

Supporting Information for
Excited State Relaxation Processes of H₂-evolution Ru–Pd supramolecular
photocatalyst containing a linear or non-linear bridge: A DFT and TDDFT
Study

Jun Cao*^{ab} and Yun Zhou^a

^a*Guizhou Provincial Key Laboratory of Computational Nano-material Science,
Guizhou Synergetic Innovation Center of Scientific Big Data for Advanced
Manufacturing Technology, Guizhou Education University, Guiyang, Guizhou,
550018, China*

^b*Key Laboratory of Theoretical and Computational Photochemistry, Ministry of
Education, College of Chemistry, Beijing Normal University, Beijing 100875, China*

Contents:

1. **Table S1.** Selected geometrical parameters for the optimized minima.
2. **Table S2.** The relative energies for all optimized structures.
3. **Table S3.** Singlet excitation energies of Ru_1 and RuPd_1.
4. **Table S4.** Singlet excitation energies of Ru_2 and RuPd_2.
5. **Table S5.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{bpy}-³MC_{Ru} conversion of Ru_1.
6. **Table S6.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{bpy}-³MC_{Ru} conversion of RuPd_1.
7. **Table S7.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of Ru_1.
8. **Table S8.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of RuPd_1.
9. **Table S9.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{bpy} - ³MLCT_{tpy} conversion of Ru_1.
10. **Table S10.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{bpy}-³MLCT_{tpy} conversion of RuPd_1.
11. **Table S11.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MC_{Ru}-S₀ conversion of Ru_1.
12. **Table S12.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MC_{Ru}-S₀ conversion of RuPd_1.
13. **Table S13.** The MOs involved in the TDDFT excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of RuPd_2.
14. **Table S14.** Spin density on the Ru atom for the ³MLCT_{tpy}-³MC_{Ru} crossing of RuPd_2.
15. **Figure S1.** UV absorption of the studied system calculated with TD-PBE0.
16. **Figure S2.** UV absorption of the studied system calculated with TD-CAM-B3LYP based on the PBE0 optimized structures.
17. **Figure S3.** UV absorption of the studied system calculated with TD-wB97xD

based on the PBE0 optimized structures.

18. **Figure S4.** Natural Transition Orbital (NTO) analysis for vertical excitations with maximum oscillator strength in both the strongest and the weaker transition regions of RuPd_1.
19. **Figure S5.** The calculated HOMO and LUMO levels of Ru_1 and RuPd_1.
20. **Figure S6.** The calculated HOMO and LUMO levels of Ru_2 and RuPd_2.
21. **S1.** Cartesian coordinates of all optimized structures.

Table S1. Selected geometrical parameters for the optimized minima with the PBE0 functional. Bond-length in Å, and dihedral angle in °. The TD-PBE0 calculated parameters is in italic. Some structural parameters obtained by the CAM-B3LYP optimization are also given in underline.

species	Ru-N2	Ru-N9	Ru-N14	Ru-N21	Ru-N30	Ru-N37	C7-C8	C31-C32	C35-C40	C34C35C40N41	Ru-N (averaged value)	Pd-Cl	Pd-N	Pd-ACN	Pd-C
Ru_1_S0	2.072 <u>2.094</u>	2.071 <u>2.094</u>	2.071 <u>2.093</u>	2.071 <u>2.094</u>	2.073 <u>2.095</u>	2.073 <u>2.095</u>	1.470 <u>1.478</u>	1.468 <u>1.476</u>	1.480 <u>1.485</u>	20.6 <u>21.5</u>	2.072 <u>2.094</u>				
Ru_1_T _{tpy}	2.075 <u>2.071</u>	2.094 <u>2.085</u>	2.096 <u>2.090</u>	2.077 <u>2.077</u>	2.047 <u>2.044</u>	2.049 <u>2.025</u>	1.469 <u>1.471</u>	1.413 <u>1.406</u>	1.469 <u>1.453</u>	0.72 <u>0.77</u>					
Ru_1_T _{bpy}	2.047 <u>2.048</u>	2.044 <u>2.001</u>	2.073 <u>2.067</u>	2.096 <u>2.088</u>	2.096 <u>2.101</u>	2.076 <u>2.083</u>	1.414 <u>1.409</u>	1.467 <u>1.468</u>	1.480 <u>1.480</u>	18.9 <u>19.3</u>					
Ru_1_T _{tpy'}	2.073 <u>2.110</u>	2.094 <u>2.105</u>	2.096 <u>2.067</u>	2.047 <u>2.034</u>	2.049 <u>2.041</u>	1.469 <u>1.469</u>	1.413 <u>1.424</u>	1.469 <u>1.472</u>	0.72 <u>15.6</u>						
Ru_1_ ³ MC _{Ru}	2.138	2.429	2.083	2.086	2.415	2.136	1.478	1.476	1.480	19.2					
Ru_1_Q	2.050	2.045	2.073	2.095	2.094	2.071	1.414	1.405	1.422	0.4					
Ru_1_S _{tpy}	2.070 <u>2.070</u>	2.086 <u>2.086</u>	2.086 <u>2.070</u>	2.070 <u>2.054</u>	2.054 <u>2.058</u>	2.058 <u>1.469</u>	1.469 <u>1.417</u>	1.417 <u>1.470</u>	1.470 <u>1.3</u>						
Ru_1_S _{bpy}	2.054 <u>2.054</u>	2.055 <u>2.055</u>	2.068 <u>2.068</u>	2.087 <u>2.087</u>	2.085 <u>2.085</u>	2.070 <u>2.070</u>	1.418 <u>1.418</u>	1.467 <u>1.467</u>	1.480 <u>1.480</u>	18.8					
RuPd_1_S0	2.072 <u>2.095</u>	2.072 <u>2.095</u>	2.070 <u>2.093</u>	2.069 <u>2.092</u>	2.070 <u>2.093</u>	2.074 <u>2.096</u>	1.470 <u>1.478</u>	1.469 <u>1.478</u>	1.460 <u>1.466</u>	0.2 <u>0.2</u>	2.071 <u>2.094</u> 2.08 ^a 2.05 ^b	2.334 <u>2.345</u> 2.35 ^a 2.36 ^c	2.053 <u>2.064</u> 2.08 ^a 2.02 ^c	2.110 <u>2.123</u> 2.14 ^a 2.14 ^c	1.962 <u>1.972</u> 1.98 ^a 1.99 ^c
RuPd_1_T _{tpy}	2.071 <u>2.068</u>	2.091 <u>2.086</u>	2.095 <u>2.096</u>	2.078 <u>2.080</u>	2.052 <u>2.054</u>	2.040 <u>2.006</u>	1.469 <u>1.471</u>	1.418 <u>1.414</u>	1.438 <u>1.430</u>	0.2 <u>0.7</u>					
RuPd_1_T _{bp}	2.044 <u>1.994</u>	2.046 <u>2.055</u>	2.077 <u>2.085</u>	2.098 <u>2.107</u>	2.095 <u>2.086</u>	2.069 <u>2.061</u>	1.414 <u>1.410</u>	1.468 <u>1.471</u>	1.461 <u>1.461</u>	0.4 <u>0.2</u>					
RuPd_1_ ³ M C _{Ru}	2.137	2.420	2.079	2.080	2.424	2.135	1.478	1.478	1.460	0.2					
RuPd_1_Q	2.052	2.042	2.071	2.094	2.092	2.066	1.414	1.416	1.399	0.9					
RuPd_1_S _{tpy}	2.067 <u>2.067</u>	2.087 <u>2.087</u>	2.087 <u>2.072</u>	2.072 <u>2.054</u>	2.054 <u>2.051</u>	2.051 <u>1.470</u>	1.470 <u>1.421</u>	1.421 <u>1.439</u>	1.439 <u>0.7</u>						
RuPd_1_S _{bp}	2.054 <u>2.054</u>	2.054 <u>2.071</u>	2.071 <u>2.089</u>	2.089 <u>2.086</u>	2.086 <u>2.062</u>	2.062 <u>1.418</u>	1.418 <u>1.468</u>	1.468 <u>1.461</u>	1.461 <u>0.3</u>						
species	Ru-N2	Ru-N9	Ru-N14	Ru-N21	Ru-N30	Ru-N37	C7-C8	C31-C32	C36-C40	C35C36C40N41	Ru-N (averaged value)	Pd-Cl	Pd-N	Pd-ACN	Pd-C
Ru_2_S0	2.076 <u>2.090</u>	2.087 <u>2.106</u>	2.064 <u>2.088</u>	2.068 <u>2.101</u>	2.060 <u>2.086</u>	2.133 <u>2.168</u>	1.468 <u>1.477</u>	1.470 <u>1.478</u>	1.493 <u>1.492</u>	75.1 <u>108.3</u>	2.081 <u>2.106</u>				
Ru_2_ ³ MC _{Ru}	2.078	2.089	2.383	2.134	2.129	2.647	1.465	1.480	1.484	26.4					

u															
RuPd_2_S0	2.082 <i>2.104</i>	2.086 <i>2.109</i>	2.050 <i>2.073</i>	2.069 <i>2.093</i>	2.063 <i>2.086</i>	2.186 <i>2.221</i>	1.469 <i>1.477</i>	1.469 <i>1.476</i>	1.469 <i>1.476</i>	11.5 <i>11.6</i>	2.089 <i>2.114</i> 2.11 ^a 2.05 ^b	2.336 <i>2.347</i> 2.35 ^a 2.36 ^c	2.039 <i>2.050</i> 2.07 ^a 2.02 ^c	2.112 <i>2.126</i> 2.14 ^a 2.14 ^c	1.965 <i>1.974</i> 1.98 ^a 1.99 ^c
RuPd_2_T _{tp} y	2.070 <i>2.068</i>	2.090 <i>2.091</i>	2.163 <i>2.154</i>	2.118 <i>2.109</i>	2.080 <i>2.089</i>	2.122 <i>1.998</i>	1.467 <i>1.471</i>	1.458 <i>1.457</i>	1.444 <i>1.430</i>	11.1 <i>12.0</i>					
RuPd_2_T _{bp} y	<i>2.068</i>	<i>1.998</i>	<i>2.046</i>	<i>2.084</i>	<i>2.096</i>	<i>2.189</i>	<i>1.409</i>	<i>1.469</i>	<i>1.469</i>	<i>12.6</i>					
RuPd_2_ ³ M C _{Ru}	2.077	2.094	2.358	2.129	2.129	2.708	1.465	1.478	1.466	6.7					
RuPd_2_Q	2.069	2.097	2.118	2.096	2.052	2.065	1.468	1.403	1.406	15.6					
RuPd_2_S _{tpy}	<i>2.071</i>	<i>2.085</i>	<i>2.109</i>	<i>2.088</i>	<i>2.070</i>	<i>2.135</i>	<i>1.466</i>	<i>1.452</i>	<i>1.442</i>	<i>12.1</i>					

^aG. S. Bindra, M. Schulz, A. Paul, R. Groarke, S. Soman, J. L. Inglis, W. R. Browne, M. G. Pfeffer, S. Rau, B. J. MacLean, M. T. Prycea and J. G. Vos, *Dalton Trans.*, 2012, 41, 13050.

^bM. Biner, H. B. Buergi, A. Ludi and C. Roehr, *J. Am. Chem. Soc.*, 1992, 114, 5197.

^cJ. E. Bercaw, A. C. Durrell, H. B. Gray, J. C. Green, N. Hazari, J. A. Labinger and J. R. Winkler, *Inorg. Chem.*, 2010, 49, 1801.

Table S2. Relative energies of all optimized structures. The TD-PBE0 energies are given in *italic*. Unit is kcal/mol.

species	Relative energy with zero-point correction	Relative energy without zero-point correction	Exp. Emission maximum ^a
Ru_1_S0	0.0	0.0	
Ru_1_T _{tpy}	45.6(<i>45.7</i>)	47.2(<i>48.7</i>)	
Ru_1_T _{tpy} '	<i>54.4</i>	<i>48.7</i>	
Ru_1_T _{bp}	<i>47.6/49.1</i>	<i>49.2/51.7</i>	
Ru_1_ ³ MC _{Ru}	49.5	51.3	
Ru_1_S _{bp}	57.4	58.5	
Ru_1_S _{tpy}	55.6	56.6	
RuPd_1_S0	0.0	0.0	
RuPd_1_T _{tpy}	44.3(<i>45.6</i>)	45.8(<i>48.0</i>)	45.0 (635nm)
RuPd_1_T _{bp}	<i>46.7/48.5</i>	<i>48.4/51.0</i>	
RuPd_1_ ³ MC _{Ru}	49.6	51.3	
RuPd_1_S _{tpy}	54.5	55.4	
RuPd_1_S _{bp}	56.5	57.7	
Ru_2_S0	0.0	0.0	
Ru_2_ ³ MC _{Ru}	41.4	42.7	
RuPd_2_S0	0.0	0.0	
RuPd_2_ ³ MC _{Ru}	38.8	39.8	
RuPd_2_T _{tpy}	42.4(<i>43.2</i>)	44.5(<i>45.5</i>)	
RuPd_2_T _{bp}	<i>48.6</i>	<i>51.3</i>	

RuPd_2_S _{typ}	53.6	55.3	
-------------------------	------	------	--

^a G. S. Bindra, M. Schulz, A. Paul, R. Groarke, S. Soman, J. L. Inglis, W. R. Browne, M. G. Pfeffer, S. Rau, B. J. MacLean, M. T. Prycea and J. G. Vos, *Dalton Trans.*, 2012, 41, 13050.

Table S3. Singlet excitation energies of Ru_1 and RuPd_1 calculated at the PBE0 optimized ground-state geometry by the TD-PBE0 method. Only transitions with excitation energy in the range of 370-500 nm and an oscillator strength $f > 0.001$ are listed.

State	Transition	Transition amplitude	E (eV)	λ (nm)	f
Ru_1					
S4	148 ->151	0.62780	2.8980	427.83	0.0035
	148 ->152	0.22613			
	149 ->153	-0.16860			
S5	148 ->152	0.10136	2.9742	416.87	0.0653
	149 ->151	0.58705			
	149 ->152	-0.31115			
	149 ->153	-0.20026			
S6	148 ->151	0.29241	2.9867	415.12	0.0196
	148 ->152	-0.37023			
	149 ->151	0.21433			
	149 ->153	0.46300			
S7	148 ->153	-0.41451	3.0481	406.76	0.0552
	149 ->151	0.25081			
	149 ->152	0.49479			
S8	148 ->152	0.53028	3.1103	398.63	0.1457
	149 ->153	0.44238			
S9	148 ->153	0.53080	3.3087	374.72	0.0106
	149 ->151	0.14855			
	149 ->152	0.35837			
	150 ->157	-0.17816			
S10	150 ->154	0.68629	3.6216	342.34	0.0053
RuPd_1					
S1	178 ->179	0.68107	2.6173	473.70	0.0010
	178 ->180	-0.10540			
S3	178 ->179	0.12092	2.7474	451.27	0.0011
	178 ->180	0.60638			
	178 ->181	0.32269			
S4	176 ->179	0.50315	2.8281	438.41	0.0153
	176 ->180	-0.10053			
	177 ->179	0.44578			
	177 ->181	-0.12465			

S5	176 ->179	-0.44244	2.8832	430.02	0.1148
	177 ->179	0.49397			
	177 ->180	0.20164			
S6	176 ->179	0.14914	2.9395	421.79	0.0028
	176 ->180	0.32699			
	176 ->181	-0.18609			
	177 ->180	0.24149			
	177 ->181	0.51042			
S7	176 ->180	-0.28822	2.9881	414.93	0.0192
	176 ->181	0.35253			
	177 ->179	-0.13138			
	177 ->180	0.49880			
S8	176 ->180	0.50912	3.0703	403.81	0.1461
	176 ->181	0.14344			
	177 ->180	0.23589			
	177 ->181	-0.38510			
S9	176 ->180	0.15784	3.2553	380.87	0.0349
	176 ->181	0.53483			
	177 ->179	0.12038			
	177 ->180	-0.26896			
	177 ->181	0.22133			
	178 ->187	0.13750			
S10	174 ->179	-0.29064	3.4678	357.53	0.0045
	174 ->184	0.54040			
	175 ->179	-0.28049			

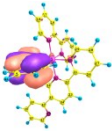
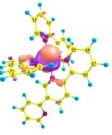
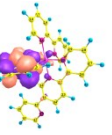
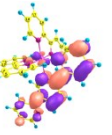
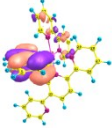
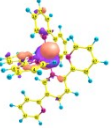
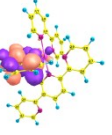
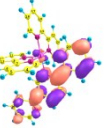
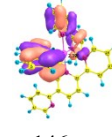
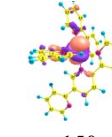
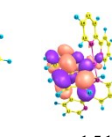
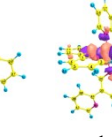
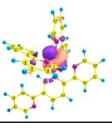
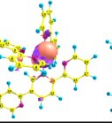
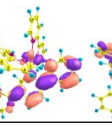
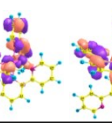
Table S4. Singlet excitation energies of Ru_2 and RuPd_2 calculated at the PBE0 optimized ground-state geometry by TD-PBE0 method. Only transitions with excitation energy in the range of 370-500 nm and an oscillator strength $f > 0.001$ are listed.

