.968535000	3.144158000	-1.559238000
N	1.138499000	-1.290002000	0.216089000
C	0.042339000	-0.468593000	0.134330000
N	-1.070285000	-1.253604000	0.316550000
C	2.516199000	-0.889509000	0.103507000
C	3.144015000	-0.962825000	-1.159723000
C	3.239876000	-0.539296000	1.263856000
C	4.503480000	-0.633448000	-1.240405000
C	4.598123000	-0.229587000	1.126581000
C	5.246403000	-0.260047000	-0.114281000
H	4.995610000	-0.681261000	-2.215243000
H	5.163470000	0.048433000	2.019845000
C	-2.456603000	-0.927214000	0.127074000
C	-3.301263000	-0.869995000	1.256418000
C	-2.983749000	-0.808250000	-1.179504000
C	-4.663880000	-0.603891000	1.060693000
C	-4.351952000	-0.540872000	-1.317494000
C	-5.207554000	-0.419356000	-0.214418000
H	-5.316164000	-0.540951000	1.935747000
H	-4.762237000	-0.439595000	-2.325805000
C	-2.788497000	-1.117306000	2.654710000

H	-4.924980000	-0.172260000	-2.157622000
C	-2.383295000	-0.993338000	2.545696000
H	-1.950729000	-2.000953000	2.643121000
H	-1.554539000	-0.268832000	2.632941000
H	-3.071708000	-0.841410000	3.387156000
C	-2.361976000	-0.986739000	-2.538225000
H	-3.043197000	-0.826997000	-3.384078000
H	-1.529211000	-0.265590000	-2.616544000
H	-1.934461000	-1.996188000	-2.639139000
C	-6.519066000	0.393044000	-0.011913000
H	-6.535850000	1.494423000	0.021921000
H	-7.056257000	0.086654000	-0.919967000
H	-7.082401000	0.032725000	0.860025000
C	2.379109000	-1.002993000	-2.542902000
H	1.551719000	-0.277268000	-2.632691000
H	3.066718000	-0.856430000	-3.385959000
H	1.944448000	-2.010196000	-2.634956000
C	2.366340000	-0.976825000	2.540997000
H	3.048358000	-0.811584000	3.385162000
H	1.532137000	-0.257049000	2.616805000
H	1.941068000	-1.986677000	2.647386000
C	6.519206000	0.393081000	0.003342000
H	6.535875000	1.494513000	0.035356000
H	7.077639000	0.034282000	0.879061000
H	7.061450000	0.085035000	-0.901135000
H	0.003792000	4.053688000	-0.920421000
H	-1.916698000	2.716007000	0.922840000
H	-1.912272000	2.715345000	-0.936725000
H	1.919763000	2.715217000	-0.920299000
H	-2.825889000	-2.190907000	2.904108000
H	-1.750001000	-0.786213000	2.781596000
H	-3.409289000	-0.595005000	3.394705000
C	-2.127302000	-0.997571000	-2.404920000
H	-2.739116000	-0.916917000	-3.312878000
H	-1.312570000	-0.260251000	-2.465547000
H	-1.656703000	-1.993779000	-2.411334000
C	-6.668939000	-0.092819000	-0.400242000
H	-6.815131000	0.989320000	-0.547228000
H	-7.084340000	-0.597610000	-1.283952000
H	-7.262355000	-0.388524000	0.475475000
C	2.388808000	-1.378635000	-2.395223000
H	1.596185000	-0.651700000	-2.630137000
H	3.068543000	-1.448886000	-3.254342000
H	1.906078000	-2.360037000	-2.267609000
C	2.580799000	-0.455163000	2.616116000
H	3.336112000	-0.367885000	3.407991000
H	1.933354000	0.433387000	2.657116000
H	1.959151000	-1.334670000	2.838209000
C	6.701660000	0.119637000	-0.236343000
H	6.812560000	1.208362000	-0.365432000
H	7.267932000	-0.159922000	0.663047000
H	7.172271000	-0.362104000	-1.104412000
C	0.799650000	-2.676264000	0.575078000
C	-0.727610000	-2.688535000	0.437580000
H	-1.064613000	-3.227945000	-0.462655000
H	1.296956000	-3.383382000	-0.104250000
H	-1.229988000	-3.133491000	1.307756000
H	1.131225000	-2.903858000	1.601948000

10 [$NHMesCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -2059.33364 Hartree

N	1.103139000	-1.537424000	0.125218000
C	0.000016000	-0.758426000	0.069540000
C	0.769583000	-2.977127000	0.231225000
C	-0.769506000	-2.977316000	0.229028000
N	-1.103105000	-1.537459000	0.125123000
H	-1.194832000	-3.525348000	-0.624635000
H	1.197571000	-3.526953000	-0.619911000
Ru	-0.000033000	1.255642000	-0.018223000
Cl	-0.001102000	1.416147000	2.368263000
Cl	0.001071000	1.302760000	-2.408343000
C	1.349249000	2.679480000	-0.050312000
H	1.916684000	2.812371000	0.875579000
H	-1.195691000	-3.398700000	1.151064000
H	1.193151000	-3.396370000	1.155478000
C	-1.349381000	2.679359000	-0.051478000
C	-0.000059000	3.508769000	-0.074914000
H	-0.000507000	4.124243000	0.831308000
C	2.477466000	-1.108913000	0.051145000
C	3.102991000	-1.030174000	-1.211870000
C	3.198162000	-0.887115000	1.245213000

10' [$NHMesCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -2059.30829702 Hartree

Ru	0.237115000	1.340388000	-0.238409000
Cl	1.805713000	2.258440000	1.132127000
Cl	0.090597000	1.195716000	-2.570453000
C	-0.934945000	1.590307000	1.560051000
C	-1.670023000	2.813116000	1.028993000
C	-1.481338000	2.522553000	-0.442917000
H	-2.725120000	2.889088000	1.351279000
H	-2.290558000	1.972711000	-0.935799000
H	-1.593369000	0.728276000	1.665533000
H	-1.157107000	3.740266000	1.320487000
H	-0.329010000	1.738769000	2.461636000
H	-1.134052000	3.345405000	-1.087995000
N	1.061990000	-1.429460000	-0.100253000
C	-0.022135000	-0.590179000	-0.070185000
N	-1.144950000	-1.377465000	-0.034865000
C	2.449717000	-1.067226000	0.019396000
C	3.255875000	-1.028682000	-1.137448000
C	3.003116000	-0.886988000	1.305331000
C	4.618009000	-0.736176000	-0.981025000
C	4.369543000	-0.607336000	1.404941000