State	Transition	Transition amplitude	E (eV)	λ (nm)	f
Ru_2					
S1	148 ->152	-0.12803	2.6692	464.49	0.0028
	150 ->152	0.68328			
S2	150 ->151	0.53184	2.7386	452.73	0.0032
	150 ->153	-0.45231			
S3	150 ->151	0.45670	2.8123	440.87	0.0020
	150 ->153	0.52784			
S4	148 ->151	-0.19148	2.9418	421.45	0.0091
	148 ->153	0.21733			
	149 ->152	0.63429			

S5	148 ->152	-0.33270	3.0128	411.53	0.0022
	149 ->151	0.58964			
	149 ->153	-0.15131			
S6	148 ->151	0.66862	3.1083	398.88	0.0865
	148 ->153	0.10233			
	149 ->152	0.15748			
S7	148 ->152	0.45881	3.1259	396.63	0.1138
	149 ->151	0.37104			
	149 ->153	0.34369			
	150 ->152	0.10536			
S8	148 ->153	0.64947	3.1480	393.86	0.0515
	149 ->152	-0.23820			
S9	148 ->152	-0.34574	3.3317	372.13	0.0095
	149 ->153	0.54652			
	150 ->155	-0.11401			
	150 ->157	0.19198			
S10	150 ->154	0.69481	3.6457	340.08	0.0122
RuPd_2					
S2	178 ->179	-0.12785	2.7118	457.21	0.0024
	178 ->180	0.51446			
	178 ->181	0.42255			
	178 ->182	0.14451			
S3	178 ->179	0.10782	2.8175	440.04	0.0022
	178 ->180	-0.41625			
	178 ->181	0.54088			
S4	176 ->179	-0.24890	2.9045	426.87	0.0166
	177 ->179	0.48758			
	177 ->180	0.33659			
	177 ->181	0.18827			
S5	176 ->179	0.44831	3.0206	410.46	0.0046
	176 ->182	-0.10803			
	177 ->179	-0.10203			
	177 ->180	0.48167			
S6	176 ->179	0.35296	3.0383	408.07	0.0332
	176 ->180	-0.11946			
	176 ->181	-0.21723			
	176 ->182	-0.14547			
	177 ->179	0.37566			
	177 ->180	-0.27909			
	178 ->179	0.11712			
	178 ->182	0.14725			
S7	176 ->179	0.12747	3.1062	399.15	0.0364
	176 ->181	0.45437			
	177 ->180	-0.19183			

	177 ->181	0.46036			
S8	176 ->180	-0.13868	3.1609	392.25	0.0442
	176 ->181	0.40782			
	177 ->181	-0.38738			
	178 ->182	0.34875			
S9	176 ->180	0.54521	3.1908	388.57	0.1453
	176 ->181	-0.16082			
	178 ->179	0.10664			
	178 ->182	0.36207			
S10	175 ->179	0.13618	3.3189	373.57	0.0021
	176 ->179	-0.10534			
	176 ->180	-0.29989			
	176 ->181	-0.15624			
	177 ->179	-0.20511			
	177 ->180	0.12006			
	177 ->181	0.23046			
	177 ->182	-0.25614			
	178 ->182	0.33542			

Table S5. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{bpy}-³MC_{Ru} conversion of Ru_1, and the selected excitation configuration with the absolute value of transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.096	2.044	2.037	2.076	2.047	2.096	1.414	1.467	146 ->151 150 ->151 150 ->152	-0.18779 0.61954 -0.19096	    146 150 151 152
2.296	2.018	2.066	2.095	2.048	2.095	1.413	1.473	146 ->151 150 ->151 150 ->152	-0.17062 0.64036 -0.12947	    146 150 151 152
2.396	2.018	2.064	2.110	2.048	2.093	1.416	1.475	146 ->151 150 ->151 150 ->162	-0.12985 0.63422 0.16257	    146 150 151 162
2.496	2.408	2.085	2.139	2.133	2.079	1.479	1.478	148 ->151 148 ->154 150 ->151	0.12477 0.28615 0.24254	    148 154 150 151

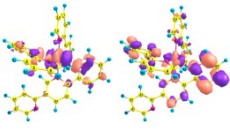
								150 ->152	0.14345	148	150	151	152	153
								150 ->153	-0.10069					
								150 ->154	0.53083					
								150 ->160	0.16207					
										154	160			

Table S6. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{bpy}-³MC_{Ru} conversion of RuPd_1, and the selected excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

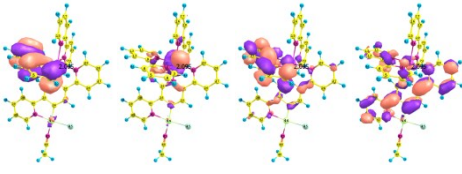
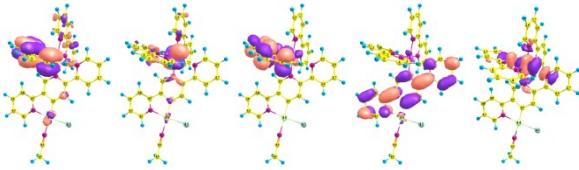
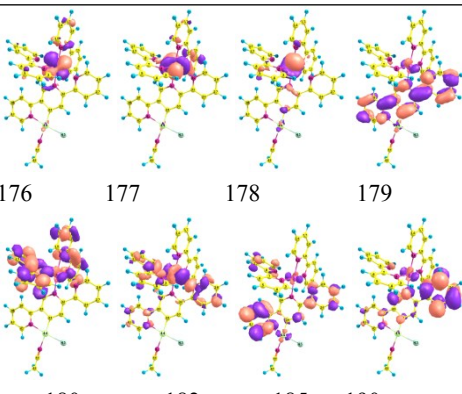
Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.095	2.046	2.077	2.069	2.044	2.098	1.414	1.468	171 ->179 178 ->179 178 ->180	-0.16997 0.57547 -0.30564	
2.395	2.016	2.067	2.099	2.044	2.095	1.414	1.477	171 ->179 178 ->179 178 ->180 178 ->191	0.15253 0.62735 -0.13777 0.13148	
2.495	2.406	2.081	2.141	2.133	2.078	1.478	1.479	176 ->180 176 ->182 177 ->182 178 ->179 178 ->180 178 ->182 178 ->185 178 ->190	0.10776 0.26983 0.15613 0.18743 0.20149 0.48771 0.10873 0.11358	

Table S7. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of Ru_1, and the excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
--------	-------	--------	--------	-------	--------	-------	---------	------------	----------------------	-----------------------------

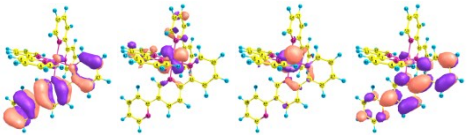
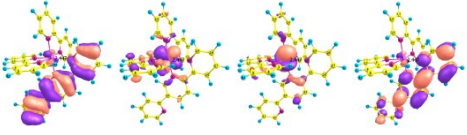
2.047	2.094	2.096	2.049	2.075	2.077	1.469	1.413	147 -> 151 148 -> 151 150 -> 151	-0.24710 -0.10554 0.61595	 147 148 150 151
2.447	2.037	2.097	2.049	2.062	2.082	1.465	1.425	147 -> 151 149 -> 151 150 -> 151	0.29566 -0.20347 0.55848	 147 149 150 151

Table S8. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of RuPd_1, and the selected excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

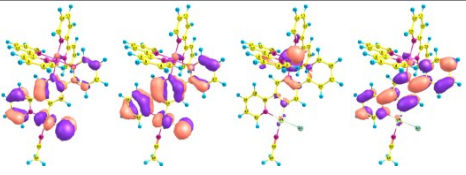
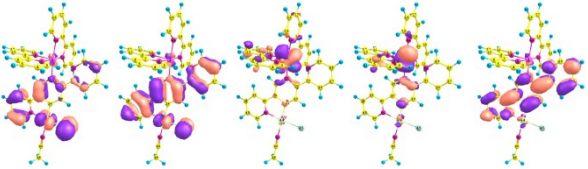
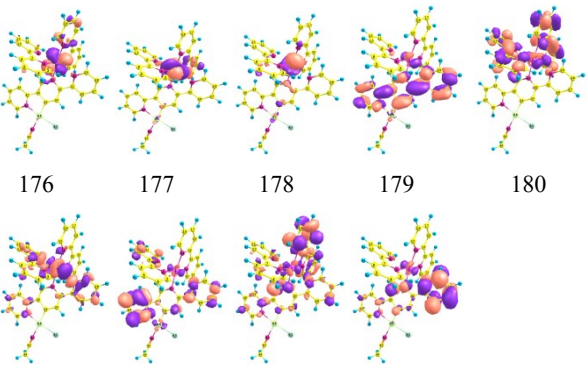
Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.052	2.091	2.095	2.040	2.071	2.078	1.469	1.418	173 -> 179 175 -> 179 178 -> 179	-0.13618 -0.20890 0.62039	 173 175 178 179
2.452	2.039	2.097	2.048	2.057	2.084	1.466	1.431	173 -> 179 175 -> 179 177 -> 179 178 -> 179	-0.14463 0.24936 -0.16801 0.57967	 173 175 177 178 179
2.552	2.394	2.086	2.136	2.134	2.076	1.478	1.480	176 -> 182 177 -> 182 178 -> 179 178 -> 180 178 -> 182 178 -> 185 178 -> 186 178 -> 190	0.21896 0.24099 0.21205 0.19357 0.49795 0.10396 0.10072 0.10517	 176 177 178 179 180 182 185 186 190

Table S9. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{bpy}-³MLCT_{tpy} conversion of Ru_1, and the selected excitation configuration

with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

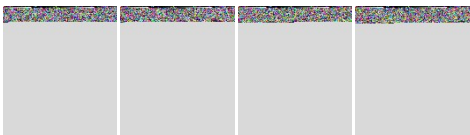
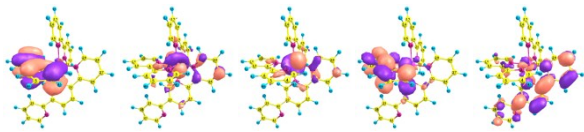
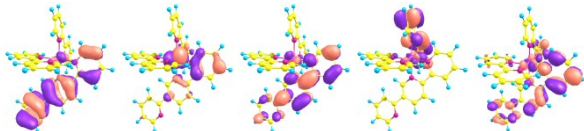
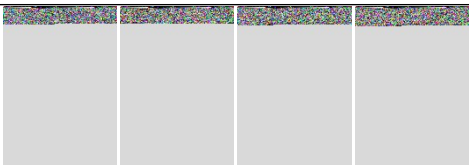
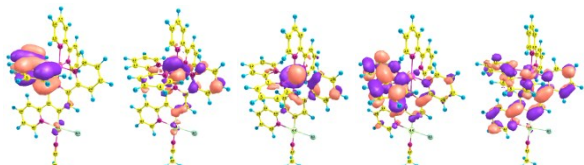
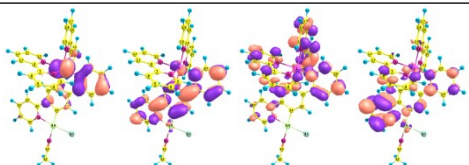
Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.096	2.044	2.073	2.076	2.047	2.096	1.414	1.467	146 → 151 150 → 151 150 → 152	-0.18779 0.61954 -0.19096	 146 150 151 152
1.896	2.085	2.083	2.062	2.046	2.097	1.417	1.458	146 → 151 149 → 151 150 → 151 150 → 152	-0.20374 -0.20573 0.58024 -0.18292	 146 149 150 151 152
1.846	2.145	2.096	2.053	2.092	2.067	1.472	1.407	147 → 151 150 → 151 150 → 152 150 → 159	0.13295 0.64744 -0.10541 -0.11653	 147 150 151 152 159

Table S10. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{bpy}-³MLCT_{tpy} conversion of RuPd_1, and the selected excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.095	2.046	2.077	2.069	2.044	2.098	1.414	1.468	171 → 179 178 → 179 178 → 180	-0.16997 0.57547 -0.30564	 171 178 179 180
1.845	2.100	2.089	2.052	2.046	2.100	1.419	1.456	171 → 179 177 → 179 177 → 180 178 → 179 178 → 180	-0.17914 -0.17051 0.13718 0.56916 -0.20785	 171 177 178 179 180
1.795	2.160	2.098	2.053	2.096	2.066	1.472	1.408	178 → 179 178 → 182 178 → 183	0.64214 -0.12095 0.12882	

										178	179	182	183
--	--	--	--	--	--	--	--	--	--	-----	-----	-----	-----

Table S11. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MC_{Ru}-S₀ conversion of Ru_1, and the selected excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures. The highest and lowest singly occupied MOs (HSOMO and LSOMO) from uDFT calculations are also displayed with the label in *italic*.

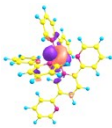
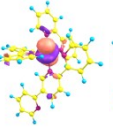
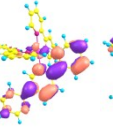
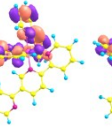
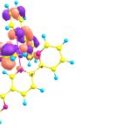
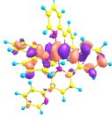
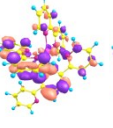
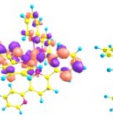
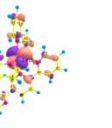
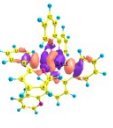
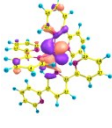
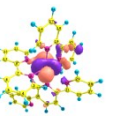
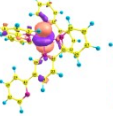
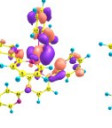
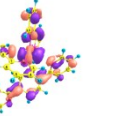
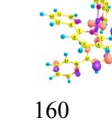
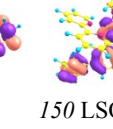
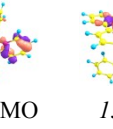
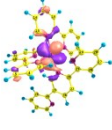
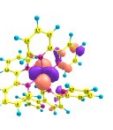
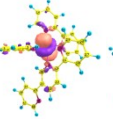
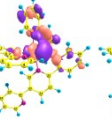
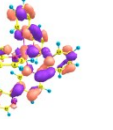
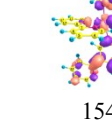
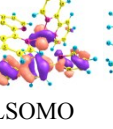
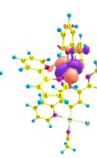
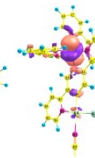
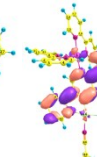
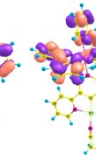
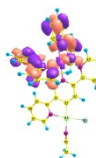
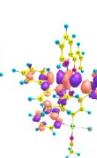
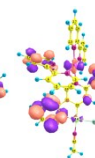
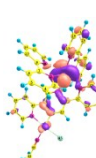
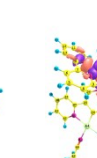
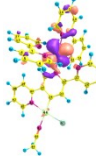
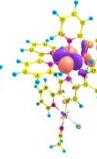
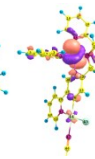
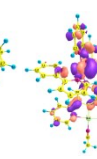
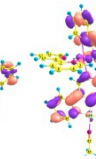
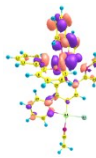
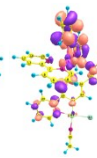
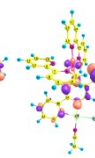
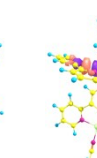
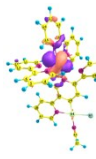
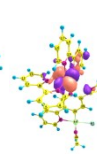
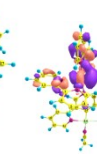
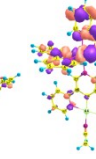
Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.415	2.429	2.083	2.136	2.138	2.086	1.478	1.476	148 ->151	0.11339	     148 150 151 152 153      154 155 160 <i>150 LSOMO</i> <i>151 HSOMO</i>
								148 ->154	0.25609	
								148 ->160	0.10615	
								150 ->151	0.23584	
								150 ->152	0.11443	
								150 ->153	-0.15469	
								150 ->154	0.50081	
								150 ->155	-0.12279	
								150 ->160	0.21215	
2.815	2.335	2.086	2.145	2.124	2.071	1.478	1.482	148 ->151	0.23059	     148 149 150 151 154    160 <i>150 LSOMO</i> <i>151 HSOMO</i>
								148 ->154	0.19479	
								149 ->151	0.20397	
								149 ->154	0.17503	
								150 ->151	0.55702	
								150 ->154	0.46227	
								150 ->160	-0.11454	
3.015	2.322	2.084	2.142	2.120	2.071	1.477	1.485	148 ->151	0.22852	     148 149 150 151 153    154 <i>150 LSOMO</i> <i>151 HSOMO</i>
								148 ->154	0.11452	
								149 ->151	0.25453	
								149 ->154	0.12882	
								150 ->151	0.58666	
								150 ->153	0.21403	
								150 ->154	0.28907	

Table S12. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MC_{Ru}-S₀ conversion of RuPd_1, and the selected excitation configuration with transition amplitude > 0.1. Additionally, the first eight columns list some chosen

structural parameters of the partially optimized T₁ structures. The highest and lowest singly occupied MOs (HSOMO and LSOMO) from uDFT calculations are also displayed with the label in *italic*.

Ru-N30	Ru-N9	Ru-N14	Ru-N37	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.424	2.420	2.079	2.135	2.137	2.080	1.478	1.478	176 ->182 177 ->182 178 ->179 178 ->180 178 ->181 178 ->182 178 ->185 178 ->189 178 ->190	0.25216 0.14092 0.18479 0.16152 -0.14033 0.44955 0.14271 -0.10080 0.16316	     176 177 178 179 180    181 182 185   <i>178 LSOMO</i> <i>179 HSOMO</i>
2.824	2.345	2.089	2.141	2.126	2.071	1.478	1.483	176 ->179 176 ->182 177 ->179 177 ->182 178 ->179 178 ->180 178 ->182 178 ->186 178 ->190	0.24853 0.22201 0.30940 0.28027 0.58726 0.14830 0.51631 -0.12786 0.10718	     176 177 178 179 180    182 186 190   <i>178 LSOMO</i> <i>179 HSOMO</i>
3.024	2.320	2.088	2.151	2.119	2.090	1.476	1.486	176 ->179 176 ->182 177 ->179 177 ->182 178 ->179 178 ->182	0.61861 0.36655 0.36334 0.21671 0.57495 0.33377	     176 177 178 179 182

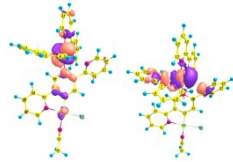
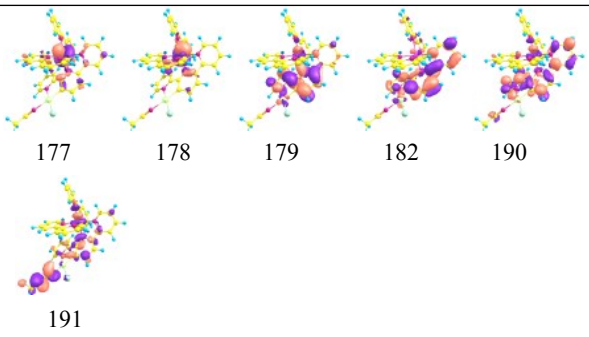
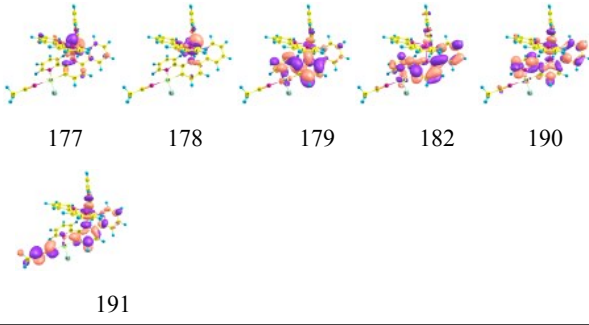
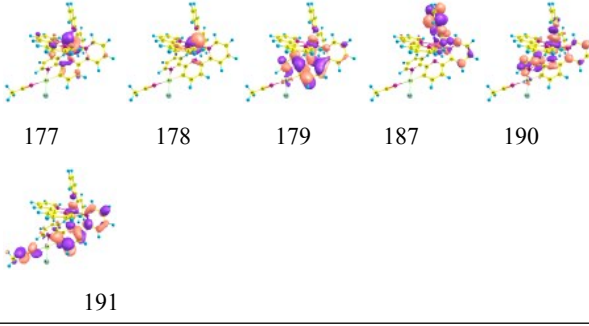
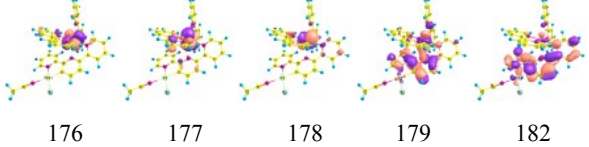
										 178 LSOMO 179 HSOMO
--	--	--	--	--	--	--	--	--	--	--

Table S13. The MOs involved in the TD-PBE0 excitation for the T₁ state along the ³MLCT_{tpy}-³MC_{Ru} conversion of RuPd_2, and the selected excitation configuration with transition amplitude > 0.11. Additionally, the first eight columns list some chosen structural parameters of the partially optimized T₁ structures.

Ru-N37	Ru-N14	Ru-N30	Ru-N9	Ru-N2	Ru-N21	C7-C8	C31-C32	transition	Transition amplitude	MOs involved in excitations
2.122	2.163	2.080	2.090	2.070	2.118	1.467	1.458	177 ->179 178 ->179 178 ->182 178 ->190 178 ->191	0.15827 0.61153 0.10385 0.15330 0.14535	
2.172	2.198	2.085	2.091	2.074	2.128	1.467	1.461	177 ->179 178 ->179 178 ->182 178 ->190 178 ->191	-0.14191 0.57697 0.10342 0.22619 0.19444	
2.222	2.289	2.088	2.091	2.086	2.156	1.466	1.466	177 ->179 178 ->179 178 ->187 178 ->190 178 ->191	-0.13465 0.50833 -0.10230 0.34517 0.15314	
2.522	2.367	2.112	2.090	2.079	2.140	1.466	1.475	176 ->179 176 ->183 177 ->179 177 ->183 178 ->179 178 ->182	-0.16110 -0.12249 -0.17374 -0.13310 0.43627 0.14247	

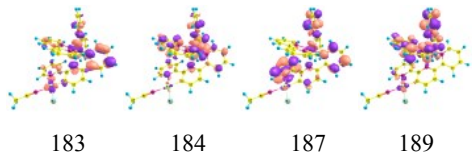
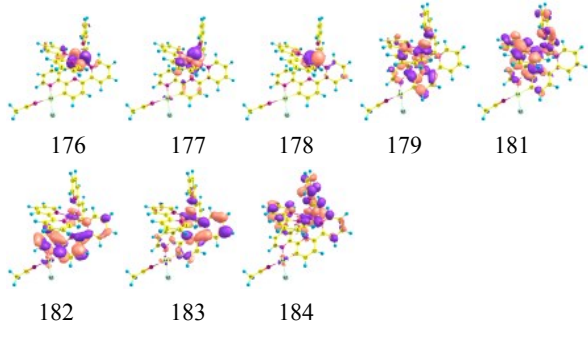
								178 ->183	0.31697	
								178 ->184	0.20717	
								178 ->187	0.12991	
								178 ->189	0.13185	
2.722	2.347	2.119	2.090	2.074	2.136	1.465	1.480	176 ->179	-0.22315	
								176 ->183	-0.14260	
								177 ->179	-0.20609	
								177 ->183	-0.13293	
								178 ->179	0.52438	
								178 ->181	-0.13169	
								178 ->182	0.19334	
								178 ->183	0.32297	
								178 ->184	0.13141	

Table S14. Spin density on the Ru atom for the $^3\text{MLCT}_{\text{tpy}}\text{-}^3\text{MC}_{\text{Ru}}$ crossing of RuPd_2

Ru-N37	2.122	2.172	2.222	2.272	2.322	2.372	2.422	2.472	2.522	2.572	2.622	2.672	2.722
Spin density	1.23	1.37	1.59	1.69	1.75	1.79	1.82	1.84	1.86	1.87	1.88	1.89	1.89

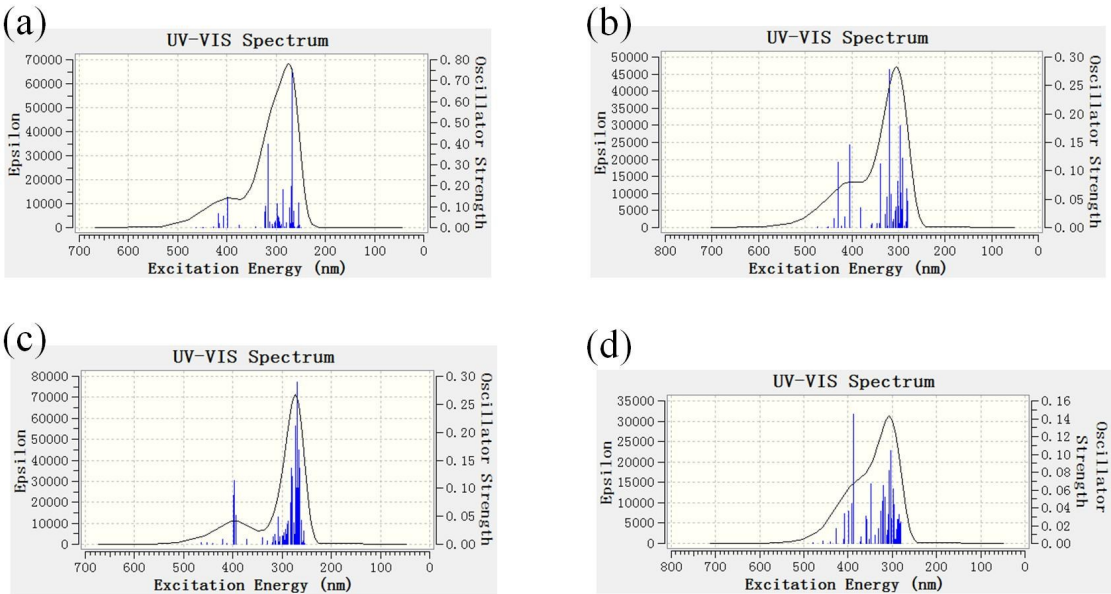


Figure S1. The UV absorption spectrum of Ru_1 (a), RuPd_1 (b), Ru_2 (c), and RuPd_2 (d). The spectra are calculated with the default settings of Gaussview based on the TD-PBE0//PBE0/SDD[Ru,Pd]6-31G**[C,N,H,Cl]/PCM(CH₃CN) calculations. In the TDDFT calculation 50 singlet states are considered. The experimental maximum absorption and $^1\text{MLCT}$ peak are at ~ 300 and ~ 450 nm, respectively (ref.58 in main text).

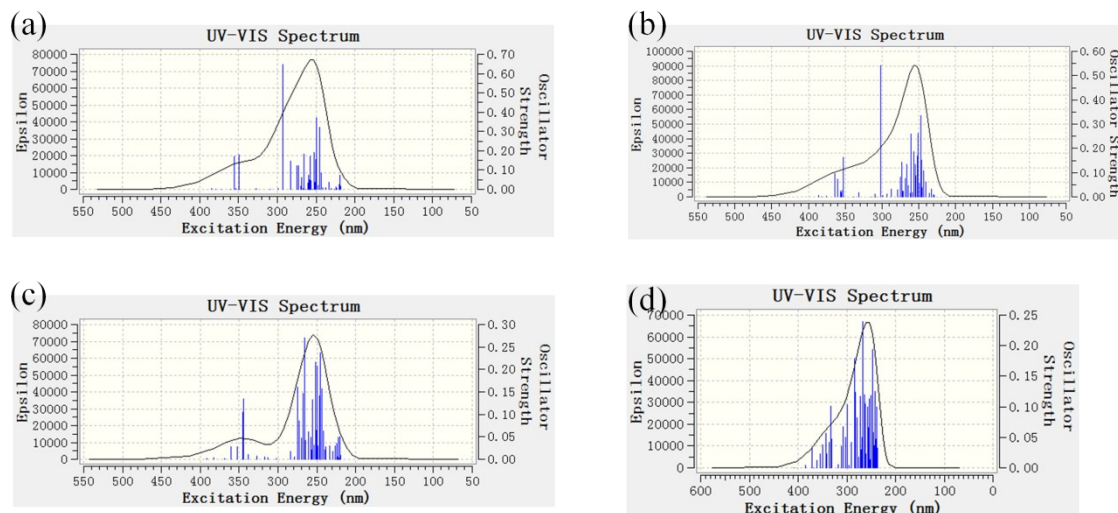


Figure S2. The UV absorption spectrum of Ru_1 (a), RuPd_1 (b), Ru_2 (c), and RuPd_2 (d). The spectra are calculated with the default settings of Gaussview based on the TD-CAM-B3LYP//PBE0/SDD[Ru,Pd]6-31G**[C,N,H,Cl]/PCM(CH₃CN) calculations. In the TDDFT calculation 50 singlet states are considered. As seen in this figure, the TD-CAM-B3LYP calculation predicts the maximum absorption is at ~250 nm and the low energy ¹MLCT peak is at 350 nm for each complex. Experimentally, the maximum absorption and ¹MLCT peak are at ~300 and ~450 nm, respectively (ref.58 in main text).

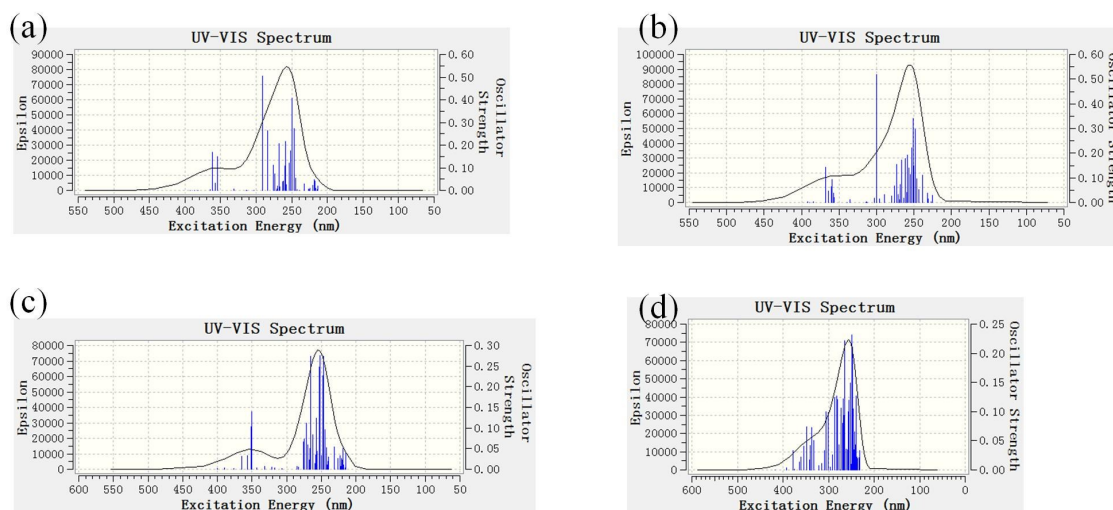


Figure S3. The UV absorption spectrum of Ru_1 (a), RuPd_1 (b), Ru_2 (c), and RuPd_2 (d). The spectra are calculated with the default settings of Gaussview based on the TD-wB97xD//PBE0/SDD[Ru,Pd]6-31G**[C,N,H,Cl]/PCM(CH₃CN) calculations. In the TDDFT calculation 50 singlet states are considered. As seen in

this figure, the TD-wB97xD calculation predicts the maximum absorption is at ~250 nm and the low energy ¹MLCT peak is at 350 nm for each complex. Experimentally, the maximum absorption and ¹MLCT peak are at ~300 and ~450 nm, respectively (ref.58 in main text).