C	4.450405000	-0.647311000	-1.256419000	C	5.192345000	-0.512221000	0.274846000
C	4.542423000	-0.506335000	1.139897000	H	5.247320000	-0.690860000	-1.873480000
C	5.182880000	-0.365386000	-0.097495000	H	4.801408000	-0.453699000	2.397178000
H	4.940271000	-0.577110000	-2.230955000	C	-2.536595000	-1.021460000	0.052556000
H	5.105756000	-0.323660000	2.058659000	C	-3.167109000	-1.063678000	1.316680000
C	-2.477427000	-1.108968000	0.050832000	C	-3.290618000	-0.793670000	-1.120571000
C	-3.198350000	-0.887942000	1.244902000	C	-4.531156000	-0.751462000	1.395872000
C	-3.102735000	-1.029459000	-1.212249000	C	-4.650467000	-0.483126000	-0.983789000
C	-4.542599000	-0.507132000	1.139616000	C	-5.287131000	-0.435007000	0.262326000
C	-4.450151000	-0.646588000	-1.256773000	H	-5.014047000	-0.760674000	2.376595000
C	-5.182838000	-0.365404000	-0.097799000	H	-5.231186000	-0.286233000	-1.888764000
H	-5.106085000	-0.325033000	2.058396000	C	-2.437504000	-1.488216000	2.569724000
H	-4.939851000	-0.575789000	-2.231350000	H	-2.535469000	-2.575831000	2.724304000
C	-2.566769000	-1.067580000	2.600266000	H	-1.366912000	-1.253712000	2.535055000
H	-2.221011000	-2.102400000	2.752844000	H	-2.865558000	-0.999069000	3.454778000
H	-1.696770000	-0.405199000	2.729826000	C	-2.697607000	-0.944319000	-2.497244000
H	-3.292067000	-0.843226000	3.392994000	H	-3.373838000	-0.528834000	-3.255552000
C	-2.367317000	-1.350257000	-2.486350000	H	-1.724685000	-0.445862000	-2.595012000
H	-3.057651000	-1.340604000	-3.339650000	H	-2.552279000	-2.009867000	-2.741579000
H	-1.569664000	-0.614897000	-2.678960000	C	-6.741697000	-0.051204000	0.376516000
H	-1.896278000	-2.344649000	-2.449476000	H	-6.856527000	1.043865000	0.417844000
C	-6.620929000	0.084293000	-0.178643000	H	-7.320117000	-0.404872000	-0.488368000
H	-6.688177000	1.184185000	-0.177510000	H	-7.197065000	-0.462601000	1.287611000
H	-7.102950000	-0.271453000	-1.099445000	C	2.694531000	-1.313613000	-2.505875000
H	-7.205162000	-0.277151000	0.679108000	H	1.847596000	-0.652216000	-2.740915000
C	2.367733000	-1.351738000	-2.485864000	H	3.466875000	-1.176321000	-3.273602000
H	1.570571000	-0.616050000	-2.679280000	H	2.331017000	-2.351013000	-2.585260000
H	3.058286000	-1.343252000	-3.338999000	C	2.157751000	-0.983316000	2.549457000
H	1.896059000	-2.345796000	-2.448185000	H	2.770667000	-0.819492000	3.444803000
C	2.566428000	-1.065882000	2.600626000	H	1.360581000	-0.226754000	2.542330000
H	3.291681000	-0.841107000	3.393276000	H	1.680675000	-1.971059000	2.648941000
H	1.696436000	-0.403397000	2.729765000	C	6.652456000	-0.158646000	0.411080000
H	2.220577000	-2.100573000	2.753841000	H	6.784080000	0.933375000	0.475504000
C	6.620988000	0.084254000	-0.178358000	H	7.088709000	-0.592283000	1.321987000
H	6.688276000	1.184143000	-0.177388000	H	7.234878000	-0.509374000	-0.451719000
H	7.205181000	-0.277077000	0.679471000	C	0.695988000	-2.855069000	-0.014337000
H	7.103027000	-0.271657000	-1.099084000	C	-0.829122000	-2.818396000	-0.151231000
H	0.000285000	4.074869000	-1.012780000	H	-1.173897000	-3.197902000	-1.126246000
H	-1.917603000	2.812213000	0.873938000	H	1.182813000	-3.424568000	-0.818353000
H	-1.920774000	2.763631000	-0.980702000	H	-1.343571000	-3.386399000	0.636536000
H	1.921430000	2.763703000	-0.979055000	H	1.026835000	-3.277417000	0.948770000

11 [$NHMesCl_2Ru(CH_2CH_2CHC_6H_4O\text{-}iPr)$]

Total SCF energy = -2483.67916 Hartree

N	-0.669812000	2.220169000	-0.284194000
C	-1.385305000	1.077475000	-0.178406000
C	-1.522131000	3.403004000	-0.542326000
C	-2.941151000	2.813233000	-0.530138000
N	-2.701427000	1.365634000	-0.319066000
H	-3.563704000	3.215222000	0.283245000
H	-1.365598000	4.158479000	0.241418000
Ru	-0.593992000	-0.763885000	0.090891000

11' [$NHMesCl_2Ru(CH_2CH_2CHC_6H_4O\text{-}iPr)$]

Total SCF energy = -2483.66211646 Hartree

Ru	0.391022000	-0.437591000	-0.543842000
Cl	1.878884000	-1.194941000	-2.116878000
Cl	-0.432579000	-1.125935000	1.558608000
C	-0.157168000	0.814837000	-2.191437000
C	-1.351113000	-0.029077000	-2.584711000
C	-1.645606000	-0.669546000	-1.238469000
H	-2.212641000	0.541015000	-2.982803000
H	-2.299580000	-0.078408000	-0.593090000

Cl	-0.545614000	-0.980975000	-2.307978000	H	-0.457009000	1.786657000	-1.799137000
Cl	-0.839335000	-0.665844000	2.464744000	H	-1.078759000	-0.782867000	-3.335334000
C	1.177525000	-1.730550000	-0.016877000	H	0.631834000	0.916460000	-2.946708000
H	1.465955000	-1.785613000	-1.068663000	N	2.302881000	1.177601000	0.935953000
H	-3.475803000	2.971285000	-1.477676000	C	1.050166000	1.172428000	0.376528000
H	-1.257505000	3.855738000	-1.509465000	N	0.440540000	2.346060000	0.742848000
C	-1.397276000	-2.557084000	0.159121000	C	3.373676000	0.234896000	0.739254000
C	0.750393000	2.387429000	-0.109911000	C	3.640778000	-0.729850000	1.734130000
C	1.252425000	2.656679000	1.183309000	C	4.224861000	0.389095000	-0.376279000
C	1.587290000	2.416989000	-1.245277000	C	4.728625000	-1.592086000	1.539853000
C	2.626370000	2.887230000	1.320803000	C	5.302810000	-0.491932000	-0.515188000
C	2.954035000	2.657792000	-1.047435000	C	5.562140000	-1.501609000	0.419854000
C	3.495502000	2.882290000	0.222737000	H	4.931903000	-2.352761000	2.298072000
H	3.023871000	3.087851000	2.318940000	H	5.955415000	-0.385629000	-1.385584000
H	3.610005000	2.678746000	-1.921439000	C	-0.803936000	2.939598000	0.326638000
C	1.047860000	2.219412000	-2.637589000	C	-0.780699000	3.861248000	-0.746918000
H	0.539504000	1.247805000	-2.739850000	C	-1.980473000	2.744517000	1.080769000
H	0.317369000	2.999814000	-2.905151000	C	-1.975211000	4.491474000	-1.116615000
C	0.352091000	2.725711000	2.389040000	C	-3.149892000	3.398774000	0.665038000
H	0.921185000	3.043851000	3.272088000	C	-3.177091000	4.259772000	-0.437035000
C	4.974887000	3.109937000	0.411288000	H	-1.961558000	5.187381000	-1.959548000
H	5.466491000	2.194894000	0.777893000	H	-4.066246000	3.236403000	1.238611000
H	5.462285000	3.395397000	-0.530839000	C	0.497457000	4.208346000	-1.471416000
H	1.861416000	2.265619000	-3.373149000	H	1.076078000	4.961724000	-0.911197000
H	5.169265000	3.899475000	1.151410000	H	1.146189000	3.335335000	-1.611768000
H	-0.106119000	1.748617000	2.608375000	H	0.279763000	4.637571000	-2.457961000
H	-0.468622000	3.445715000	2.244373000	C	-1.999519000	1.915726000	2.337327000
C	-3.827878000	0.469248000	-0.228916000	H	-3.028032000	1.797702000	2.702552000
C	-4.373936000	-0.078806000	-1.410630000	H	-1.561511000	0.919772000	2.186224000
C	-4.448588000	0.271527000	1.024403000	H	-1.423167000	2.405006000	3.139732000
C	-5.492275000	-0.915132000	-1.293154000	C	-4.461126000	4.915027000	-0.882341000
C	-5.567719000	-0.570364000	1.081016000	H	-4.968926000	4.305031000	-1.646729000
C	-6.092683000	-1.189827000	-0.058765000	H	-5.161370000	5.037726000	-0.044702000
H	-5.912007000	-1.352915000	-2.202592000	H	-4.276522000	5.903590000	-1.325371000
H	-6.046928000	-0.734937000	2.049612000	C	2.817278000	-0.831446000	2.991019000
C	-3.955349000	0.943675000	2.278466000	H	1.747798000	-0.953485000	2.766292000
H	-2.984644000	0.529277000	2.594426000	H	3.146902000	-1.685259000	3.597249000
H	-3.816088000	2.026330000	2.138620000	H	2.919374000	0.072092000	3.614268000
C	-3.809327000	0.231973000	-2.771508000	C	3.994387000	1.463489000	-1.408463000
H	-4.397413000	-0.268142000	-3.552016000	H	4.820325000	1.482199000	-2.130981000
C	-7.270773000	-2.127258000	0.040867000	H	3.064011000	1.277960000	-1.964851000
H	-7.865163000	-2.128041000	-0.883291000	H	3.921849000	2.464583000	-0.956734000
H	-6.934199000	-3.162308000	0.213623000	C	6.699194000	-2.471908000	0.216790000
H	-4.674612000	0.801801000	3.095618000	H	6.374073000	-3.331657000	-0.390919000
H	-7.931312000	-1.856540000	0.876248000	H	7.541752000	-2.001795000	-0.309442000
H	-2.761857000	-0.096527000	-2.857612000	H	7.066902000	-2.867736000	1.173493000
H	-3.832749000	1.313072000	-2.982311000	C	2.608443000	2.419544000	1.670212000
C	2.365871000	-1.572430000	0.849243000	C	1.258120000	3.137568000	1.690067000
C	3.635550000	-1.374639000	0.222634000	H	0.789090000	3.123826000	2.686682000
C	2.338007000	-1.678275000	2.253188000	H	2.981450000	2.185037000	2.676769000
C	4.799866000	-1.301829000	1.005515000	H	1.322308000	4.182707000	1.357187000
C	3.496739000	-1.614625000	3.021920000	H	3.390322000	2.991664000	1.143765000
C	4.731431000	-1.427087000	2.393333000	C	-1.927157000	-2.119293000	-1.159821000
H	1.369936000	-1.786478000	2.742566000	C	-2.943360000	-2.617779000	-0.283833000
H	5.762951000	-1.134568000	0.528957000	C	-1.222016000	-3.051892000	-1.947910000
H	3.435705000	-1.699611000	4.107512000	C	-3.203462000	-3.994792000	-0.234011000