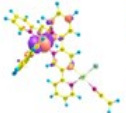
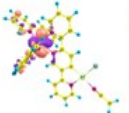
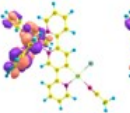
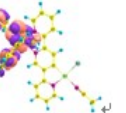
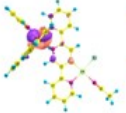
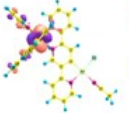
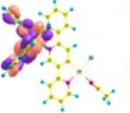
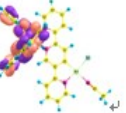
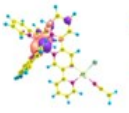
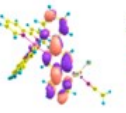
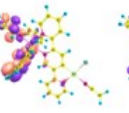
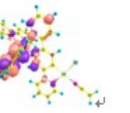
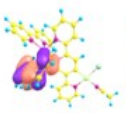
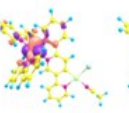
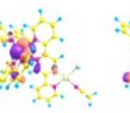
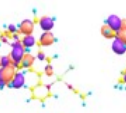
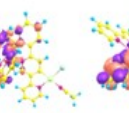
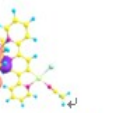
functional [⊃]	state [⊃]	oscillator strength [⊃]	energy [⊃] (nm) [⊃]	NTOs and their eigenvalues [⊃]					
weaker absorption [⊃]									
PBE0 [⊃]	S ₈ [⊃]	0.1461 [⊃]	403.81 [⊃]						
				177 (0.34)	178 (0.65)	179 (0.65)	180 (0.34) [⊃]		
CAM-B3LY P [⊃]	S ₉ [⊃]	0.1618 [⊃]	353.00 [⊃]						
				177 (0.22)	178 (0.74)	179 (0.74)	180 (0.22) [⊃]		
Strongest absorption [⊃]									
PBE0 [⊃]	S ₃₅ [⊃]	0.1794 [⊃]	296.26 [⊃]						
				176 (0.12)	177 (0.27)	178 (0.48)	179 (0.48)	180 (0.27)	181 (0.12) [⊃]
CAM-B3LY P [⊃]	S ₄₁ [⊃]	0.3358 [⊃]	247.42 [⊃]						
				176 (0.05)	177 (0.20)	178 (0.64)	179 (0.64)	180 (0.20)	181 (0.05) [⊃]

Figure S4. Natural Transition Orbital (NTO) analysis for vertical excitations with maximum oscillator strength in both the strongest and the weaker transition regions of RuPd_1. We found that both functionals predicted the same nature of excitation for the transition with maximum oscillator strength in the weaker transition region (~400 nm for PBE0, and 350 nm for CAM-B3LYP, see Figures S1 and S2). In the strongest transition region (~300 nm for PBE0, and 250 nm for CAM-B3LYP, see Figures S1 and S2), the transition with maximum oscillator strength predicted by the PBE0 was found to have mixed character with ligand centered π - π^* and Ru→ligand charge transfer, while the transition with maximum oscillator strength predicted by the CAM-B3LYP mainly involves Ru→ligand transitions. It is seen that both PBE0 and CAM-B3LYP predict consistent results for the lower UV absorption of RuPd_1. Combined

with the results in Tables S1 and S2, we believe that the PBE0 can give a suitable description of the molecular structures and the lower UV absorption of these studied systems.

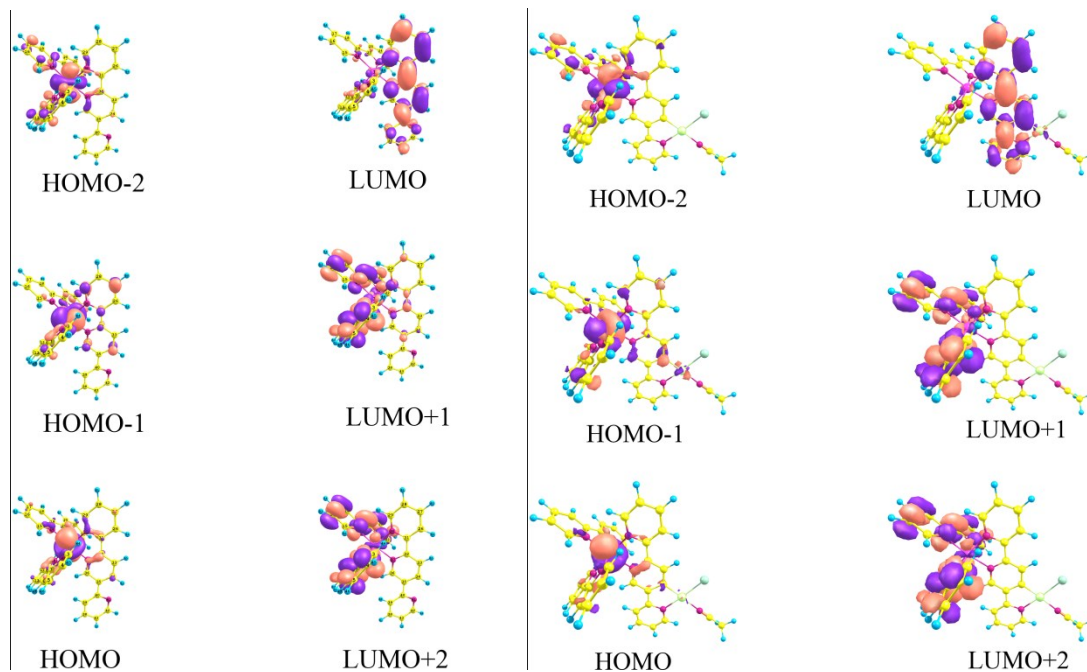


Figure S5. The calculated HOMO and LUMO levels of Ru_1 and RuPd_1 with PBE0/SDD[Ru,Pd]6-31G**[C,N,H,Cl]/PCM(CH₃CN).

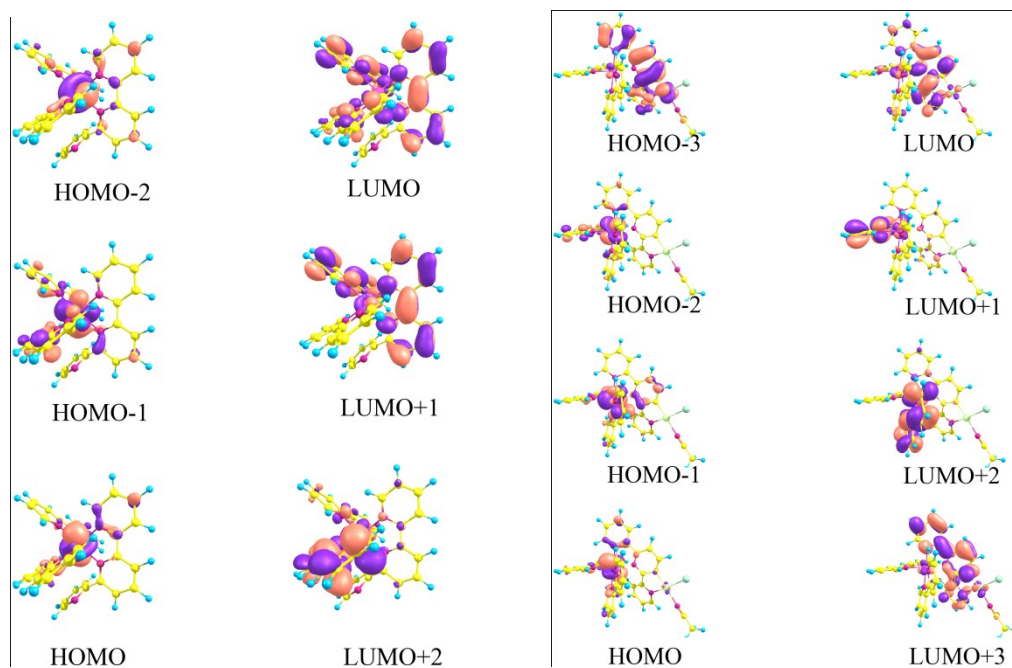


Figure S6. The calculated HOMO and LUMO levels of Ru_2 and RuPd_2 with PBE0/SDD[Ru,Pd]6-31G**[C,N,H,Cl]/PCM(CH₃CN)

S1. Cartesian coordinates of all optimized structures.

Ru_1_S0:

Ru	14.105896000	4.784547000	15.376317000
N	13.039107000	4.086242000	17.009205000
C	11.865752000	4.576610000	17.437689000
C	11.213561000	4.083805000	18.557919000
C	11.799046000	3.042077000	19.268752000
C	13.013209000	2.530839000	18.831734000
C	13.617104000	3.068954000	17.697063000
C	14.896805000	2.594979000	17.150805000
N	15.337507000	3.264953000	16.056136000
C	16.496382000	2.895494000	15.489305000
C	17.271926000	1.857299000	15.982494000
C	16.830747000	1.168092000	17.106794000
C	15.629947000	1.541708000	17.694663000
N	13.336520000	3.451549000	13.990931000
C	12.385409000	2.538333000	14.239706000
C	11.933315000	1.648411000	13.277160000
C	12.489576000	1.700569000	12.003809000
C	13.474796000	2.642147000	11.740106000
C	13.883565000	3.510511000	12.750414000
C	14.914745000	4.543023000	12.573628000
N	15.208162000	5.259412000	13.688310000
C	16.142476000	6.219886000	13.616815000
C	16.826844000	6.511742000	12.446624000
C	16.531157000	5.783916000	11.299339000
C	15.564432000	4.790104000	11.365899000
C	12.390674000	8.693675000	15.305797000
C	11.361393000	8.655409000	14.375550000
C	11.093303000	7.459840000	13.717954000
C	11.865905000	6.347166000	14.014869000
N	12.861363000	6.376482000	14.913813000
C	13.130709000	7.539844000	15.559822000
C	14.235638000	7.474394000	16.523836000
C	14.648641000	8.545852000	17.314504000
C	15.695776000	8.379193000	18.203425000
C	16.327836000	7.135940000	18.304887000
C	15.875025000	6.118696000	17.465615000
N	14.862461000	6.273883000	16.603230000
C	18.854234000	5.538993000	20.611333000
C	17.798423000	5.655060000	19.714615000
C	17.440639000	6.928030000	19.258131000
N	18.065208000	8.041273000	19.669736000

C	19.071478000	7.914747000	20.531883000
C	19.511767000	6.689993000	21.029672000
H	11.444633000	5.384775000	16.851730000
H	10.266248000	4.516032000	18.858958000
H	11.319465000	2.631360000	20.150728000
H	13.484516000	1.719850000	19.373243000
H	16.803204000	3.460949000	14.617268000
H	18.201480000	1.602000000	15.486964000
H	17.410395000	0.350299000	17.521178000
H	15.266830000	1.014324000	18.567904000
H	11.978844000	2.534866000	15.243986000
H	11.160943000	0.931845000	13.531763000
H	12.163317000	1.019019000	11.225633000
H	13.922527000	2.696029000	10.755443000
H	16.342500000	6.760036000	14.534501000
H	17.574008000	7.297003000	12.445461000
H	17.044097000	5.985216000	10.365038000
H	15.317730000	4.214533000	10.482318000
H	10.779227000	9.546917000	14.168500000
H	10.300230000	7.379915000	12.983440000
H	11.690353000	5.395157000	13.528151000
H	16.035015000	9.197468000	18.828488000
H	16.348643000	5.144689000	17.456428000
H	14.151770000	9.505504000	17.243299000
H	12.615183000	9.616174000	15.827025000
H	19.150485000	4.563022000	20.983144000
H	17.253448000	4.771675000	19.399514000
H	19.555262000	8.838645000	20.842783000
H	20.339585000	6.647073000	21.729264000

Ru_1_T_{ipy}:

Ru	14.106877000	4.784898000	15.376910000
N	13.059589000	4.159914000	17.055293000
C	11.932648000	4.739938000	17.493582000
C	11.279442000	4.302619000	18.635479000
C	11.818232000	3.236597000	19.347161000
C	12.990734000	2.642630000	18.897894000
C	13.600270000	3.123344000	17.742949000
C	14.845258000	2.580506000	17.182887000
N	15.294075000	3.203445000	16.065950000
C	16.418272000	2.779293000	15.472399000
C	17.160008000	1.719143000	15.970467000
C	16.712871000	1.073781000	17.118016000
C	15.542867000	1.506643000	17.728825000

N	13.381793000	3.397003000	13.983354000
C	12.481563000	2.442485000	14.257069000
C	12.054769000	1.534799000	13.299949000
C	12.588138000	1.616152000	12.018604000
C	13.526681000	2.599966000	11.735400000
C	13.909908000	3.485762000	12.738261000
C	14.893178000	4.561055000	12.553397000
N	15.163867000	5.292505000	13.662419000
C	16.036438000	6.308849000	13.598488000
C	16.694137000	6.637276000	12.423264000
C	16.429058000	5.894020000	11.278597000
C	15.518415000	4.847286000	11.343464000
C	12.386164000	8.680794000	15.273105000
C	11.402530000	8.632683000	14.320585000
C	11.160535000	7.426630000	13.619352000
C	11.925973000	6.328210000	13.929238000
N	12.883234000	6.349277000	14.881049000
C	13.158048000	7.525783000	15.563020000
C	14.216354000	7.465574000	16.497870000
C	14.647818000	8.527733000	17.335146000
C	15.671467000	8.344662000	18.218166000
C	16.326647000	7.076945000	18.322395000
C	15.864678000	6.073969000	17.484158000
N	14.872898000	6.242608000	16.596221000
C	19.128570000	5.552188000	20.348290000
C	18.097700000	5.651024000	19.427167000
C	17.429671000	6.879093000	19.271619000
N	17.772843000	7.957850000	20.000925000
C	18.765158000	7.844456000	20.881981000
C	19.480121000	6.671492000	21.100705000
H	11.557465000	5.565612000	16.900669000
H	10.368506000	4.796165000	18.952639000
H	11.334180000	2.869633000	20.245747000
H	13.423358000	1.814750000	19.445237000
H	16.726509000	3.317491000	14.583621000
H	18.066596000	1.414000000	15.461579000
H	17.266571000	0.239756000	17.535335000
H	15.180936000	1.010444000	18.620378000
H	12.093122000	2.420485000	15.268545000
H	11.320524000	0.783238000	13.564712000
H	12.280031000	0.920750000	11.245421000
H	13.954959000	2.672892000	10.743635000
H	16.203186000	6.855837000	14.518830000
H	17.395423000	7.463267000	12.415788000

H	16.922949000	6.126460000	10.341326000
H	15.296694000	4.264348000	10.458421000
H	10.815245000	9.518603000	14.101337000
H	10.392947000	7.353119000	12.858733000
H	11.774980000	5.378319000	13.428253000
H	16.006587000	9.150431000	18.860653000
H	16.309256000	5.086063000	17.491250000
H	14.153720000	9.490643000	17.271620000
H	12.585609000	9.602646000	15.806993000
H	19.652706000	4.609884000	20.478287000
H	17.821758000	4.780132000	18.842650000
H	19.004850000	8.743892000	21.447457000
H	20.280230000	6.638307000	21.832256000

Ru_1_T_{ipy} (optimized by TD-PBE0):

Ru	14.105646000	4.788966000	15.394087000
N	13.034769000	4.117528000	17.034706000
C	11.876106000	4.641983000	17.461381000
C	11.213293000	4.162839000	18.580798000
C	11.773947000	3.104443000	19.286986000
C	12.974850000	2.561413000	18.850121000
C	13.591803000	3.084886000	17.716707000
C	14.860712000	2.580243000	17.169990000
N	15.317876000	3.235579000	16.075082000
C	16.463590000	2.840877000	15.503106000
C	17.215154000	1.784326000	15.995987000
C	16.758819000	1.108974000	17.122074000
C	15.568211000	1.510478000	17.713550000
N	13.343032000	3.430868000	14.000586000
C	12.413200000	2.500903000	14.259223000
C	11.972863000	1.602314000	13.298853000
C	12.521391000	1.666873000	12.023262000
C	13.487353000	2.626825000	11.752242000
C	13.883584000	3.502955000	12.759894000
C	14.897292000	4.553127000	12.579277000
N	15.190399000	5.273163000	13.690816000
C	16.105638000	6.251075000	13.619583000
C	16.774438000	6.557319000	12.444211000
C	16.480185000	5.827763000	11.298186000
C	15.531503000	4.816399000	11.367666000
C	12.409100000	8.703054000	15.289254000
C	11.398790000	8.659847000	14.362716000
C	11.125547000	7.448322000	13.691765000
C	11.885368000	6.330226000	13.999044000

N	12.867927000	6.341689000	14.908719000
C	13.172735000	7.532536000	15.565689000
C	14.248431000	7.478071000	16.469284000
C	14.711393000	8.570617000	17.267598000
C	15.727981000	8.397452000	18.152962000
C	16.353689000	7.104228000	18.296885000
C	15.875521000	6.074932000	17.472761000
N	14.895970000	6.222580000	16.585809000
C	19.094369000	5.574359000	20.380754000
C	18.073057000	5.667673000	19.449545000
C	17.434674000	6.911033000	19.248700000
N	17.800661000	8.009808000	19.948777000
C	18.780380000	7.899354000	20.836191000
C	19.466156000	6.710571000	21.097325000
H	11.480239000	5.462645000	16.875222000
H	10.277862000	4.617684000	18.884859000
H	11.284464000	2.703863000	20.168160000
H	13.424099000	1.737590000	19.390487000
H	16.781285000	3.399942000	14.630694000
H	18.137416000	1.505813000	15.499721000
H	17.319709000	0.278360000	17.536704000
H	15.196229000	0.992396000	18.588465000
H	12.011838000	2.490276000	15.265682000
H	11.216056000	0.870843000	13.557025000
H	12.204102000	0.979185000	11.246827000
H	13.928328000	2.687912000	10.765163000
H	16.302410000	6.789268000	14.538878000
H	17.508059000	7.354982000	12.438635000
H	16.981062000	6.041263000	10.360092000
H	15.287188000	4.241035000	10.483522000
H	10.816007000	9.549130000	14.147317000
H	10.336297000	7.372825000	12.953555000
H	11.697171000	5.379014000	13.513839000
H	16.089190000	9.212585000	18.767610000
H	16.313743000	5.085263000	17.508705000
H	14.240982000	9.541198000	17.164465000
H	12.633330000	9.624697000	15.812158000
H	19.594683000	4.625339000	20.547139000
H	17.778110000	4.785562000	18.892743000
H	19.041515000	8.807853000	21.376516000
H	20.259619000	6.683052000	21.836108000

Ru_1_T_{ipy}:

Ru	14.094858000	4.816728000	15.379172000
----	--------------	-------------	--------------

N	13.027248000	4.048339000	16.981668000
C	11.836073000	4.530237000	17.369114000
C	11.185177000	4.053152000	18.495967000
C	11.787714000	3.043345000	19.237511000
C	13.018486000	2.542169000	18.831605000
C	13.625977000	3.063442000	17.694131000
C	14.922859000	2.613937000	17.170055000
N	15.370868000	3.292848000	16.086824000
C	16.549533000	2.959147000	15.544412000
C	17.340045000	1.940134000	16.055604000
C	16.888996000	1.236822000	17.165446000
C	15.665383000	1.577103000	17.727764000
N	13.283800000	3.473942000	13.975344000
C	12.293690000	2.604912000	14.217262000
C	11.829028000	1.721695000	13.253324000
C	12.416983000	1.735801000	11.994767000
C	13.442707000	2.636710000	11.739582000
C	13.856988000	3.501765000	12.748047000
C	14.916612000	4.505163000	12.579295000
N	15.230305000	5.206118000	13.696813000
C	16.185919000	6.148156000	13.654407000
C	16.874014000	6.439968000	12.487525000
C	16.563451000	5.729084000	11.333682000
C	15.576653000	4.751947000	11.380271000
C	12.390929000	8.695613000	15.265324000
C	11.383554000	8.650634000	14.330431000
C	11.096608000	7.427209000	13.671990000
C	11.840367000	6.324066000	13.993228000
N	12.832618000	6.344499000	14.922184000
C	13.131935000	7.536519000	15.573637000
C	14.196627000	7.476788000	16.517336000
C	14.607083000	8.533992000	17.356955000
C	15.645344000	8.365319000	18.235013000
C	16.318899000	7.107450000	18.319395000
C	15.888454000	6.113888000	17.465981000
N	14.874418000	6.265291000	16.587129000
C	18.963325000	5.541876000	20.514128000
C	17.900716000	5.641474000	19.628262000
C	17.433448000	6.913983000	19.261821000
N	17.971249000	8.036110000	19.770552000
C	18.985086000	7.922017000	20.627991000
C	19.528459000	6.706089000	21.029562000
H	11.415135000	5.313247000	16.750227000
H	10.225607000	4.470839000	18.776347000

H	11.306315000	2.645419000	20.124254000
H	13.497498000	1.755524000	19.400708000
H	16.866089000	3.530056000	14.680219000
H	18.286847000	1.710772000	15.581259000
H	17.478439000	0.431605000	17.590136000
H	15.294182000	1.037035000	18.589430000
H	11.863052000	2.624994000	15.210742000
H	11.024290000	1.038902000	13.498980000
H	12.084045000	1.055563000	11.218462000
H	13.915205000	2.660024000	10.765604000
H	16.386441000	6.667757000	14.583477000
H	17.636536000	7.209647000	12.494691000
H	17.083095000	5.930784000	10.403261000
H	15.322752000	4.193978000	10.487990000
H	10.818462000	9.546361000	14.095251000
H	10.309293000	7.351714000	12.931906000
H	11.657114000	5.366202000	13.520697000
H	15.968007000	9.172237000	18.882504000
H	16.378144000	5.148115000	17.438684000
H	14.087049000	9.484299000	17.314426000
H	12.628424000	9.629180000	15.762398000
H	19.337944000	4.565988000	20.808625000
H	17.430336000	4.741381000	19.246658000
H	19.388452000	8.855973000	21.016284000
H	20.357159000	6.674971000	21.728714000

Ru_1_T_{bpy}:

Ru	13.987490000	4.605057000	15.169605000
N	13.045895000	4.185500000	16.938663000
C	11.949572000	4.814032000	17.417560000
C	11.407385000	4.534131000	18.647501000
C	12.042575000	3.556255000	19.456519000
C	13.167959000	2.924889000	18.999675000
C	13.698131000	3.237374000	17.719997000
C	14.861483000	2.667303000	17.153571000
N	15.231139000	3.158266000	15.904007000
C	16.289454000	2.621219000	15.255671000
C	17.069210000	1.629507000	15.795778000
C	16.735663000	1.137057000	17.085286000
C	15.650197000	1.645958000	17.746084000
N	13.135366000	3.084258000	14.047347000
C	12.259017000	2.196493000	14.540258000
C	11.743006000	1.168873000	13.766365000
C	12.158898000	1.053082000	12.444815000

C	13.074777000	1.965904000	11.937972000
C	13.553109000	2.981146000	12.761253000
C	14.530449000	3.993094000	12.338654000
N	14.914612000	4.860181000	13.306896000
C	15.799795000	5.825403000	13.021714000
C	16.354945000	5.967615000	11.759300000
C	15.968629000	5.084784000	10.757270000
C	15.045351000	4.089073000	11.048775000
C	12.386618000	8.560465000	14.772781000
C	11.325918000	8.462674000	13.882090000
C	11.005216000	7.222884000	13.340183000
C	11.759301000	6.119950000	13.710209000
N	12.778454000	6.210660000	14.575802000
C	13.104477000	7.414900000	15.107048000
C	14.245851000	7.401533000	16.027765000
C	14.733071000	8.522071000	16.696046000
C	15.811848000	8.389551000	17.553269000
C	16.400986000	7.136686000	17.753224000
C	15.871600000	6.062543000	17.039439000
N	14.833682000	6.193377000	16.205244000
C	18.998124000	5.676502000	20.071198000
C	17.905204000	5.739809000	19.214147000
C	17.548635000	6.979376000	18.673909000
N	18.207225000	8.110021000	18.966646000
C	19.248847000	8.034420000	19.791168000
C	19.691260000	6.844407000	20.366279000
H	11.499191000	5.549917000	16.760130000
H	10.515680000	5.054106000	18.975696000
H	11.642336000	3.313876000	20.435712000
H	13.666516000	2.185252000	19.615617000
H	16.508604000	3.038724000	14.278796000
H	17.917749000	1.247189000	15.241700000
H	17.333194000	0.354937000	17.542404000
H	15.379116000	1.264767000	18.724009000
H	11.973141000	2.330698000	15.576813000
H	11.033019000	0.475798000	14.201828000
H	11.779057000	0.257678000	11.812769000
H	13.414906000	1.881456000	10.913529000
H	16.069831000	6.490578000	13.833831000
H	17.071965000	6.758975000	11.575760000
H	16.378696000	5.169290000	9.756727000
H	14.729779000	3.398616000	10.276841000
H	10.758223000	9.347211000	13.614230000
H	10.186181000	7.101535000	12.641236000

H	11.544062000	5.132591000	13.318455000
H	16.293267000	5.067019000	17.103589000
H	14.272884000	9.491890000	16.553763000
H	12.650466000	9.519420000	15.200848000
H	19.296069000	4.727945000	20.506794000
H	17.335579000	4.843053000	18.994830000
H	19.760457000	8.970668000	20.004849000
H	20.549065000	6.841338000	21.030086000
H	16.212257000	9.247601000	18.081441000

Ru_1_T_{bpy} (optimized by TD-PBE0):

Ru	13.986395000	4.568376000	15.178140000
N	13.002211000	4.151859000	16.925617000
C	11.882263000	4.739252000	17.378169000
C	11.334267000	4.462418000	18.615304000
C	11.988838000	3.525925000	19.452182000
C	13.140330000	2.923529000	19.019469000
C	13.672782000	3.237513000	17.736718000
C	14.855604000	2.696634000	17.195997000
N	15.218849000	3.174440000	15.913789000
C	16.281655000	2.612897000	15.283300000
C	17.066983000	1.647050000	15.857079000
C	16.754864000	1.194472000	17.178153000
C	15.668269000	1.712307000	17.825647000
N	13.104060000	3.097095000	14.025075000
C	12.182075000	2.232166000	14.474064000
C	11.645474000	1.242058000	13.666247000
C	12.087262000	1.140618000	12.351938000
C	13.046702000	2.030942000	11.887173000
C	13.543912000	3.009055000	12.743899000
C	14.561842000	3.998378000	12.358291000
N	14.962185000	4.829235000	13.351131000
C	15.885749000	5.765113000	13.096380000
C	16.461138000	5.917031000	11.843214000
C	16.057852000	5.071150000	10.817036000
C	15.097129000	4.102435000	11.076888000
C	12.354008000	8.519295000	14.812727000
C	11.290590000	8.423841000	13.925180000
C	10.978446000	7.187114000	13.372792000
C	11.742746000	6.086506000	13.730782000
N	12.765409000	6.174190000	14.591895000
C	13.082355000	7.375670000	15.132226000
C	14.229606000	7.366419000	16.048449000
C	14.707968000	8.492808000	16.714092000

C	15.800109000	8.377093000	17.556102000
C	16.412676000	7.133761000	17.739493000
C	15.887791000	6.053607000	17.030802000
N	14.833331000	6.164812000	16.214660000
C	19.083524000	5.710750000	19.997497000
C	17.968779000	5.758812000	19.167958000
C	17.583013000	6.992581000	18.634322000
N	18.234558000	8.131839000	18.909433000
C	19.297179000	8.070844000	19.708092000
C	19.769125000	6.887719000	20.273593000
H	11.409216000	5.444703000	16.703754000
H	10.419725000	4.955989000	18.920686000
H	11.582047000	3.288218000	20.429455000
H	13.653150000	2.207727000	19.650665000
H	16.498413000	2.996354000	14.292827000
H	17.915137000	1.250436000	15.312309000
H	17.371793000	0.441396000	17.656249000
H	15.410461000	1.368213000	18.820427000
H	11.875870000	2.353201000	15.506234000
H	10.899947000	0.567017000	14.069464000
H	11.692751000	0.374947000	11.692686000
H	13.404255000	1.957494000	10.867802000
H	16.169842000	6.401195000	13.926696000
H	17.207756000	6.686636000	11.686460000
H	16.483431000	5.162264000	9.823560000
H	14.768879000	3.439363000	10.286460000
H	10.715098000	9.306763000	13.668825000
H	10.158016000	7.065347000	12.675451000
H	11.531655000	5.101987000	13.330215000
H	16.332395000	5.067751000	17.083677000
H	14.231387000	9.455736000	16.579491000
H	12.611720000	9.475823000	15.249784000
H	19.404200000	4.766743000	20.426877000
H	17.405198000	4.854583000	18.964304000
H	19.801739000	9.014001000	19.907915000
H	20.643294000	6.896642000	20.915659000
H	16.194436000	9.240272000	18.080339000

Ru_1_³MC_{Ru}:

Ru	14.181698000	4.786063000	15.435568000
N	13.255211000	4.040873000	17.212473000
C	12.279007000	4.756889000	17.793155000
C	11.675065000	4.376468000	18.981176000
C	12.112315000	3.212850000	19.604657000

C	13.124379000	2.472257000	19.010641000
C	13.678036000	2.898994000	17.803025000
C	14.748860000	2.147647000	17.114141000
N	15.412684000	2.820965000	16.159544000
C	16.395935000	2.212003000	15.492728000
C	16.773824000	0.899431000	15.746987000
C	16.081640000	0.191445000	16.724873000
C	15.053263000	0.818573000	17.416605000
N	13.321589000	3.488067000	14.052589000
C	12.389276000	2.569178000	14.350422000
C	11.809588000	1.757474000	13.388578000
C	12.211087000	1.899486000	12.064096000
C	13.173728000	2.848068000	11.749433000
C	13.717052000	3.635945000	12.762437000
C	14.731980000	4.669302000	12.541470000
N	15.092504000	5.364516000	13.649981000
C	16.022769000	6.326652000	13.546106000
C	16.634980000	6.643712000	12.344065000
C	16.269456000	5.938722000	11.201651000
C	15.308662000	4.942601000	11.302613000
C	13.278816000	9.207740000	15.441110000
C	12.278450000	9.455075000	14.509747000
C	11.619812000	8.381842000	13.917005000
C	12.001996000	7.095267000	14.276129000
N	12.958641000	6.852604000	15.174819000
C	13.590511000	7.883992000	15.760743000
C	14.629127000	7.520534000	16.744522000
C	15.164078000	8.435752000	17.652424000
C	16.133483000	8.029594000	18.551695000
C	16.564629000	6.699145000	18.554931000
C	15.986934000	5.844532000	17.618069000
N	15.051255000	6.234962000	16.741947000
C	18.747987000	4.531925000	20.745083000
C	17.758004000	4.886897000	19.836287000
C	17.594444000	6.238070000	19.513016000
N	18.344583000	7.203882000	20.063573000
C	19.285480000	6.849358000	20.935973000
C	19.534900000	5.530048000	21.308025000
H	11.982221000	5.660206000	17.270547000
H	10.887132000	4.988981000	19.403862000
H	11.677844000	2.888244000	20.544294000
H	13.495686000	1.576229000	19.492696000
H	16.896410000	2.804179000	14.731317000
H	17.584739000	0.447293000	15.186989000

H	16.333103000	-0.841321000	16.943177000
H	14.489366000	0.272635000	18.163619000
H	12.105762000	2.496158000	15.393848000
H	11.059533000	1.031786000	13.680815000
H	11.779556000	1.281371000	11.284168000
H	13.494180000	2.976155000	10.722881000
H	16.277201000	6.847277000	14.462025000
H	17.382194000	7.428180000	12.313312000
H	16.727601000	6.159046000	10.243434000
H	15.016355000	4.379875000	10.424658000
H	12.021991000	10.475824000	14.245490000
H	10.831129000	8.533106000	13.188511000
H	11.526918000	6.223078000	13.834892000
H	16.561568000	8.725021000	19.265045000
H	16.287170000	4.805533000	17.535390000
H	14.806550000	9.458076000	17.670250000
H	13.815486000	10.032862000	15.894174000
H	18.894108000	3.490439000	21.014338000
H	17.115611000	4.124691000	19.408690000
H	19.874427000	7.659650000	21.361271000
H	20.317624000	5.299307000	22.022600000

Ru_1_S_{bpy}:

Ru	14.014532000	4.618348000	15.179675000
N	13.057997000	4.183221000	16.945010000
C	11.968050000	4.811483000	17.433953000
C	11.422623000	4.518341000	18.659700000
C	12.050486000	3.525269000	19.452702000
C	13.170173000	2.890327000	18.983350000
C	13.698360000	3.215143000	17.707575000
C	14.854840000	2.630808000	17.130663000
N	15.243270000	3.135804000	15.896650000
C	16.301663000	2.599899000	15.253081000
C	17.061694000	1.584715000	15.780220000
C	16.701996000	1.068887000	17.050578000
C	15.615363000	1.582234000	17.709043000
N	13.142505000	3.124901000	14.046098000
C	12.254699000	2.242859000	14.527200000
C	11.717496000	1.237875000	13.737659000
C	12.124933000	1.138896000	12.412305000
C	13.054395000	2.044517000	11.917150000
C	13.553217000	3.036216000	12.756628000
C	14.549642000	4.036643000	12.350008000
N	14.943533000	4.885762000	13.330427000

C	15.845350000	5.839599000	13.060937000
C	16.408906000	5.987606000	11.802824000
C	16.012786000	5.123334000	10.788670000
C	15.072107000	4.139396000	11.063730000
C	12.453570000	8.585632000	14.865704000
C	11.384798000	8.513087000	13.982337000
C	11.051451000	7.287035000	13.417455000
C	11.800965000	6.171461000	13.758530000
N	12.826853000	6.237208000	14.617861000
C	13.165915000	7.428519000	15.170117000
C	14.316508000	7.388819000	16.078750000
C	14.824681000	8.494404000	16.755837000
C	15.910231000	8.335861000	17.600169000
C	16.483643000	7.072591000	17.778727000
C	15.931234000	6.014487000	17.058049000
N	14.888462000	6.169885000	16.235001000
C	19.088427000	5.547696000	20.045724000
C	17.986082000	5.637055000	19.203214000
C	17.639266000	6.888428000	18.684346000
N	18.316078000	8.006355000	18.984379000
C	19.366525000	7.905882000	19.794891000
C	19.800358000	6.702352000	20.348070000
H	11.524196000	5.562198000	16.788922000
H	10.535492000	5.040578000	18.996109000
H	11.651390000	3.272681000	20.429668000
H	13.663850000	2.139416000	19.589320000
H	16.538669000	3.034561000	14.287804000
H	17.912107000	1.202693000	15.229115000
H	17.278571000	0.265544000	17.497531000
H	15.324556000	1.181276000	18.673160000
H	11.975941000	2.363733000	15.567155000
H	10.997670000	0.549314000	14.163964000
H	11.728330000	0.361689000	11.768046000
H	13.387987000	1.972114000	10.889642000
H	16.122281000	6.490316000	13.882219000
H	17.139930000	6.768892000	11.632013000
H	16.428875000	5.213145000	9.791093000
H	14.749806000	3.463158000	10.282167000
H	10.820710000	9.406616000	13.737751000
H	10.225849000	7.185677000	12.723105000
H	11.576632000	5.193688000	13.348561000
H	16.338723000	5.012310000	17.106440000
H	14.376298000	9.472062000	16.630522000
H	12.727989000	9.533552000	15.311252000