H	5.648448000	-1.365482000	2.982487000
O	3.626214000	-1.227288000	-1.136828000
C	4.711939000	-1.666671000	-2.008320000
C	5.201208000	-3.077092000	-1.687166000
H	4.355364000	-3.775149000	-1.627081000
H	5.868709000	-3.417914000	-2.491722000
H	5.758171000	-3.125695000	-0.742672000
C	5.830614000	-0.629523000	-2.134684000
H	6.432911000	-0.855221000	-3.027294000
H	5.405693000	0.375492000	-2.255523000
H	6.509549000	-0.620645000	-1.271843000
H	4.188211000	-1.701998000	-2.976050000
C	0.127858000	-2.889532000	0.319913000
H	0.344593000	-3.634420000	-0.456964000
H	0.320288000	-3.255153000	1.332201000
H	-1.839169000	-2.922064000	-0.772996000
H	-1.974067000	-2.767799000	1.065636000

C	-1.473348000	-4.421121000	-1.879901000
C	-2.468038000	-4.887360000	-1.019334000
H	-0.432701000	-2.687868000	-2.607515000
H	-3.986603000	-4.383599000	0.410633000
H	-0.896225000	-5.115010000	-2.491547000
H	-2.685807000	-5.955052000	-0.954706000
O	-3.633230000	-1.665988000	0.403872000
C	-4.549759000	-1.943927000	1.501952000
C	-3.903266000	-2.720625000	2.649500000
H	-2.915982000	-2.299532000	2.879974000
H	-4.539885000	-2.629326000	3.541916000
H	-3.780339000	-3.789185000	2.434924000
C	-5.892081000	-2.502307000	1.021893000
H	-6.624434000	-2.431968000	1.839833000
H	-6.269866000	-1.913227000	0.175249000
H	-5.837312000	-3.553737000	0.713115000
H	-4.734784000	-0.920902000	1.864293000

12 $[PCy_3Cl_2Ru(CH_2CH_2CH_2)]$

Total SCF energy = -2181.05655 Hartree

Ru	-1.912410000	0.150789000	-0.021044000
C	-3.319728000	0.551634000	-1.325893000
C	-3.337065000	-0.179444000	1.280920000
Cl	-2.098209000	-2.153543000	-0.675318000
Cl	-1.955054000	2.446200000	0.617698000
C	-4.149708000	0.211552000	-0.021836000
C	0.745515000	-1.855873000	-3.767065000
C	0.378958000	-0.804221000	-2.708164000
C	1.092329000	-1.106076000	-1.368997000
C	2.619230000	-1.147071000	-1.583470000
P	0.479549000	-0.022622000	0.034288000
C	2.989327000	-2.198582000	-2.646116000
C	2.262777000	-1.947684000	-3.974608000
C	0.435906000	-2.712834000	3.329178000
C	2.186212000	3.639826000	-1.242950000
C	1.233861000	2.432998000	-1.202628000
C	1.531110000	1.530228000	0.015691000
C	1.453135000	2.353189000	1.320667000
C	2.413672000	3.552792000	1.270666000
C	2.134217000	4.450564000	0.058173000
C	0.230857000	-2.219065000	1.887206000
C	0.897978000	-0.845221000	1.678496000
C	2.405429000	-0.947259000	2.009912000
C	2.604430000	-1.416092000	3.462396000
C	1.919557000	-2.764743000	3.716045000
H	-3.405764000	1.601630000	-1.623941000
H	-3.461532000	-0.186589000	-2.121854000
H	-3.436542000	0.562466000	2.080080000
H	-3.488007000	-1.223697000	1.574251000
H	-4.710572000	1.118814000	0.229949000
H	-4.762214000	-0.662126000	-0.271146000
H	0.241631000	-1.614035000	-4.715807000
H	0.352505000	-2.835347000	-3.445086000

12' $[PCy_3Cl_2Ru(CH_2CH_2CH_2)]$

Total SCF energy = -2181.0468 Hartree

Ru	1.002754000	-1.751537000	-0.131247000
Cl	1.637277000	-1.790438000	2.080446000
Cl	2.103511000	-1.360202000	-2.098263000
P	-0.070222000	0.202633000	0.008459000
C	-1.061883000	0.723043000	-1.521543000
C	-2.385905000	-0.042157000	-1.730453000
C	-2.951178000	0.212389000	-3.138569000
C	-3.186111000	1.709151000	-3.378547000
C	-1.915664000	2.521185000	-3.096422000
C	-1.341315000	2.235395000	-1.694628000
C	-1.107226000	0.412722000	1.577707000
C	-2.346181000	-0.503640000	1.660148000
C	-2.951200000	-0.484375000	3.074411000
C	-3.326086000	0.940325000	3.503508000
C	-2.128127000	1.888232000	3.372800000
C	-1.512220000	1.853671000	1.960420000
C	1.166596000	1.631300000	0.173783000
C	2.024944000	1.586086000	1.453762000
C	2.824973000	2.890051000	1.620974000
C	3.696411000	3.183089000	0.392897000
C	2.858103000	3.184191000	-0.891977000
C	2.068256000	1.872638000	-1.052160000
H	-0.366325000	0.412809000	-2.324364000
H	-3.125852000	0.306932000	-0.991474000
H	-2.256653000	-1.117559000	-1.562331000
H	-2.242313000	-0.177913000	-3.890016000
H	-3.888917000	-0.350888000	-3.268497000
H	-3.996370000	2.057788000	-2.713095000
H	-3.532150000	1.886465000	-4.409135000
H	-2.117703000	3.599514000	-3.196420000
H	-1.147428000	2.275163000	-3.850773000
H	-0.388262000	0.046813000	2.333537000
H	-2.068638000	2.564142000	-0.932893000

H	-0.708920000	-0.796984000	-2.555519000
H	0.673611000	0.193069000	-3.073999000
H	0.741539000	-2.103640000	-1.047462000
H	3.150398000	-1.366113000	-0.647091000
H	2.970599000	-0.157332000	-1.922181000
H	4.080460000	-2.200434000	-2.796995000
H	2.722747000	-3.200639000	-2.267643000
H	2.506063000	-2.742227000	-4.697144000
H	2.628931000	-1.002662000	-4.413788000
H	-0.027270000	-3.704946000	3.444236000
H	-0.098746000	-2.037234000	4.020122000
H	1.931243000	4.276659000	-2.104481000
H	3.219283000	3.284992000	-1.411007000
H	1.326357000	1.866104000	-2.140277000
H	0.190832000	2.780963000	-1.132621000
H	2.564164000	1.146262000	-0.089379000
H	1.694650000	1.732865000	2.195728000
H	0.419658000	2.707634000	1.451785000
H	2.324550000	4.129203000	2.204707000
H	3.457268000	3.191079000	1.224174000
H	2.855119000	5.282262000	0.020213000
H	1.132994000	4.901177000	0.164814000
H	-0.837650000	-2.181578000	1.641064000
H	0.672518000	-2.948697000	1.187428000
H	0.444895000	-0.139292000	2.399955000
H	2.922367000	0.008486000	1.848756000
H	2.874176000	-1.682243000	1.335804000
H	3.681558000	-1.481177000	3.683051000
H	2.189659000	-0.655984000	4.147654000
H	2.033571000	-3.058914000	4.771046000
H	2.424180000	-3.544031000	3.117999000