H	19.379299000	4.589391000	20.464423000
H	17.402233000	4.750889000	18.978479000
H	19.892962000	8.832358000	20.015033000
H	20.666210000	6.679008000	21.000930000
H	16.328178000	9.181521000	18.134701000

Ru_1_S_{ipy}:

Ru	14.105248000	4.775241000	15.377474000
N	13.055451000	4.154388000	17.049808000
C	11.929283000	4.734447000	17.488369000
C	11.269484000	4.290270000	18.624190000
C	11.801844000	3.217325000	19.329870000
C	12.975089000	2.623683000	18.881842000
C	13.590261000	3.112288000	17.733417000
C	14.839361000	2.574382000	17.176861000
N	15.287692000	3.198445000	16.060306000
C	16.413543000	2.777035000	15.468769000
C	17.158505000	1.720134000	15.969426000
C	16.712323000	1.074922000	17.117215000
C	15.539855000	1.504049000	17.725761000
N	13.379055000	3.399622000	13.987777000
C	12.470472000	2.451988000	14.255363000
C	12.037462000	1.552442000	13.293080000
C	12.574320000	1.634863000	12.013426000
C	13.521924000	2.611636000	11.736230000
C	13.910471000	3.489359000	12.744107000
C	14.903718000	4.557360000	12.566449000
N	15.167769000	5.289115000	13.677173000
C	16.044564000	6.301520000	13.618417000
C	16.715176000	6.624140000	12.448639000
C	16.457352000	5.879543000	11.303387000
C	15.540793000	4.837457000	11.361506000
C	12.392017000	8.675496000	15.270309000
C	11.402151000	8.631069000	14.322647000
C	11.147156000	7.424630000	13.629055000
C	11.909803000	6.323912000	13.938827000
N	12.873271000	6.342263000	14.881808000
C	13.155223000	7.516452000	15.561681000
C	14.214307000	7.455589000	16.501643000
C	14.640838000	8.520656000	17.335879000
C	15.669374000	8.343962000	18.216723000
C	16.330064000	7.082571000	18.320685000
C	15.868263000	6.076717000	17.485538000
N	14.872889000	6.238418000	16.603538000

C	19.14000000	5.56928500	20.34481100
C	18.10417000	5.66267100	19.42834400
C	17.43832300	6.89052800	19.26643700
N	17.78677400	7.97425100	19.98511400
C	18.78339800	7.86620000	20.86194100
C	19.49754200	6.69379100	21.08609000
H	11.55905400	5.56535600	16.89988400
H	10.35847100	4.78372900	18.94116400
H	11.31255000	2.84494100	20.22336100
H	13.40343700	1.79091600	19.42506500
H	16.72137600	3.31533700	14.58007300
H	18.06704500	1.41772700	15.46248100
H	17.26872800	0.24371400	17.53652300
H	15.17834800	1.00809200	18.61757200
H	12.08019900	2.42929400	15.26598600
H	11.29582900	0.80639300	13.55262700
H	12.26168600	0.94558500	11.23659900
H	13.95252900	2.68510200	10.74556000
H	16.20505100	6.85000400	14.53878500
H	17.42056400	7.44660300	12.44563800
H	16.96121400	6.10755500	10.37034900
H	15.32438600	4.25422000	10.47543300
H	10.82115300	9.52088600	14.10269500
H	10.37402800	7.35250800	12.87410300
H	11.75115100	5.37372400	13.44062900
H	16.00186600	9.15280500	18.85676400
H	16.31637600	5.09027100	17.49349900
H	14.14153300	9.48084600	17.27487000
H	12.60107900	9.59927100	15.79703100
H	19.66277000	4.62697500	20.47988800
H	17.82257200	4.78744200	18.85316200
H	19.02743000	8.76960400	21.41910500
H	20.30139200	6.66503000	21.81366500

Ru_1_Q:

Ru	14.11626000	4.78629300	15.34184500
N	13.07916800	4.13676900	16.98603300
C	11.92916200	4.66621500	17.45595200
C	11.31138700	4.21510000	18.59726300
C	11.92153400	3.15810600	19.32003900
C	13.10006000	2.62314000	18.87337800
C	13.70918800	3.11599500	17.68923500
C	14.93325000	2.65848300	17.14930700
N	15.37034700	3.31088600	15.99826800

C	16.500510000	2.901435000	15.378598000
C	17.286538000	1.884280000	15.857793000
C	16.879918000	1.222820000	17.048128000
C	15.723893000	1.602029000	17.675249000
N	13.390090000	3.386114000	13.996266000
C	12.510809000	2.426480000	14.319520000
C	12.073381000	1.491266000	13.394674000
C	12.572145000	1.549882000	12.097963000
C	13.490161000	2.538033000	11.766306000
C	13.888697000	3.452560000	12.736830000
C	14.858490000	4.531294000	12.503686000
N	15.150726000	5.287157000	13.589935000
C	16.019459000	6.301137000	13.479186000
C	16.648293000	6.607077000	12.281851000
C	16.357825000	5.838327000	11.160387000
C	15.452695000	4.790973000	11.271664000
C	12.376262000	8.732982000	15.290439000
C	11.365838000	8.690966000	14.355069000
C	11.115558000	7.498672000	13.664794000
C	11.903536000	6.386226000	13.950644000
N	12.879538000	6.404725000	14.856730000
C	13.150366000	7.570565000	15.549103000
C	14.198489000	7.510414000	16.483401000
C	14.642159000	8.600588000	17.313697000
C	15.639795000	8.427199000	18.206283000
C	16.277519000	7.130422000	18.341160000
C	15.810334000	6.096073000	17.469094000
N	14.851929000	6.261450000	16.595667000
C	18.937591000	5.522953000	20.433860000
C	17.950186000	5.648655000	19.474980000
C	17.305098000	6.908958000	19.298437000
N	17.645393000	7.990654000	20.059920000
C	18.588222000	7.844112000	20.965288000
C	19.274838000	6.634933000	21.203144000
H	11.499782000	5.467163000	16.863799000
H	10.379875000	4.663539000	18.920533000
H	11.460037000	2.777698000	20.225691000
H	13.578837000	1.821721000	19.424443000
H	16.769587000	3.444219000	14.478707000
H	18.192709000	1.607298000	15.333043000
H	17.479313000	0.414756000	17.454986000
H	15.399637000	1.093358000	18.575867000
H	12.157566000	2.428116000	15.343926000
H	11.358346000	0.734756000	13.695542000

H	12.253831000	0.831958000	11.349822000
H	13.892145000	2.591318000	10.762389000
H	16.214206000	6.869206000	14.381319000
H	17.347657000	7.433716000	12.239912000
H	16.828460000	6.050761000	10.206542000
H	15.212541000	4.186696000	10.405815000
H	10.772198000	9.576749000	14.156156000
H	10.333532000	7.422330000	12.919273000
H	11.739047000	5.444479000	13.438226000
H	15.984125000	9.233803000	18.840732000
H	16.250530000	5.105941000	17.490950000
H	14.163502000	9.567195000	17.215702000
H	12.581129000	9.649022000	15.830134000
H	19.438085000	4.571950000	20.582269000
H	17.678970000	4.788497000	18.874864000
H	18.834544000	8.725792000	21.554103000
H	20.041926000	6.585623000	21.967814000

RuPd_1_S0:

Ru	13.972320000	4.559098000	15.194963000
N	12.960498000	4.124399000	16.949783000
C	11.843546000	4.735979000	17.372872000
C	11.234595000	4.429881000	18.580469000
C	11.805705000	3.453414000	19.389028000
C	12.961140000	2.816671000	18.957331000
C	13.521833000	3.166951000	17.730514000
C	14.736415000	2.548400000	17.180409000
N	15.153388000	3.054946000	15.992099000
C	16.256245000	2.547100000	15.419822000
C	16.993985000	1.523763000	15.995637000
C	16.572781000	0.997989000	17.212225000
C	15.431767000	1.516754000	17.808253000
N	13.054518000	3.130272000	14.011257000
C	12.069708000	2.308828000	14.407734000
C	11.514600000	1.349738000	13.574319000
C	11.997646000	1.230388000	12.275934000
C	13.017437000	2.074809000	11.859609000
C	13.532929000	3.018972000	12.745628000
C	14.609674000	3.958656000	12.402661000
N	15.001502000	4.775702000	13.412907000
C	15.978062000	5.668034000	13.187007000
C	16.610987000	5.788495000	11.959261000
C	16.218023000	4.953433000	10.919152000
C	15.207055000	4.029661000	11.145447000

C	12.397022000	8.512688000	14.866717000
C	11.312611000	8.433019000	14.004345000
C	10.976750000	7.198851000	13.458403000
C	11.736545000	6.090097000	13.799143000
N	12.782827000	6.159020000	14.636477000
C	13.122638000	7.361149000	15.168630000
C	14.291602000	7.343377000	16.058878000
C	14.778768000	8.473489000	16.713789000
C	15.908855000	8.390415000	17.522816000
C	16.522872000	7.122084000	17.630380000
C	15.978208000	6.031861000	16.961663000
N	14.887515000	6.130457000	16.193308000
C	19.618670000	6.025285000	19.513400000
C	18.495406000	5.923033000	18.702643000
C	17.722636000	7.055363000	18.459609000
N	18.055846000	8.252354000	19.006308000
C	19.138247000	8.350238000	19.786961000
C	19.948014000	7.258237000	20.065455000
Pd	16.793948000	9.806701000	18.553332000
Cl	15.241123000	11.439681000	17.944091000
C	18.314199000	12.099240000	20.308164000
N	17.812212000	11.256173000	19.699258000
C	18.942523000	13.155042000	21.071583000
H	11.432826000	5.489923000	16.711900000
H	10.332407000	4.954683000	18.872768000
H	11.360314000	3.189689000	20.342223000
H	13.422454000	2.055716000	19.574395000
H	16.548439000	2.987167000	14.473554000
H	17.878279000	1.152041000	15.490983000
H	17.122185000	0.194902000	17.691590000
H	15.086437000	1.116547000	18.753577000
H	11.720769000	2.437332000	15.425499000
H	10.719941000	0.713265000	13.946119000
H	11.588642000	0.491195000	11.595596000
H	13.408274000	1.995278000	10.852717000
H	16.253571000	6.295809000	14.026057000
H	17.394809000	6.526155000	11.831393000
H	16.689556000	5.019057000	9.944519000
H	14.885751000	3.372639000	10.346818000
H	10.740704000	9.322458000	13.762559000
H	10.140137000	7.085879000	12.778551000
H	11.507496000	5.108299000	13.402116000
H	16.418370000	5.043467000	17.025571000
H	14.280433000	9.428227000	16.598681000

H	12.677497000	9.464838000	15.299846000
H	20.229465000	5.150422000	19.710305000
H	18.223108000	4.970738000	18.262298000
H	19.350834000	9.331629000	20.192835000
H	20.815589000	7.383640000	20.702618000
H	19.968034000	13.299280000	20.723509000
H	18.381887000	14.083639000	20.940961000
H	18.954078000	12.884969000	22.130218000

RuPd_1_T_{ipy}:

Ru	13.978956000	4.565212000	15.203046000
N	13.040569000	4.144906000	17.000968000
C	11.967080000	4.807154000	17.457025000
C	11.394716000	4.517060000	18.685521000
C	11.962052000	3.516911000	19.467330000
C	13.079302000	2.837543000	18.998442000
C	13.606212000	3.168180000	17.753644000
C	14.784968000	2.523304000	17.159572000
N	15.168438000	3.019417000	15.957557000
C	16.227009000	2.492186000	15.326850000
C	16.963521000	1.449647000	15.868458000
C	16.582251000	0.933719000	17.101981000
C	15.481099000	1.474411000	17.753376000
N	13.115563000	3.075958000	14.009620000
C	12.220443000	2.176877000	14.443575000
C	11.698477000	1.196472000	13.614221000
C	12.128455000	1.141333000	12.293461000
C	13.062812000	2.065511000	11.844734000
C	13.544537000	3.030884000	12.724434000
C	14.536649000	4.051838000	12.362410000
N	14.919732000	4.868498000	13.374799000
C	15.812281000	5.843112000	13.145948000
C	16.376749000	6.042728000	11.895656000
C	15.994868000	5.211939000	10.848847000
C	15.064423000	4.207923000	11.084043000
C	12.434686000	8.509866000	14.758821000
C	11.361857000	8.403386000	13.910263000
C	10.993222000	7.139143000	13.400782000
C	11.732092000	6.042348000	13.782007000
N	12.777644000	6.126960000	14.628355000
C	13.169217000	7.355232000	15.127010000
C	14.301328000	7.348828000	15.981023000
C	14.846078000	8.490275000	16.625862000
C	15.920569000	8.386429000	17.471982000

C	16.477910000	7.069961000	17.693023000
C	15.918162000	5.985667000	17.035701000
N	14.885111000	6.101409000	16.194285000
C	19.350660000	5.924573000	19.853891000
C	18.296190000	5.833703000	18.965615000
C	17.593473000	6.990928000	18.596333000
N	17.954085000	8.201347000	19.116073000
C	18.978822000	8.281420000	19.978636000
C	19.704599000	7.172792000	20.375444000
Pd	16.843610000	9.798535000	18.475618000
Cl	15.483835000	11.521621000	17.643745000
C	18.424814000	12.104445000	20.177318000
N	17.899597000	11.253364000	19.599226000
C	19.081767000	13.171463000	20.901035000
H	11.569521000	5.579140000	16.808961000
H	10.525303000	5.073201000	19.015291000
H	11.542868000	3.267764000	20.436154000
H	13.535460000	2.061841000	19.600350000
H	16.485603000	2.930564000	14.369944000
H	17.815196000	1.057061000	15.325751000
H	17.133348000	0.116492000	17.554559000
H	15.169549000	1.078184000	18.711708000
H	11.914119000	2.258243000	15.479899000
H	10.972490000	0.494387000	14.006684000
H	11.744447000	0.385171000	11.617362000
H	13.412772000	2.029415000	10.820751000
H	16.074652000	6.464582000	13.993686000
H	17.097973000	6.839302000	11.756458000
H	16.413029000	5.343213000	9.856752000
H	14.751978000	3.557673000	10.276784000
H	10.801261000	9.289627000	13.630667000
H	10.152113000	7.016850000	12.729416000
H	11.486887000	5.048034000	13.425537000
H	16.313896000	4.983658000	17.162284000
H	14.398118000	9.460704000	16.446838000
H	12.729440000	9.476074000	15.150801000
H	19.897521000	5.032380000	20.142092000
H	18.009797000	4.872382000	18.553681000
H	19.210921000	9.271571000	20.351888000
H	20.524671000	7.287720000	21.074301000
H	20.114257000	13.267760000	20.557038000
H	18.553386000	14.111566000	20.725749000
H	19.076617000	12.948090000	21.970497000

RuPd_1_T_{py} (optimized by TD-PBE0) :

Ru	13.977200000	4.579652000	15.228834000
N	12.956845000	4.133354000	16.971914000
C	11.843805000	4.756797000	17.386337000
C	11.225346000	4.445429000	18.587073000
C	11.785239000	3.457235000	19.389023000
C	12.938552000	2.811018000	18.962905000
C	13.510234000	3.163645000	17.743358000
C	14.725073000	2.539421000	17.196039000
N	15.160057000	3.053772000	16.019494000
C	16.257585000	2.543452000	15.444704000
C	16.978025000	1.502232000	16.012190000
C	16.540410000	0.967635000	17.218225000
C	15.401293000	1.491334000	17.815341000
N	13.092556000	3.109271000	14.024457000
C	12.152685000	2.244017000	14.430893000
C	11.634055000	1.264215000	13.597640000
C	12.112212000	1.173184000	12.295971000
C	13.088830000	2.064404000	11.872336000
C	13.565117000	3.029285000	12.756855000
C	14.595962000	4.019070000	12.410285000
N	14.975089000	4.838136000	13.422166000
C	15.906415000	5.776579000	13.196106000
C	16.508127000	5.941405000	11.957848000
C	16.127799000	5.107436000	10.913327000
C	15.161521000	4.137310000	11.143066000
C	12.408805000	8.522595000	14.817589000
C	11.336988000	8.427098000	13.963261000
C	10.981618000	7.171504000	13.434942000
C	11.727288000	6.064127000	13.803124000
N	12.768017000	6.133206000	14.643899000
C	13.147233000	7.359840000	15.161420000
C	14.277498000	7.350575000	16.011629000
C	14.802540000	8.493356000	16.679383000
C	15.898947000	8.404052000	17.491891000
C	16.514520000	7.086043000	17.643539000
C	15.953616000	5.988630000	16.989515000
N	14.890361000	6.082510000	16.193638000
C	19.561861000	5.979859000	19.559266000
C	18.451346000	5.878086000	18.742858000
C	17.681722000	7.022078000	18.466735000
N	18.033390000	8.232670000	19.004973000
C	19.109526000	8.321433000	19.792789000
C	19.903009000	7.223387000	20.097526000

Pd	16.809134000	9.800147000	18.521081000
Cl	15.300522000	11.477105000	17.886895000
C	18.372049000	12.086499000	20.260617000
N	17.857140000	11.242818000	19.662982000
C	19.015674000	13.143871000	21.009526000
H	11.450626000	5.519903000	16.725536000
H	10.326532000	4.975094000	18.879914000
H	11.331692000	3.190357000	20.337463000
H	13.387712000	2.042731000	19.579393000
H	16.561752000	2.994486000	14.507188000
H	17.861227000	1.125447000	15.509809000
H	17.076241000	0.151516000	17.690800000
H	15.045015000	1.081475000	18.752224000
H	11.807221000	2.350328000	15.452355000
H	10.872780000	0.590556000	13.973113000
H	11.732914000	0.417496000	11.616625000
H	13.476218000	2.003038000	10.863070000
H	16.173172000	6.401689000	14.039504000
H	17.257695000	6.712997000	11.826756000
H	16.574584000	5.209151000	9.930244000
H	14.849666000	3.482779000	10.339006000
H	10.771299000	9.313996000	13.697490000
H	10.143651000	7.054129000	12.758506000
H	11.482710000	5.076370000	13.428612000
H	16.378962000	4.996399000	17.088638000
H	14.315810000	9.451654000	16.542818000
H	12.698072000	9.482350000	15.227925000
H	20.161124000	5.101909000	19.776945000
H	18.172841000	4.922182000	18.314155000
H	19.334556000	9.305093000	20.186893000
H	20.765605000	7.348534000	20.741222000
H	20.045734000	13.263462000	20.665594000
H	18.473257000	14.080317000	20.859301000
H	19.016174000	12.892856000	22.072887000

RuPd_1_T_{bpy} (optimized by TD-PBE0):

Ru	13.966835000	4.581387000	15.229840000
N	12.979081000	4.124220000	16.900359000
C	11.893816000	4.771741000	17.405849000
C	11.306626000	4.430305000	18.593168000
C	11.860546000	3.351854000	19.356789000
C	12.970185000	2.701886000	18.892602000
C	13.568472000	3.084124000	17.661668000
C	14.746509000	2.524505000	17.124611000

N	15.197962000	3.097418000	15.941266000
C	16.296851000	2.608376000	15.344396000
C	17.033927000	1.563319000	15.866158000
C	16.604012000	0.973705000	17.077999000
C	15.476180000	1.446128000	17.697275000
N	13.103289000	3.095187000	14.049161000
C	12.190347000	2.218247000	14.491928000
C	11.675501000	1.216290000	13.683422000
C	12.128305000	1.114829000	12.373613000
C	13.076670000	2.019181000	11.914840000
C	13.551567000	3.007657000	12.773106000
C	14.554955000	4.012022000	12.388989000
N	14.936874000	4.852631000	13.379551000
C	15.844170000	5.805237000	13.124160000
C	16.420492000	5.963728000	11.872728000
C	16.034716000	5.108201000	10.847831000
C	15.091192000	4.123288000	11.108511000
C	12.454199000	8.553653000	14.803798000
C	11.355001000	8.468734000	13.959553000
C	10.971002000	7.225679000	13.470077000
C	11.703605000	6.108196000	13.843404000
N	12.761684000	6.186446000	14.660301000
C	13.146825000	7.393329000	15.142367000
C	14.318129000	7.369847000	16.031211000
C	14.841725000	8.500546000	16.649578000
C	15.945513000	8.397888000	17.495832000
C	16.486375000	7.105518000	17.693143000
C	15.925567000	6.016652000	17.039895000
N	14.871858000	6.143139000	16.224111000
C	19.375767000	5.936475000	19.840909000
C	18.312836000	5.856318000	18.949837000
C	17.624596000	7.015304000	18.603952000
N	17.979817000	8.216730000	19.125508000
C	19.002819000	8.293223000	19.984302000
C	19.727666000	7.173564000	20.368317000
Pd	16.867462000	9.817647000	18.481656000
Cl	15.513216000	11.510381000	17.621066000
C	18.440588000	12.128272000	20.157934000
N	17.915903000	11.272940000	19.586647000
C	19.096622000	13.200986000	20.872547000
H	11.498768000	5.573683000	16.792914000
H	10.432379000	4.970454000	18.935909000
H	11.407154000	3.061158000	20.298172000
H	13.409703000	1.894984000	19.467398000

H	16.592199000	3.095704000	14.421317000
H	17.920602000	1.218466000	15.348315000
H	17.160981000	0.150615000	17.513403000
H	15.132501000	0.997611000	18.621798000
H	11.869112000	2.339159000	15.519337000
H	10.936067000	0.533233000	14.084582000
H	11.750815000	0.340818000	11.714195000
H	13.444108000	1.949650000	10.898730000
H	16.116433000	6.449794000	13.951755000
H	17.153285000	6.746497000	11.716177000
H	16.460113000	5.204879000	9.854800000
H	14.775560000	3.453189000	10.318931000
H	10.806400000	9.364535000	13.689159000
H	10.119416000	7.111981000	12.809610000
H	11.440367000	5.117427000	13.491404000
H	16.312840000	5.010586000	17.150083000
H	14.394921000	9.472628000	16.481074000
H	12.767880000	9.513909000	15.193719000
H	19.921578000	5.041084000	20.119173000
H	18.022485000	4.900617000	18.528978000
H	19.237953000	9.278954000	20.366203000
H	20.549043000	7.281765000	21.066881000
H	20.131387000	13.288721000	20.533147000
H	18.572060000	14.140305000	20.682140000
H	19.083715000	12.989730000	21.944380000

RuPd_1_T_{bpy} :

Ru	13.984063000	4.580098000	15.175430000
N	13.034090000	4.155506000	16.934739000
C	11.950646000	4.800548000	17.422081000
C	11.396284000	4.508841000	18.643404000
C	12.004256000	3.498911000	19.434921000
C	13.117563000	2.851486000	18.971152000
C	13.662504000	3.178064000	17.701276000
C	14.819419000	2.597539000	17.132184000
N	15.207775000	3.106997000	15.896980000
C	16.267853000	2.572949000	15.251308000
C	17.029773000	1.560022000	15.779399000
C	16.673248000	1.043373000	17.052629000
C	15.586476000	1.552374000	17.711506000
N	13.111350000	3.075059000	14.040675000
C	12.228761000	2.190721000	14.528374000
C	11.699389000	1.175592000	13.746905000
C	12.108363000	1.068742000	12.422506000

C	13.030753000	1.977822000	11.920849000
C	13.522113000	2.980508000	12.751973000
C	14.507251000	3.987209000	12.334209000
N	14.907646000	4.839086000	13.309056000
C	15.801303000	5.797689000	13.028003000
C	16.348329000	5.948542000	11.763012000
C	15.944587000	5.081872000	10.753827000
C	15.013136000	4.092745000	11.041421000
C	12.468591000	8.565601000	14.766803000
C	11.391108000	8.484389000	13.895042000
C	11.029706000	7.246646000	13.374022000
C	11.762037000	6.129655000	13.745333000
N	12.797496000	6.205003000	14.592912000
C	13.163268000	7.406365000	15.104071000
C	14.316497000	7.375349000	16.012313000
C	14.831135000	8.498390000	16.652250000
C	15.917523000	8.382995000	17.518560000
C	16.446954000	7.086092000	17.716152000
C	15.896612000	6.004970000	17.040623000
N	14.863775000	6.146664000	16.201481000
C	19.280313000	5.881864000	19.918673000
C	18.233257000	5.814439000	19.007931000
C	17.566006000	6.981783000	18.649040000
N	17.924982000	8.178710000	19.178501000
C	18.932877000	8.242876000	20.055882000
C	19.637627000	7.114681000	20.452291000
Pd	16.832962000	9.791073000	18.527551000
Cl	15.493815000	11.495229000	17.666457000
C	18.411632000	12.082400000	20.224078000
N	17.881255000	11.234251000	19.647373000
C	19.075481000	13.145627000	20.945624000
H	11.522512000	5.560836000	16.777704000
H	10.516141000	5.043517000	18.979106000
H	11.593072000	3.245632000	20.406816000
H	13.595856000	2.088514000	19.574653000
H	16.503338000	3.008721000	14.286133000
H	17.880479000	1.179363000	15.227453000
H	17.254666000	0.243376000	17.499581000
H	15.299270000	1.154497000	18.678134000
H	11.948351000	2.317452000	15.567371000
H	10.984639000	0.485186000	14.178841000
H	11.718201000	0.283309000	11.784296000
H	13.365832000	1.900025000	10.894205000
H	16.085117000	6.450493000	13.845490000

H	17.072480000	6.734244000	11.583110000
H	16.347350000	5.173847000	9.750974000
H	14.683777000	3.414943000	10.264051000
H	10.841350000	9.379852000	13.625911000
H	10.196009000	7.137706000	12.690483000
H	11.516243000	5.143034000	13.369734000
H	16.277823000	4.996197000	17.148285000
H	14.391181000	9.473589000	16.483042000
H	12.764595000	9.521786000	15.179770000
H	19.809522000	4.979840000	20.207370000
H	17.938565000	4.861784000	18.583207000
H	19.172178000	9.225546000	20.443037000
H	20.447373000	7.213077000	21.165731000
H	20.113384000	13.221960000	20.613069000
H	18.563326000	14.091573000	20.754307000
H	19.053209000	12.931822000	22.016804000

RuPd_1_³MC_{Ru}:

Ru	14.185780000	4.483044000	15.275134000
N	13.381575000	3.956059000	17.183484000
C	12.490156000	4.772148000	17.768274000
C	11.970219000	4.533475000	19.030652000
C	12.403635000	3.409615000	19.725473000
C	13.328645000	2.565666000	19.127061000
C	13.800069000	2.852091000	17.845482000
C	14.777236000	1.988880000	17.148634000
N	15.379228000	2.537597000	16.080097000
C	16.278289000	1.825355000	15.396627000
C	16.629948000	0.527953000	15.747019000
C	16.000527000	-0.052258000	16.844238000
C	15.059193000	0.682398000	17.554054000
N	13.127691000	3.133070000	14.100816000
C	12.185309000	2.295091000	14.562479000
C	11.472168000	1.445218000	13.732414000
C	11.744461000	1.459503000	12.368024000
C	12.716978000	2.322966000	11.884224000
C	13.398404000	3.154947000	12.770438000
C	14.438898000	4.103871000	12.367373000
N	14.949920000	4.854801000	13.376393000
C	15.917586000	5.745086000	13.104410000
C	16.417887000	5.934063000	11.826216000
C	15.895614000	5.173573000	10.784752000
C	14.897334000	4.249823000	11.059378000
C	13.534384000	8.931656000	14.941725000

C	12.454401000	9.162133000	14.099339000
C	11.664199000	8.089236000	13.697578000
C	12.000594000	6.818955000	14.148437000
N	13.033724000	6.592809000	14.963349000
C	13.792360000	7.626458000	15.368600000
C	14.909698000	7.290058000	16.276116000
C	15.564220000	8.259176000	17.037666000
C	16.617867000	7.912676000	17.878747000
C	16.972025000	6.545132000	17.925884000
C	16.267117000	5.627557000	17.157510000
N	15.262966000	5.983513000	16.346585000
C	19.654032000	4.749671000	19.904670000
C	18.596647000	4.919470000	19.020171000
C	18.076032000	6.194295000	18.814426000
N	18.591037000	7.266864000	19.467692000
C	19.610148000	7.102590000	20.319444000
C	20.171402000	5.857892000	20.566312000
Pd	17.698232000	9.066601000	19.040462000
Cl	16.567100000	11.014129000	18.427294000
C	19.541556000	10.924948000	20.994666000
N	18.916613000	10.227727000	20.318741000
C	20.325101000	11.797540000	21.841358000
H	12.192680000	5.638964000	17.187503000
H	11.248732000	5.222833000	19.453703000
H	12.033588000	3.195088000	20.722475000
H	13.696312000	1.697535000	19.660256000
H	16.730797000	2.319663000	14.541146000
H	17.372353000	-0.010842000	15.168951000
H	16.233169000	-1.069596000	17.141591000
H	14.544214000	0.235461000	18.396113000
H	12.004960000	2.319844000	15.630834000
H	10.720384000	0.789138000	14.155497000
H	11.206348000	0.808363000	11.687544000
H	12.938641000	2.350567000	10.824547000
H	16.295416000	6.313203000	13.946363000
H	17.200666000	6.664937000	11.659666000
H	16.261893000	5.295162000	9.771008000
H	14.483920000	3.645303000	10.261618000
H	12.237907000	10.168333000	13.755462000
H	10.809876000	8.227333000	13.044332000
H	11.422959000	5.946966000	13.853264000
H	16.498260000	4.567298000	17.170282000
H	15.240442000	9.291720000	16.991503000
H	14.173235000	9.752681000	15.245013000

H	20.068901000	3.761497000	20.073990000
H	18.180130000	4.067848000	18.494759000
H	19.976576000	7.996684000	20.808643000
H	20.996057000	5.770924000	21.263978000
H	21.366218000	11.791786000	21.510089000
H	19.931892000	12.815047000	21.781640000
H	20.272738000	11.449246000	22.875570000

RuPd_1_Q:

Ru	13.988562289	4.557272891	15.171906918
N	13.025338249	4.137922205	16.934079593
C	11.934805912	4.777098106	17.407536436
C	11.380678008	4.497689750	18.633637635
C	11.997119867	3.507684331	19.440112811
C	13.117545692	2.863896360	18.986955896
C	13.659844049	3.178114730	17.712727984
C	14.820352511	2.597234456	17.150576484
N	15.208015593	3.092494179	15.905478774
C	16.265428896	2.544592126	15.262361461
C	17.026657671	1.539679444	15.802109237
C	16.673787094	1.041590893	17.086380721
C	15.589668279	1.560037613	17.741063256
N	13.115763370	3.074360466	14.018870175
C	12.219981754	2.193173352	14.488793172
C	11.690338564	1.190604439	13.691994901
C	12.112915861	1.093565582	12.370834630
C	13.048366403	1.999216025	11.887418936
C	13.539748807	2.989611978	12.733150756
C	14.536037693	3.993289893	12.335678951
N	14.934268074	4.830926957	13.324114952
C	15.834501447	5.788074814	13.060401957
C	16.391103254	5.951300912	11.801072343
C	15.991408639	5.097908325	10.779053272
C	15.052737207	4.110396437	11.048116937
C	12.427340282	8.552268899	14.815822172
C	11.350567823	8.465314123	13.957931552
C	10.999355158	7.224224878	13.417194267
C	11.756792855	6.111288499	13.765900748
N	12.795840056	6.178307951	14.600184930
C	13.162829876	7.388565054	15.144420976
C	14.278008909	7.376018102	16.016494499
C	14.823419252	8.527776618	16.664623596
C	15.894861415	8.435791430	17.498739658
C	16.460199885	7.096149538	17.717601601

C	15.889571653	5.980521657	17.019446414
N	14.870733149	6.104950437	16.217947726
C	19.249325680	5.865453016	19.890382959
C	18.209170593	5.802711592	18.988527287
C	17.528708183	6.992079688	18.615053247
N	17.909671034	8.209311664	19.159649134
C	18.912435356	8.250253208	20.026341876
C	19.613981669	7.106150988	20.423114533
Pd	16.833837864	9.820682793	18.506428663
Cl	15.512028293	11.542199521	17.649108073
C	18.441486179	12.097165535	20.205868539
N	17.902963607	11.252435871	19.631371016
C	19.115206923	13.156572196	20.923893590
H	11.500204173	5.522686232	16.750307447
H	10.493715449	5.027494889	18.959044865
H	11.587171014	3.264460613	20.415126867
H	13.602137006	2.114043345	19.601674118
H	16.497264465	2.965894052	14.289932701
H	17.874644686	1.148798838	15.253173674
H	17.256083949	0.247407406	17.542360745
H	15.304733900	1.174571098	18.713405443
H	11.930636312	2.312461122	15.526328990
H	10.965229470	0.501933522	14.109138712
H	11.722799990	0.317781715	11.720877066
H	13.393161312	1.928054285	10.863503134
H	16.114901782	6.430713804	13.886979731
H	17.119550874	6.736171422	11.635327097
H	16.402363193	5.199321684	9.780444473
H	14.725850662	3.443373859	10.260434696
H	10.784398280	9.355615633	13.705818598
H	10.163383695	7.111652896	12.737686810
H	11.519627307	5.129971937	13.369522858
H	16.296025819	4.980244330	17.127040690
H	14.372942990	9.495586931	16.480367253
H	12.711345055	9.507159138	15.239769138
H	19.776266467	4.963761253	20.182465834
H	17.907927660	4.851758829	18.565467275
H	19.170777731	9.225606731	20.421438152
H	20.424778372	7.202986032	21.135231055
H	20.153329705	13.223351243	20.589940200
H	18.610813849	14.106285176	20.730556777
H	19.092395309	12.946025481	21.995704590