H	-0.436444000	2.840232000	-1.550993000
H	-2.088424000	-1.531346000	1.374675000
H	-3.111481000	-0.156134000	0.947804000
H	-2.219695000	-0.905389000	3.785659000
H	-3.835691000	-1.140210000	3.106961000
H	-3.706365000	0.944562000	4.537144000
H	-4.150856000	1.306109000	2.865917000
H	-1.352473000	1.601016000	4.104197000
H	-2.423026000	2.920682000	3.619326000
H	-0.650348000	2.533696000	1.933276000
H	-2.246898000	2.239842000	1.233897000
H	0.494577000	2.505021000	0.260098000
H	2.718201000	0.733172000	1.398650000
H	1.407364000	1.413111000	2.346770000
H	2.126025000	3.730884000	1.782850000
H	3.446721000	2.824252000	2.527745000
H	4.218332000	4.145610000	0.512892000
H	4.479426000	2.409085000	0.311196000
H	2.155849000	4.037797000	-0.869386000
H	3.502693000	3.333392000	-1.772446000
H	1.482180000	1.900414000	-1.982413000
H	2.767774000	1.031408000	-1.163165000
C	-0.257864000	-2.806736000	-1.562647000
C	-1.201218000	-3.439284000	-0.566917000
C	-0.294620000	-3.296477000	0.629924000
H	-2.134390000	-2.869253000	-0.442845000
H	-0.735315000	-3.086810000	1.609113000
H	-1.484105000	-4.482015000	-0.808380000
H	0.440858000	-3.530256000	-2.006009000
H	0.435735000	-4.117512000	0.729121000
H	-0.665785000	-2.170396000	-2.354158000

13 [$PyCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1381.98280 Hartree

Ru	0.713888000	0.000004000	-0.000003000
Cl	0.699822000	2.344288000	-0.380606000
Cl	0.699881000	-2.344279000	0.380588000
C	2.111645000	0.238377000	1.339256000
H	2.237443000	1.252174000	1.732799000
C	2.927288000	-0.000047000	0.000023000
H	3.513142000	-0.910747000	0.160898000
C	2.111703000	-0.238297000	-1.339239000
H	2.230868000	0.576419000	-2.060606000
H	2.237462000	-1.252067000	-1.732864000
H	3.513309000	0.910561000	-0.160777000
H	2.230789000	-0.576285000	2.060688000
N	-1.310297000	0.000000000	-0.000006000
C	-1.995300000	-0.943303000	-0.696378000
C	-1.995311000	0.943290000	0.696371000
C	-3.384906000	-0.952230000	-0.732990000
C	-3.384918000	0.952187000	0.732998000
C	-4.096993000	-0.000029000	0.000008000
H	-1.389993000	-1.700352000	-1.191880000

13' [$PyCl_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -1381.96168 Hartree

Ru	0.248220000	-0.080716000	0.030944000
Cl	2.573047000	0.010389000	0.357000000
Cl	-1.590192000	-1.093261000	-0.939059000
C	0.517475000	1.829615000	-0.491124000
C	-0.708508000	2.465983000	0.108963000
C	-1.189173000	1.229840000	0.874605000
H	-0.462685000	3.322690000	0.754504000
H	-0.997687000	1.289605000	1.953545000
H	1.488658000	2.332842000	-0.484365000
H	-1.432101000	2.805974000	-0.649237000
H	0.366134000	1.315292000	-1.499895000
H	-2.211544000	0.891121000	0.674546000
N	0.215229000	-1.060882000	1.769533000
C	-0.304272000	-2.317499000	1.843512000
C	0.746163000	-0.511502000	2.892301000
C	-0.313331000	-3.037692000	3.031160000
C	0.754461000	-1.185459000	4.109667000
C	0.219335000	-2.470392000	4.191779000
H	-0.719771000	-2.716490000	0.921030000

H	-1.390014000	1.700352000	1.191865000
H	-3.894375000	-1.718966000	-1.315586000
H	-3.894397000	1.718913000	1.315600000
H	-5.187422000	-0.000040000	0.000015000

H	1.182229000	0.476873000	2.775212000
H	-0.742752000	-4.039110000	3.031424000
H	1.193258000	-0.694537000	4.977808000
H	0.220975000	-3.019461000	5.133449000

14 [$PyF_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -661.19054 Hartree

Ru	-0.811907000	0.057854000	-0.001268000
F	-0.744423000	-1.987677000	0.009802000
F	-0.803910000	2.061503000	-0.010619000
C	-2.182890000	-0.163314000	1.347670000
H	-2.295751000	-1.167045000	1.771792000
C	-3.000653000	0.052663000	0.001973000
H	-3.473340000	1.037961000	-0.004317000
C	-2.187294000	-0.182925000	-1.342785000
H	-2.301437000	-1.192743000	-1.751771000
H	-2.318745000	0.642639000	-2.053278000
H	-3.712377000	-0.781503000	0.009333000
H	-2.312662000	0.672604000	2.046263000
N	1.228538000	0.000288000	-0.000423000
C	1.920882000	1.168420000	0.003308000
C	1.890845000	-1.184744000	-0.003888000
C	3.312487000	1.181278000	0.004277000
C	3.279525000	-1.228024000	-0.003492000
C	4.005461000	-0.031195000	0.000771000
H	1.295250000	2.064443000	0.004107000
H	1.230605000	-2.057152000	-0.005252000
H	3.838215000	2.135826000	0.007232000
H	3.782851000	-2.194580000	-0.006233000
H	5.096342000	-0.045420000	0.001226000

14'[$PyF_2Ru(CH_2CH_2CH_2)$]

Total SCF energy = -661.18079 Hartree

Ru	0.358926000	-0.178163000	-0.112755000
F	2.273227000	0.130909000	0.230540000
F	-0.941704000	-1.347414000	-0.958483000
C	0.420116000	1.866509000	-0.237072000
C	-0.860813000	2.188149000	0.499495000
C	-1.448729000	0.787730000	0.420346000
H	-0.646364000	2.487193000	1.535394000
H	-1.877420000	0.384969000	1.348238000
H	1.370742000	2.308360000	0.080376000
H	-1.484060000	2.979171000	0.043472000
H	0.327957000	1.898858000	-1.347968000
H	-2.127847000	0.606967000	-0.422783000
N	0.367875000	-0.964909000	1.683835000
C	-0.552875000	-1.931909000	1.961920000
C	1.260069000	-0.607742000	2.648650000
C	-0.597929000	-2.562969000	3.199084000
C	1.247088000	-1.203802000	3.904019000
C	0.309140000	-2.197582000	4.196440000
H	-1.233523000	-2.171425000	1.146285000
H	1.983127000	0.149485000	2.356074000
H	-1.352696000	-3.330569000	3.368746000
H	1.976223000	-0.877492000	4.645501000
H	0.282639000	-2.671102000	5.177946000

15 [$PyF_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -818.50491 Hartree

Ru	-0.332250000	0.000248000	0.083697000
F	-0.237192000	0.002247000	-1.971237000
F	-0.237389000	-0.001312000	2.109182000
C	-1.731869000	-1.386338000	-0.029698000
C	-2.492519000	-0.001153000	0.272762000
H	-2.855322000	-0.002440000	1.305476000
C	-1.734229000	1.385140000	-0.027528000
H	-3.299599000	-0.001580000	-0.468097000
N	1.725011000	0.000648000	-0.028620000
C	2.440393000	-0.000596000	1.125640000
C	2.371614000	0.001815000	-1.221750000
C	3.832474000	-0.000724000	1.116143000
C	3.759817000	0.001734000	-1.289822000
C	4.506641000	0.000455000	-0.106715000
H	1.833184000	-0.001493000	2.034348000
H	1.698366000	0.002716000	-2.083593000
H	4.373383000	-0.001731000	2.062250000

15' [$PyF_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -818.498551040 Hartree

Ru	-0.054926000	0.199488000	-0.958935000
F	1.858553000	-0.260827000	-0.995762000
F	-1.880202000	-0.454704000	-1.329035000
C	0.754789000	2.110808000	-1.296151000
C	-0.134567000	2.861029000	-0.335267000
C	-1.185565000	1.804252000	0.027764000
H	0.450709000	3.161145000	0.547952000
H	-0.574547000	3.784843000	-0.763465000
C	0.177571000	1.785171000	-2.644520000
H	0.942769000	1.677530000	-3.422312000
H	-0.360452000	0.742481000	-2.681474000
H	-0.635996000	2.446164000	-2.973019000
C	-2.548386000	2.055919000	-0.610937000
H	-2.503355000	2.163445000	-1.702354000
H	-3.259292000	1.251854000	-0.390024000
H	-2.953799000	3.002388000	-0.203898000
N	-0.004276000	-0.948909000	0.719309000

H	4.245762000	0.002633000	-2.265404000
H	5.597221000	0.000374000	-0.139220000
C	-1.783274000	-2.365918000	1.135785000
H	-2.792044000	-2.809567000	1.218270000
H	-1.086858000	-3.197609000	0.948589000
H	-1.513562000	-1.887817000	2.083959000
C	-1.786213000	2.362978000	1.139368000
H	-2.795320000	2.805720000	1.222638000
H	-1.516014000	1.883690000	2.086805000
H	-1.090473000	3.195491000	0.953325000
C	-2.099513000	2.030414000	-1.353473000
H	-1.408983000	2.861033000	-1.561229000
H	-2.032174000	1.324624000	-2.187345000
H	-3.116649000	2.458640000	-1.300292000
C	-2.096361000	-2.030145000	-1.356596000
H	-1.404622000	-2.859470000	-1.565516000
H	-3.112863000	-2.459934000	-1.303990000
H	-2.030039000	-1.323123000	-2.189503000

C	-1.033691000	-1.783531000	1.015559000
C	1.091525000	-0.957279000	1.520223000
C	-0.998341000	-2.633715000	2.115050000
C	1.178426000	-1.777795000	2.640757000
C	0.120779000	-2.634405000	2.951765000
H	-1.879988000	-1.728114000	0.330622000
H	1.898739000	-0.297603000	1.211090000
H	-1.851563000	-3.283950000	2.307580000
H	2.076569000	-1.738008000	3.256927000
H	0.167173000	-3.286796000	3.824348000
C	-1.339616000	1.619421000	1.529680000
H	-2.031717000	0.802238000	1.778307000
H	-0.381290000	1.431111000	2.033335000
H	-1.761397000	2.544869000	1.966368000
C	2.230412000	2.419197000	-1.247534000
H	2.615007000	2.347811000	-0.220791000
H	2.821257000	1.748896000	-1.881667000
H	2.390770000	3.460036000	-1.586988000

16 $[C_5F_5NF_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -1314.87521 Hartree

Ru	-1.062837000	-0.000007000	-0.000012000
F	-0.984649000	0.000106000	2.025343000
F	-0.984653000	-0.000176000	-2.025362000
C	-2.447656000	1.407749000	-0.000080000
C	-3.232672000	0.000036000	0.000033000
H	-3.826900000	-0.000082000	-0.918525000
C	-2.447603000	-1.407750000	0.000123000
H	-3.826856000	0.000048000	0.918620000
N	0.981097000	0.000002000	-0.000019000
C	1.676386000	1.151188000	-0.000092000
C	1.676391000	-1.151183000	0.000062000
C	3.065342000	1.204313000	-0.000084000
C	3.065347000	-1.204302000	0.000076000
C	3.780550000	0.000008000	0.000002000
C	-2.640641000	2.220420000	-1.269053000
H	-3.653019000	2.662189000	-1.280681000
H	-1.927040000	3.057395000	-1.280655000
H	-2.479083000	1.617372000	-2.168275000
C	-2.640623000	-2.220581000	-1.268740000
H	-3.653010000	-2.662331000	-1.280308000
H	-2.479047000	-1.617656000	-2.168042000
H	-1.927039000	-3.057573000	-1.280228000
C	-2.640612000	-2.220410000	1.269096000
H	-1.927066000	-3.057434000	1.280665000
H	-2.478979000	-1.617374000	2.168314000
H	-3.653018000	-2.662113000	1.280755000
C	-2.640595000	2.220607000	1.268778000
H	-1.926951000	3.057547000	1.280255000
H	-3.652951000	2.662429000	1.280349000
H	-2.479057000	1.617680000	2.168083000
F	3.705123000	2.378084000	-0.000157000
F	3.705134000	-2.378069000	0.000159000

16' $[C_5F_5NF_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -1314.8648 Hartree

Ru	-1.171345000	-0.534790000	-0.462580000
F	-0.719100000	0.275787000	-2.181306000
F	-1.081559000	-2.198758000	0.559868000
C	-2.628629000	1.002221000	-0.518642000
C	-2.668245000	1.270053000	0.965996000
C	-1.952363000	0.045579000	1.536532000
H	-2.116862000	2.197510000	1.180100000
H	-3.694459000	1.401019000	1.368515000
C	-3.364865000	-0.199148000	-1.027782000
H	-3.596290000	-0.135753000	-2.097215000
H	-2.747738000	-1.218070000	-0.968287000
H	-4.244866000	-0.500656000	-0.442640000
C	-2.906282000	-1.001591000	2.108214000
H	-3.677807000	-1.334654000	1.402306000
H	-2.370282000	-1.890851000	2.456255000
H	-3.432830000	-0.549466000	2.970106000
N	0.845698000	-0.171432000	-0.090237000
C	1.767857000	-1.147705000	-0.237032000
C	1.319027000	1.075755000	0.099424000
C	3.140648000	-0.938468000	-0.119312000
C	2.669529000	1.386189000	0.230235000
C	3.606967000	0.354823000	0.130033000
C	-0.859473000	0.328757000	2.553232000
H	-0.242927000	-0.565323000	2.724353000
H	-0.212800000	1.169876000	2.275865000
H	-1.320346000	0.591455000	3.524640000
C	-2.565388000	2.200157000	-1.433025000
H	-1.770098000	2.892221000	-1.126327000
H	-2.397024000	1.919699000	-2.478370000
H	-3.522386000	2.751461000	-1.365356000
F	0.441648000	2.072676000	0.174404000
F	1.343816000	-2.362069000	-0.550794000

F	0.964130000	-2.276309000	0.000132000	F	3.063531000	2.647676000	0.442033000
F	0.964121000	2.276311000	-0.000174000	F	4.910915000	0.601504000	0.248799000
F	5.113626000	0.000010000	0.000013000	F	3.997781000	-1.954304000	-0.267004000

17 $[(PH_3)_2Cl_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -1977.30847 Hartree

Ru	0.001770000	-0.102470000	0.031032000
Cl	1.728625000	-1.870483000	0.003501000
Cl	-1.595249000	-1.907256000	0.528784000
C	1.409284000	1.279305000	-0.464891000
C	0.000576000	2.046912000	-0.199577000
H	-0.159799000	2.603641000	-1.128128000
C	-1.443954000	1.329601000	0.053874000
H	0.166621000	2.699256000	0.662156000
P	0.458624000	-0.139448000	2.311141000
H	-0.424685000	-0.955091000	3.064255000
H	1.699047000	-0.710398000	2.693304000
H	0.480894000	0.992469000	3.187349000
P	-0.522519000	-0.963276000	-2.098903000
H	-1.886061000	-1.147777000	-2.440409000
H	-0.088239000	-0.440492000	-3.357925000
H	-0.048157000	-2.285580000	-2.252424000
C	-2.417643000	1.481215000	-1.103682000
H	-1.938638000	1.389111000	-2.087732000
H	-3.187853000	0.698343000	-1.023103000
H	-2.939594000	2.453982000	-1.070700000
C	-2.120833000	1.727843000	1.352999000
H	-2.675595000	2.677806000	1.255803000
H	-2.853094000	0.946239000	1.610755000
H	-1.423991000	1.827383000	2.193900000
C	2.510944000	1.640489000	0.514110000
H	2.151728000	1.781335000	1.541942000
H	3.246129000	0.819812000	0.518517000
H	3.044091000	2.559302000	0.213162000
C	1.928006000	1.366355000	-1.889281000
H	2.501335000	2.295030000	-2.056643000
H	2.615475000	0.522787000	-2.059133000
H	1.135274000	1.313648000	-2.644095000

17' $[(PH_3)_2Cl_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -1977.30548 Hartree

Ru	0.000052000	-0.371555000	-0.288049000
Cl	2.121523000	-1.205559000	-0.763425000
Cl	-2.121708000	-1.203672000	-0.765299000
C	1.207479000	1.241005000	0.790887000
C	0.000402000	2.147019000	0.948935000
H	0.000544000	2.906183000	0.151104000
C	-1.206985000	1.241400000	0.790859000
H	0.000451000	2.697259000	1.914918000
P	-0.001530000	-2.049692000	1.365155000
P	0.000874000	0.799900000	-2.267246000
H	1.083093000	0.535966000	-3.153205000
H	-1.080389000	0.534459000	-3.153909000
H	0.000028000	2.220295000	-2.403670000
H	1.075247000	-2.244448000	2.272890000
H	-1.079929000	-2.244022000	2.270975000
H	-0.001221000	-3.344438000	0.785085000
C	2.326320000	1.884513000	-0.022056000
H	3.188860000	1.221547000	-0.153119000
H	1.998607000	2.221326000	-1.015567000
H	2.668407000	2.787941000	0.519941000
C	1.776408000	0.711145000	2.100236000
H	2.262587000	1.548028000	2.639241000
H	1.012564000	0.304958000	2.775318000
H	2.541041000	-0.057997000	1.928631000
C	-2.325553000	1.885509000	-0.022049000
H	-3.188695000	1.223222000	-0.152600000
H	-2.666665000	2.789431000	0.519737000
H	-1.997919000	2.221580000	-1.015829000
C	-1.776327000	0.711742000	2.100083000
H	-2.262172000	1.548807000	2.639112000
H	-2.541378000	-0.056929000	1.928192000
H	-1.012809000	0.305067000	2.775238000

18 $[(PH_2Me)_2Cl_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -2055.97987 Hartree

Ru	0.103969000	-0.200940000	0.030841000
Cl	1.877807000	-1.924816000	0.082420000
Cl	-1.460387000	-2.046578000	0.568240000
C	1.429342000	1.244416000	-0.505948000
C	-0.044749000	1.923585000	-0.315667000
H	-0.270148000	2.361815000	-1.292554000
C	-1.411296000	1.154561000	0.116533000
H	0.105201000	2.675616000	0.464562000
P	0.765877000	-0.191965000	2.300465000

18' $[(PH_2Me)_2Cl_2Ru(CMe_2CH_2CMe_2)]$

Total SCF energy = -2055.97576 Hartree

Ru	0.034021000	0.053076000	-0.407130000
Cl	-0.067864000	2.130597000	-1.468162000
Cl	0.507139000	-2.097116000	-1.188076000
C	-0.508985000	1.333624000	1.404441000
C	-0.747895000	0.123704000	2.287961000
H	-1.826952000	-0.094911000	2.332284000
C	-0.023927000	-1.020062000	1.604860000
H	-0.410587000	0.281328000	3.335951000
P	2.366792000	0.464408000	-0.600411000

H	2.167095000	-0.280474000	2.491822000
H	0.545960000	0.933033000	3.160087000
P	-0.496772000	-0.974654000	-2.115915000
H	-1.859733000	-1.343639000	-2.234361000
H	-0.443631000	-0.130169000	-3.272237000
C	-2.500760000	1.196436000	-0.942160000
H	-2.117320000	1.110628000	-1.967254000
H	-3.194294000	0.359629000	-0.763243000
H	-3.090133000	2.128217000	-0.882193000
C	-1.991303000	1.581316000	1.454241000
H	-2.593479000	2.502657000	1.361539000
H	-2.668641000	0.785779000	1.803208000
H	-1.234555000	1.746832000	2.229114000
C	2.470927000	1.778673000	0.463147000
H	2.077316000	1.959011000	1.471922000
H	3.287860000	1.044000000	0.539477000
H	2.914758000	2.723393000	0.102628000
C	1.981618000	1.300608000	-1.919830000
H	2.440623000	2.280706000	-2.141075000
H	2.777934000	0.544268000	-2.004967000
H	1.234052000	1.092264000	-2.693355000
C	0.336857000	-2.474317000	-2.763682000
H	0.216184000	-3.271823000	-2.021310000
H	-0.103235000	-2.771085000	-3.724208000
H	1.409587000	-2.279964000	-2.877044000
C	0.171487000	-1.552584000	3.376251000
H	-0.920686000	-1.508837000	3.455295000
H	0.437149000	-2.499400000	2.891726000
H	0.632945000	-1.483781000	4.369567000

P	-2.167931000	-0.220946000	-1.087813000
H	-2.871427000	0.996501000	-1.300710000
H	2.927063000	1.674486000	-0.102658000
C	-1.756784000	2.197685000	1.260985000
H	-1.623306000	3.032812000	0.563463000
H	-2.636282000	1.619015000	0.946066000
H	-1.997680000	2.621181000	2.255920000
C	0.662691000	2.207083000	1.837862000
H	0.392546000	2.713362000	2.785517000
H	1.581957000	1.641665000	2.033375000
H	0.884164000	2.987932000	1.098376000
C	-0.808987000	-2.325049000	1.666438000
H	-0.287259000	-3.159416000	1.184013000
H	-0.952883000	-2.583777000	2.734338000
H	-1.806897000	-2.239049000	1.223729000
C	1.385264000	-1.268180000	2.121794000
H	1.318882000	-1.688271000	3.145166000
H	1.915791000	-2.002175000	1.501315000
H	1.990276000	-0.356144000	2.194845000
C	3.745637000	-0.723897000	-0.287849000
H	4.660524000	-0.389041000	-0.792450000
H	3.936913000	-0.814283000	0.787430000
H	3.448804000	-1.705897000	-0.677629000
C	-3.543382000	-1.293744000	-0.465778000
H	-3.224555000	-2.342928000	-0.489534000
H	-3.798472000	-1.025343000	0.567404000
H	-4.432229000	-1.174794000	-1.099016000
H	2.591072000	0.725987000	-1.977674000
H	-2.148751000	-0.661669000	-2.440686000

19 [$(PHMe_2)_2Cl_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -2134.64622 Hartree

Ru	0.000007000	0.046688000	0.065835000
Cl	0.000191000	0.979669000	-2.174777000
Cl	0.000095000	-2.183313000	-1.136232000
C	-0.000052000	1.724277000	1.203644000
C	-0.000132000	0.378854000	2.212713000
H	-0.911026000	0.528763000	2.801146000
C	-0.000103000	-1.129990000	1.754393000
H	0.910680000	0.528757000	2.801276000
P	2.370460000	0.034123000	-0.243180000
H	3.171829000	0.184472000	0.934104000
P	-2.370441000	0.034065000	-0.243355000
H	-3.171858000	0.184265000	0.933913000
C	-1.236699000	-1.930818000	2.121506000
H	-2.172405000	-1.367689000	2.022352000
H	-1.284837000	-2.809301000	1.459896000
H	-1.175576000	-2.302726000	3.159634000
C	1.236421000	-1.930858000	2.121676000
H	1.175112000	-2.302824000	3.159772000
H	1.284660000	-2.809307000	1.460026000
H	2.172151000	-1.367743000	2.022720000
C	1.229298000	2.596835000	1.422450000

19' **[**$(PHMe_2)_2Cl_2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -2134.64891 Hartree

Ru	0.009354000	0.198372000	0.063577000
Cl	0.060192000	1.128012000	2.210077000
Cl	0.269115000	1.073279000	-2.094020000
C	-0.337345000	-1.702801000	1.296806000
C	-0.718326000	-2.513437000	0.074036000
H	-1.815780000	-2.552395000	-0.015770000
C	-0.134475000	-1.763129000	-1.106107000
H	-0.365164000	-3.567391000	0.129071000
P	2.381297000	0.474960000	0.240816000
P	-2.241590000	0.824020000	0.073919000
H	-2.836168000	0.765874000	1.365106000
H	2.989637000	0.058841000	1.458597000
C	-1.455940000	-1.670195000	2.331927000
H	-1.232996000	-1.022182000	3.187591000
H	-2.419699000	-1.363318000	1.904325000
H	-1.594532000	-2.700760000	2.714429000
C	0.958357000	-2.136889000	1.970224000
H	0.805006000	-3.136011000	2.424396000
H	1.801402000	-2.228023000	1.275189000
H	1.246226000	-1.448566000	2.776049000
C	-1.059012000	-1.765389000	-2.318103000

H	2.173971000	2.041206000	1.440898000	H	-0.629068000	-1.241578000	-3.179653000
H	1.283651000	3.336345000	0.608236000	H	-1.230558000	-2.820407000	-2.610881000
H	1.157660000	3.170104000	2.364509000	H	-2.039944000	-1.329107000	-2.104920000
C	-1.229439000	2.596844000	1.422199000	C	1.235347000	-2.264269000	-1.536392000
H	-1.158008000	3.170096000	2.364285000	H	1.111337000	-3.262323000	-2.001818000
H	-1.283603000	3.336370000	0.607986000	H	1.690524000	-1.607915000	-2.288665000
H	-2.174121000	2.041223000	1.440419000	H	1.934335000	-2.390386000	-0.702009000
C	-3.160758000	-1.461006000	-0.960513000	C	2.733979000	2.284192000	0.306549000
H	-2.937872000	-2.340765000	-0.347335000	H	2.140608000	2.737303000	1.108795000
H	-4.246806000	-1.312969000	-1.036901000	H	3.802090000	2.468188000	0.483631000
H	-2.726291000	-1.635436000	-1.952165000	H	2.438608000	2.729735000	-0.652440000
C	3.122197000	1.361963000	-1.275233000	C	3.665127000	-0.068814000	-0.972154000
H	2.762545000	1.240156000	-2.303353000	H	4.621653000	0.425739000	-0.755007000
H	2.805549000	2.350043000	-0.924763000	H	3.805483000	-1.154802000	-0.936214000
H	4.217654000	1.288830000	-1.244825000	H	3.334948000	0.209969000	-1.981418000
C	-3.122211000	1.362033000	-1.275212000	C	-3.667105000	0.213393000	-0.937283000
H	-2.762487000	1.240443000	-2.303328000	H	-3.447990000	0.349346000	-2.004202000
H	-4.217665000	1.288815000	-1.244875000	H	-3.846475000	-0.852802000	-0.748606000
H	-2.805653000	2.350073000	-0.924534000	H	-4.575598000	0.778133000	-0.685635000
C	3.160827000	-1.460993000	-0.960182000	C	-2.344231000	2.639367000	-0.235538000
H	2.726393000	-1.635518000	-1.951833000	H	-2.000012000	2.844952000	-1.257358000
H	4.246874000	-1.312945000	-1.036554000	H	-3.371457000	3.006718000	-0.106233000
H	2.937933000	-2.340700000	-0.346933000	H	-1.680088000	3.155955000	0.468482000

20 **[**(PMe_3)$_2$$Cl_2$Ru($CMe_2CH_2CMe_2$)]

Total SCF energy = -2213.29924 Hartree

Ru	-0.027334000	0.103590000	0.000245000
Cl	-0.254077000	-1.433354000	1.915596000
Cl	0.303617000	-1.925374000	-1.425860000
C	-0.230912000	1.761176000	1.145117000
C	-0.227128000	2.212315000	-0.439753000
H	0.546884000	2.987804000	-0.415938000
C	0.196266000	1.287651000	-1.662623000
H	-1.218933000	2.624977000	-0.643857000
P	-2.411974000	-0.437101000	-0.049407000
P	2.436560000	-0.389911000	0.222253000
C	-2.718190000	-2.158774000	-0.612561000
H	-2.362429000	-2.295777000	-1.638976000
H	-2.154106000	-2.841319000	0.033710000
H	-3.795482000	-2.369493000	-0.543329000
C	-3.355043000	-0.468129000	1.549852000
H	-4.206934000	-1.152212000	1.428498000
H	-2.706476000	-0.830862000	2.354062000
H	-3.742215000	0.524710000	1.804123000
C	-3.688631000	0.455683000	-1.070706000
H	-3.555944000	0.241426000	-2.137725000
H	-4.687393000	0.107367000	-0.769873000
H	-3.643528000	1.543119000	-0.919635000
C	2.709310000	-1.963867000	1.135551000
H	2.365061000	-1.867956000	2.170271000
H	2.124307000	-2.754831000	0.652734000
H	3.780882000	-2.209357000	1.109278000
C	3.694172000	0.666971000	1.096686000

20' **[**(PMe_3)$_2$$Cl_2$Ru($CMe_2CH_2CMe_2$)]

Total SCF energy = -2213.31558 Hartree

Ru	-0.023173000	0.109181000	0.000209000
Cl	0.044257000	0.970009000	2.183528000
Cl	0.046801000	0.994061000	-2.173322000
C	-0.087282000	-1.850527000	1.195442000
C	-0.498512000	-2.661406000	-0.013970000
H	-1.592466000	-2.791350000	-0.015053000
C	-0.086664000	-1.837578000	-1.214458000
H	-0.053885000	-3.682148000	-0.019164000
P	2.342828000	0.681570000	0.003829000
P	-2.316673000	0.699729000	0.003025000
C	2.348772000	2.528984000	0.020288000
H	1.823883000	2.899538000	-0.868748000
H	1.827338000	2.883674000	0.917766000
H	3.381857000	2.906203000	0.021338000
C	3.473837000	0.343607000	1.424751000
H	4.367952000	0.978892000	1.347380000
H	2.949978000	0.564981000	2.363101000
H	3.783893000	-0.708333000	1.432288000
C	3.470244000	0.369977000	-1.425731000
H	2.945393000	0.615256000	-2.357560000
H	4.367163000	0.999580000	-1.335596000
H	3.775586000	-0.682831000	-1.457687000
C	-2.270648000	2.548577000	0.014081000
H	-1.735147000	2.890145000	0.908528000
H	-1.737374000	2.900979000	-0.877482000
H	-3.292290000	2.956085000	0.017792000
C	-3.461980000	0.402385000	1.421595000

H	3.415298000	0.812516000	2.147033000	H	-2.922952000	0.554837000	2.364907000
H	4.670177000	0.161417000	1.058053000	H	-4.309507000	1.100830000	1.366671000
H	3.798484000	1.651156000	0.619092000	H	-3.851661000	-0.623256000	1.393868000
C	3.425820000	-0.754515000	-1.302920000	C	-3.462610000	0.419863000	-1.418449000
H	4.308664000	-1.339834000	-1.009840000	H	-4.312650000	1.114240000	-1.351632000
H	2.816318000	-1.338255000	-2.001911000	H	-2.925529000	0.589308000	-2.359969000
H	3.766855000	0.167572000	-1.785842000	H	-3.848587000	-0.607444000	-1.406490000
C	-0.806630000	1.189301000	-2.797440000	C	-1.103994000	-1.961100000	2.324442000
H	-0.653995000	1.985588000	-3.547894000	H	-0.845799000	-1.353453000	3.199406000
H	-0.654577000	0.222659000	-3.304051000	H	-2.117495000	-1.701418000	2.002496000
H	-1.844534000	1.237293000	-2.462154000	H	-1.132867000	-3.021313000	2.645861000
C	1.550946000	1.667531000	-2.242651000	C	1.290968000	-2.188586000	1.743094000
H	2.315902000	1.845071000	-1.476686000	H	1.249711000	-3.196596000	2.201857000
H	1.902531000	0.874488000	-2.916592000	H	2.072302000	-2.221725000	0.975785000
H	1.462571000	2.586667000	-2.849708000	H	1.593081000	-1.482817000	2.526602000
C	0.938701000	2.294781000	1.956378000	C	1.291257000	-2.171602000	-1.765784000
H	1.060672000	1.660274000	2.848153000	H	1.249497000	-3.176719000	-2.230775000
H	1.880863000	2.288186000	1.404601000	H	1.592408000	-1.461056000	-2.545423000
H	0.754468000	3.324354000	2.312739000	H	2.073423000	-2.209546000	-0.999481000
C	-1.522723000	2.181022000	1.825797000	C	-1.103532000	-1.935541000	-2.344611000
H	-2.409289000	2.023312000	1.203048000	H	-0.845785000	-1.317679000	-3.212529000
H	-1.641877000	1.601115000	2.753849000	H	-1.132245000	-2.991945000	-2.678334000
H	-1.496254000	3.247566000	2.111417000	H	-2.117051000	-1.679891000	-2.019376000

21 [$PMe_3NHMeCl2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -2058.22995 Hartree

Ru	-0.188076000	0.012689000	0.061075000	Ru	0.145531000	-0.057308000	-0.028980000
Cl	0.027529000	-0.877112000	-2.148211000	Cl	0.279241000	-0.779347000	-2.270051000
Cl	-0.322619000	2.207511000	-1.378317000	Cl	0.088492000	-1.042103000	2.109544000
C	-0.173168000	-1.376378000	1.577006000	C	0.334241000	1.947434000	-1.107756000
C	-0.731508000	0.031761000	2.193297000	C	0.058605000	2.773366000	0.138111000
H	-0.184141000	0.028697000	3.144699000	H	-0.947473000	3.217076000	0.118174000
C	-0.342830000	1.415642000	1.588622000	C	0.223370000	1.802238000	1.295047000
H	-1.808286000	-0.035755000	2.360998000	H	0.755802000	3.633326000	0.224834000
P	-2.570476000	-0.246137000	-0.521655000	P	2.495721000	-0.765879000	0.024201000
C	-3.191337000	0.896150000	-1.817741000	C	2.394781000	-2.607975000	-0.115277000
H	-3.166688000	1.928044000	-1.449710000	H	1.799067000	-2.999378000	0.718916000
H	-2.516598000	0.844503000	-2.680186000	H	1.909701000	-2.869576000	-1.064137000
H	-4.214134000	0.613387000	-2.107912000	H	3.400286000	-3.051829000	-0.085964000
C	-2.994062000	-1.872185000	-1.294885000	C	3.728086000	-0.433754000	-1.315459000
H	-4.058425000	-1.885577000	-1.570071000	H	4.572426000	-1.132778000	-1.228134000
H	-2.375332000	-2.001417000	-2.189830000	H	3.244683000	-0.569466000	-2.290960000
H	-2.788795000	-2.705134000	-0.612474000	H	4.108001000	0.592882000	-1.249599000
C	-3.973799000	-0.134235000	0.701507000	C	3.579333000	-0.640998000	1.517927000
H	-4.060618000	0.879621000	1.112133000	H	2.994330000	-0.914071000	2.405018000
H	-4.916338000	-0.382090000	0.192571000	H	4.435224000	-1.324480000	1.420545000
H	-3.842872000	-0.832684000	1.539282000	H	3.953312000	0.382164000	1.643101000
C	-1.473045000	2.426124000	1.585664000	C	-0.682317000	2.159974000	-2.228657000
H	-1.644226000	2.816060000	2.606205000	H	-0.356119000	1.699737000	-3.168368000
H	-1.200204000	3.265882000	0.933089000	H	-1.673840000	1.758182000	-1.996283000
H	-2.414062000	2.012842000	1.211764000	H	-0.791545000	3.249536000	-2.399394000
C	0.889560000	2.039077000	2.232007000	C	1.732447000	2.196443000	-1.653793000
H	1.760235000	1.372244000	2.231454000	H	1.761476000	3.218482000	-2.081729000

21' [$PMe_3NHMeCl2Ru(CMe_2CH_2CMe_2)$]

Total SCF energy = -2058.23980 Hartree

H	1.155461000	2.968500000	1.715892000	H	2.501988000	2.157089000	-0.873322000
H	0.664521000	2.312976000	3.278823000	H	1.995020000	1.494618000	-2.454292000
C	1.083107000	-1.799574000	2.352021000	C	1.576196000	1.966410000	1.976177000
H	1.515835000	-2.719451000	1.938469000	H	1.579883000	2.938108000	2.509883000
H	1.865562000	-1.031969000	2.361892000	H	1.763307000	1.181460000	2.718809000
H	0.815823000	-2.031005000	3.399791000	H	2.409771000	1.993986000	1.263210000
C	-1.209192000	-2.482460000	1.740815000	C	-0.871357000	1.906000000	2.355283000
H	-2.206866000	-2.208046000	1.384856000	H	-0.627473000	1.322448000	3.250582000
H	-0.887729000	-3.372073000	1.175744000	H	-0.964373000	2.968860000	2.654834000
H	-1.302057000	-2.798122000	2.797048000	H	-1.853536000	1.572581000	2.006607000
C	1.943522000	-0.082281000	-0.124213000	C	-1.937230000	-0.382940000	-0.087371000
N	2.608188000	-1.272497000	-0.283165000	N	-2.315639000	-1.694037000	-0.192683000
C	4.000407000	-1.104675000	-0.725622000	C	-3.742492000	-1.917203000	0.071095000
C	4.236191000	0.383343000	-0.503465000	C	-4.309761000	-0.512728000	-0.077235000
N	2.870945000	0.894120000	-0.297810000	N	-3.103104000	0.323050000	0.047063000
H	4.087170000	-1.394126000	-1.788531000	H	-3.878773000	-2.320511000	1.091095000
H	4.852722000	0.591640000	0.388765000	H	-4.776853000	-0.347472000	-1.065578000
C	2.061118000	-2.594561000	-0.519101000	C	-1.466647000	-2.870487000	-0.163924000
H	2.175628000	-2.863824000	-1.581961000	H	-1.341933000	-3.252409000	0.861961000
H	2.604013000	-3.335436000	0.091507000	H	-1.927288000	-3.649522000	-0.790736000
H	0.997277000	-2.615343000	-0.282794000	H	-0.484332000	-2.638914000	-0.584129000
C	2.726317000	2.335743000	-0.308051000	C	-3.333704000	1.745652000	-0.055298000
H	3.215066000	2.786761000	0.572479000	H	-3.821536000	1.996622000	-1.014668000
H	3.219306000	2.728737000	-1.211420000	H	-3.995949000	2.077964000	0.760350000
H	1.665002000	2.600994000	-0.369729000	H	-2.393757000	2.288089000	0.012812000
H	4.704841000	0.885364000	-1.362306000	H	-5.046005000	-0.251135000	0.696443000
H	4.676326000	-1.747586000	-0.142387000	H	-4.164245000	-2.638968000	-0.643048000

22

Total SCF energy = -988.4292 Hartree

W	0.750681000	-0.723733000	-0.281639000
C	0.273759000	-2.403762000	-1.414453000
H	1.068116000	-3.068664000	-1.756500000
H	-0.625300000	-2.948097000	-1.113674000
C	-0.054981000	-1.251982000	-2.481090000
H	0.598096000	-1.419399000	-3.341756000
H	-1.110245000	-1.364820000	-2.746050000
C	0.143789000	0.266960000	-2.022433000
H	0.888986000	0.784032000	-2.630195000
H	-0.807171000	0.805957000	-1.984797000
O	-1.151858000	-0.598225000	0.211423000
C	-2.421918000	-0.155580000	0.192290000
C	-3.486530000	-1.076760000	0.141572000
C	-4.804647000	-0.619027000	0.124664000
C	-5.083535000	0.751991000	0.162194000
H	-6.115601000	1.103962000	0.151726000
C	-4.026639000	1.666556000	0.222458000
C	-2.702466000	1.224373000	0.239730000
N	2.456519000	-0.689836000	-0.811852000
C	3.707563000	-0.540553000	-1.350217000
C	4.539059000	-1.668063000	-1.548150000
H	4.171010000	-2.650560000	-1.250801000
C	5.807103000	-1.515049000	-2.104870000

23

Total SCF energy = -1794.3140 Hartree

W	0.265330000	-0.798622000	-0.269171000
C	0.231980000	-2.298832000	-1.699763000
H	1.107544000	-2.358215000	-2.350205000
H	1.343244000	-3.731803000	-0.487940000
C	0.412435000	-3.171126000	-0.368028000
H	-0.460114000	-3.823918000	-0.292122000
H	-0.700002000	-2.518775000	-2.220739000
C	0.535963000	-2.390379000	1.027352000
H	1.534377000	-2.488008000	1.459762000
H	-0.258845000	-2.652967000	1.725580000
N	-1.503558000	-0.787779000	-0.082072000
C	-2.858291000	-0.787698000	0.040294000
C	-3.701554000	-0.700671000	-1.093371000
F	-3.156143000	-0.640829000	-2.317167000
C	-5.089291000	-0.674116000	-0.970809000
F	-5.866338000	-0.591760000	-2.060516000
C	-5.676590000	-0.736889000	0.298652000
F	-7.008699000	-0.715754000	0.420486000
C	-4.871150000	-0.827620000	1.440320000
F	-5.439507000	-0.891790000	2.653138000
C	-3.484335000	-0.853561000	1.308100000
F	-2.727969000	-0.942136000	2.412437000
O	0.523581000	1.153425000	-0.222102000

C	6.274183000	-0.246769000	-2.470857000	O	2.259917000	-0.787471000	-0.504010000
H	7.268760000	-0.132887000	-2.903691000	C	-0.327534000	2.170844000	-0.075714000
C	5.461290000	0.875340000	-2.270531000	F	-1.270285000	2.216906000	-1.066952000
C	4.190904000	0.738423000	-1.714370000	F	-1.011392000	2.120633000	1.108929000
H	3.555718000	1.608107000	-1.543041000	F	0.339664000	3.347221000	-0.103006000
N	1.196101000	-0.326422000	1.682846000	C	3.457721000	-1.271954000	-0.724709000
C	0.292937000	-0.177596000	2.743376000	F	4.430255000	-0.333611000	-0.602906000
H	-0.773189000	-0.269078000	2.575724000	F	3.780427000	-2.289164000	0.151120000
C	0.986555000	0.067771000	3.906451000	F	3.580373000	-1.810404000	-1.984824000
H	0.546073000	0.220970000	4.887919000				
C	2.379499000	0.078703000	3.576004000				
H	3.211676000	0.244548000	4.254772000				
C	2.476198000	-0.162793000	2.224849000				
H	-5.621925000	-1.341492000	0.086314000				
H	-3.261035000	-2.143866000	0.125663000				
H	-1.874257000	1.931157000	0.304909000				
H	-4.233156000	2.737623000	0.261871000				
H	3.351311000	-0.235773000	1.589531000				
H	6.439257000	-2.392508000	-2.251142000				
H	5.823164000	1.867386000	-2.545930000				