RuPd_1_S_{bpy}:

Ru	13.986539000	4.584805000	15.166680000
N	13.025159000	4.157627000	16.930572000
C	11.931451000	4.785345000	17.410070000
C	11.378719000	4.495587000	18.633780000
C	12.003941000	3.506359000	19.433265000
C	13.128132000	2.871959000	18.973337000
C	13.663461000	3.193471000	17.699662000
C	14.824584000	2.609917000	17.131118000
N	15.216857000	3.110681000	15.896578000
C	16.282640000	2.578523000	15.262981000
C	17.045465000	1.570184000	15.799674000
C	16.680735000	1.057988000	17.070347000
C	15.587249000	1.568420000	17.719512000
N	13.115107000	3.079283000	14.042168000
C	12.233695000	2.194971000	14.530831000
C	11.696884000	1.184451000	13.748074000
C	12.098331000	1.081890000	12.421180000
C	13.021383000	1.989694000	11.918098000
C	13.519555000	2.987177000	12.751150000
C	14.510347000	3.989646000	12.335153000
N	14.910535000	4.840924000	13.310741000
C	15.809104000	5.795041000	13.032020000
C	16.361879000	5.941967000	11.768849000
C	15.958202000	5.076099000	10.759179000
C	15.021549000	4.091218000	11.044154000
C	12.459775000	8.557963000	14.770500000
C	11.380050000	8.474653000	13.901822000
C	11.023897000	7.237436000	13.376354000
C	11.763498000	6.122592000	13.740468000
N	12.800655000	6.199460000	14.585225000
C	13.161527000	7.400776000	15.099982000
C	14.318361000	7.371763000	16.004023000
C	14.832958000	8.495603000	16.641862000
C	15.919039000	8.380356000	17.508866000
C	16.447239000	7.083070000	17.708513000
C	15.895502000	6.001307000	17.035094000
N	14.864283000	6.142009000	16.194175000
C	19.281967000	5.880366000	19.909798000
C	18.234243000	5.812365000	18.999860000
C	17.566487000	6.979456000	18.641087000
N	17.925621000	8.176678000	19.169797000
C	18.934098000	8.241402000	20.046394000
C	19.639399000	7.113464000	20.442657000
Pd	16.833051000	9.788475000	18.518201000

Cl	15.493990000	11.492065000	17.656348000
C	18.404491000	12.077105000	20.225300000
N	17.877876000	11.231438000	19.641570000
C	19.063730000	13.136339000	20.956854000
H	11.492606000	5.534444000	16.759689000
H	10.489377000	5.018049000	18.963879000
H	11.599505000	3.256078000	20.408690000
H	13.619345000	2.124220000	19.585205000
H	16.522695000	3.010057000	14.296933000
H	17.901225000	1.190144000	15.255456000
H	17.259325000	0.260273000	17.524752000
H	15.293767000	1.171589000	18.684571000
H	11.959358000	2.318558000	15.571645000
H	10.982244000	0.494402000	14.180691000
H	11.702301000	0.300208000	11.781980000
H	13.351071000	1.914192000	10.889564000
H	16.092311000	6.447339000	13.849958000
H	17.090491000	6.723951000	11.590934000
H	16.365277000	5.165250000	9.757822000
H	14.692859000	3.413653000	10.266371000
H	10.824331000	9.368178000	13.638587000
H	10.188421000	7.127040000	12.695267000
H	11.521881000	5.136323000	13.361549000
H	16.275283000	4.992417000	17.144980000
H	14.393208000	9.470731000	16.471955000
H	12.751728000	9.513737000	15.187199000
H	19.811692000	4.978604000	20.198345000
H	17.939499000	4.859558000	18.575526000
H	19.173538000	9.224228000	20.433034000
H	20.449750000	7.212338000	21.155340000
H	20.069974000	13.285706000	20.558368000
H	18.492303000	14.061800000	20.853651000
H	19.129076000	12.866636000	22.013581000

RuPd_1_S_{tpy}:

Ru	13.977118000	4.562372000	15.196564000
N	13.010496000	4.183293000	16.983774000
C	11.937988000	4.862710000	17.414690000
C	11.340131000	4.592121000	18.635725000
C	11.881132000	3.593614000	19.437327000
C	12.998180000	2.895878000	18.995337000
C	13.550279000	3.208069000	17.756735000
C	14.732536000	2.544015000	17.189929000
N	15.134707000	3.013841000	15.983548000

C	16.194626000	2.463536000	15.376117000
C	16.914976000	1.424849000	15.946730000
C	16.514616000	0.937084000	17.185287000
C	15.411238000	1.500542000	17.812715000
N	13.108375000	3.076040000	14.016162000
C	12.188700000	2.200900000	14.445496000
C	11.664442000	1.217261000	13.620788000
C	12.119018000	1.133194000	12.310109000
C	13.078519000	2.033230000	11.865552000
C	13.560580000	3.002911000	12.740308000
C	14.576091000	4.002336000	12.380744000
N	14.941262000	4.838512000	13.383696000
C	15.843991000	5.802704000	13.153827000
C	16.441181000	5.969201000	11.913774000
C	16.080722000	5.115150000	10.878280000
C	15.136741000	4.123544000	11.112795000
C	12.416974000	8.503821000	14.791863000
C	11.358100000	8.408086000	13.924333000
C	11.010657000	7.152996000	13.377218000
C	11.755143000	6.055995000	13.744189000
N	12.785870000	6.128590000	14.608370000
C	13.157252000	7.348258000	15.143537000
C	14.282894000	7.338177000	16.010990000
C	14.796442000	8.472609000	16.692542000
C	15.897307000	8.375399000	17.507150000
C	16.514223000	7.079881000	17.651224000
C	15.957846000	5.996627000	16.988240000
N	14.894411000	6.104930000	16.188823000
C	19.560797000	5.981997000	19.588143000
C	18.457723000	5.877938000	18.761691000
C	17.682965000	7.014514000	18.487603000
N	18.021300000	8.218195000	19.035936000
C	19.093898000	8.311817000	19.836259000
C	19.891490000	7.223085000	20.140045000
Pd	16.789491000	9.779831000	18.549579000
Cl	15.277394000	11.457852000	17.911400000
C	18.326173000	12.068543000	20.314848000
N	17.819992000	11.225747000	19.708397000
C	18.959593000	13.124499000	21.074762000
H	11.559844000	5.631739000	16.752086000
H	10.471563000	5.161659000	18.944064000
H	11.441580000	3.359522000	20.400826000
H	13.433717000	2.120908000	19.613120000
H	16.469644000	2.879900000	14.414003000

H	17.769269000	1.013761000	15.422198000
H	17.052690000	0.123983000	17.660396000
H	15.085254000	1.126460000	18.775058000
H	11.864054000	2.303670000	15.474229000
H	10.917580000	0.535211000	14.009279000
H	11.734229000	0.373611000	11.638324000
H	13.446453000	1.975478000	10.848936000
H	16.088224000	6.442696000	13.992917000
H	17.170781000	6.757823000	11.773339000
H	16.525239000	5.219515000	9.894477000
H	14.840165000	3.456824000	10.313145000
H	10.793842000	9.295792000	13.657198000
H	10.182017000	7.039214000	12.689213000
H	11.526184000	5.068294000	13.359406000
H	16.380184000	5.001439000	17.078957000
H	14.305856000	9.430858000	16.569719000
H	12.696771000	9.464293000	15.208122000
H	20.163728000	5.105514000	19.803256000
H	18.190561000	4.922610000	18.323734000
H	19.304725000	9.296070000	20.236779000
H	20.748275000	7.348177000	20.791419000
H	19.990044000	13.254221000	20.735663000
H	18.411382000	14.058465000	20.930333000
H	18.958251000	12.865066000	22.136101000

Ru_2_S0:

Ru	13.718436000	4.961141000	14.991288000
N	12.915916000	4.706834000	16.889406000
C	12.198753000	5.623843000	17.556995000
C	11.725495000	5.413715000	18.843041000
C	12.006819000	4.205058000	19.470485000
C	12.744018000	3.249936000	18.784465000
C	13.186095000	3.521475000	17.491022000
C	13.963070000	2.575870000	16.679464000
N	14.451570000	3.080044000	15.519942000
C	15.168092000	2.279516000	14.719458000
C	15.420205000	0.948564000	15.020271000
C	14.908450000	0.420195000	16.199558000
C	14.175476000	1.246855000	17.039698000
N	12.308001000	3.839194000	13.984657000
C	11.209928000	3.299962000	14.536133000
C	10.342255000	2.483369000	13.826487000
C	10.622914000	2.206807000	12.493173000
C	11.753359000	2.767756000	11.914736000

C	12.581925000	3.586582000	12.679003000
C	13.772803000	4.267541000	12.151762000
N	14.460331000	5.003243000	13.061586000
C	15.517926000	5.719027000	12.650855000
C	15.963119000	5.710747000	11.337756000
C	15.283305000	4.934022000	10.405861000
C	14.172301000	4.211093000	10.817820000
C	12.926442000	9.150329000	14.949267000
C	11.795530000	9.322371000	14.164155000
C	11.192469000	8.202967000	13.601558000
C	11.744173000	6.955335000	13.845095000
N	12.835397000	6.782667000	14.608058000
C	13.429238000	7.866436000	15.159987000
C	14.628197000	7.583865000	15.962404000
C	15.239539000	8.566723000	16.735460000
C	16.378857000	8.254698000	17.459913000
C	16.893145000	6.972938000	17.353171000
C	16.245773000	6.027997000	16.557089000
N	15.101898000	6.307318000	15.899590000
C	18.473600000	3.267179000	15.303097000
C	17.723122000	4.438171000	15.315281000
C	16.919741000	4.702394000	16.425442000
N	16.839127000	3.888602000	17.483374000
C	17.553246000	2.760511000	17.449179000
C	18.387728000	2.407111000	16.391663000
H	11.994965000	6.549595000	17.032353000
H	11.150395000	6.189893000	19.334600000
H	11.659158000	4.007350000	20.478763000
H	12.982738000	2.304966000	19.256649000
H	15.548319000	2.729800000	13.810341000
H	16.004664000	0.346935000	14.333738000
H	15.075987000	-0.618544000	16.463442000
H	13.759817000	0.855326000	17.960108000
H	11.028981000	3.541228000	15.576825000
H	9.468299000	2.074898000	14.320530000
H	9.970895000	1.566868000	11.908500000
H	11.986750000	2.567797000	10.876256000
H	16.010741000	6.315049000	13.409324000
H	16.825912000	6.305786000	11.061360000
H	15.604746000	4.898858000	9.370532000
H	13.617059000	3.616647000	10.102798000
H	11.396446000	10.316051000	13.991511000
H	10.309386000	8.284528000	12.978430000
H	11.305297000	6.058085000	13.427132000

H	14.820240000	9.563341000	16.785782000
H	13.418589000	10.012405000	15.381259000
H	19.118906000	3.037437000	14.460797000
H	17.783991000	5.145591000	14.495650000
H	17.460386000	2.110483000	18.316272000
H	18.956799000	1.484434000	16.429094000
H	16.861677000	9.000962000	18.081493000
H	17.799774000	6.684194000	17.872544000

Ru_2_³MC_{Ru}:

Ru	13.613829000	4.848630000	14.930677000
N	13.098296000	4.690760000	16.937176000
C	12.460245000	5.645452000	17.633128000
C	12.120618000	5.493088000	18.967619000
C	12.456287000	4.306426000	19.611591000
C	13.104999000	3.310969000	18.894814000
C	13.411460000	3.521726000	17.552017000
C	14.056255000	2.525691000	16.692787000
N	14.225529000	2.907834000	15.402630000
C	14.779510000	2.049547000	14.533450000
C	15.189163000	0.777545000	14.900050000
C	15.026804000	0.379400000	16.223027000
C	14.455978000	1.263268000	17.127659000
N	11.937503000	3.684880000	13.699685000
C	10.902675000	3.025621000	14.225462000
C	10.165884000	2.094481000	13.504310000
C	10.539506000	1.832109000	12.189931000
C	11.618877000	2.512661000	11.640929000
C	12.296354000	3.447383000	12.426187000
C	13.443679000	4.237744000	11.934232000
N	14.154224000	4.912512000	12.867582000
C	15.186760000	5.677908000	12.479432000
C	15.579019000	5.792280000	11.155226000
C	14.860112000	5.097250000	10.188680000
C	13.779589000	4.320758000	10.582812000
C	13.361969000	9.229645000	14.721372000
C	12.317819000	9.450489000	13.834918000
C	11.621952000	8.356113000	13.333211000
C	12.019132000	7.086633000	13.719315000
N	13.034137000	6.866262000	14.573434000
C	13.694390000	7.925572000	15.091940000
C	14.757798000	7.655091000	16.084757000
C	15.009414000	8.569526000	17.109261000
C	15.967927000	8.252276000	18.063556000

C	16.642866000	7.046184000	17.960426000
C	16.344014000	6.188164000	16.896964000
N	15.410167000	6.486065000	15.979970000
C	18.051757000	3.146472000	15.453593000
C	17.304558000	4.317608000	15.516182000
C	17.096490000	4.915823000	16.760606000
N	17.595344000	4.410065000	17.897993000
C	18.301019000	3.283196000	17.824691000
C	18.558878000	2.610469000	16.631605000
H	12.217209000	6.551873000	17.091080000
H	11.604927000	6.294358000	19.483935000
H	12.211196000	4.154034000	20.657170000
H	13.364148000	2.376289000	19.376379000
H	14.900240000	2.406469000	13.517245000
H	15.630767000	0.121684000	14.158812000
H	15.340642000	-0.606699000	16.548349000
H	14.321370000	0.970268000	18.161560000
H	10.661601000	3.256864000	15.259257000
H	9.327755000	1.586322000	13.967671000
H	10.000779000	1.099952000	11.597436000
H	11.932114000	2.303858000	10.625022000
H	15.701271000	6.213303000	13.271329000
H	16.424324000	6.419428000	10.896816000
H	15.127840000	5.167145000	9.139723000
H	13.189560000	3.796881000	9.840995000
H	12.055606000	10.460637000	13.538334000
H	10.792665000	8.472836000	12.645235000
H	11.515992000	6.201883000	13.345076000
H	14.442141000	9.490076000	17.181802000
H	13.934651000	10.061997000	15.113143000
H	18.238226000	2.665195000	14.498379000
H	16.903964000	4.774698000	14.619706000
H	18.684933000	2.895663000	18.766301000
H	19.145992000	1.698372000	16.632104000
H	16.177764000	8.936348000	18.879434000
H	17.398240000	6.748654000	18.677609000

RuPd_2_S0:

Ru	13.678442000	4.907950000	14.913048000
N	12.845632000	4.743790000	16.814003000
C	12.042764000	5.653654000	17.386600000
C	11.627875000	5.560945000	18.706815000
C	12.066594000	4.486013000	19.471803000
C	12.880675000	3.529530000	18.879977000

C	13.248470000	3.673727000	17.543666000
C	14.032207000	2.678549000	16.799201000
N	14.339463000	3.026180000	15.525802000
C	14.930187000	2.118861000	14.734251000
C	15.280954000	0.851850000	15.174144000
C	15.018849000	0.508010000	16.495704000
C	14.381272000	1.430645000	17.313469000
N	12.256091000	3.837924000	13.895695000
C	11.139824000	3.331780000	14.442000000
C	10.259250000	2.531514000	13.730032000
C	10.545932000	2.235043000	12.402068000
C	11.695964000	2.761262000	11.829803000
C	12.536630000	3.566816000	12.594677000
C	13.745846000	4.219622000	12.074322000
N	14.450475000	4.928018000	12.993527000
C	15.512601000	5.641934000	12.587007000
C	15.950773000	5.646855000	11.271453000
C	15.258652000	4.889883000	10.332354000
C	14.138912000	4.176731000	10.738153000
C	13.079274000	9.125547000	14.862517000
C	12.082268000	9.366611000	13.928338000
C	11.502643000	8.287345000	13.268867000
C	11.948728000	7.009018000	13.563016000
N	12.913310000	6.770607000	14.466512000
C	13.475088000	7.812873000	15.119010000
C	14.516693000	7.458283000	16.092081000
C	14.872715000	8.329725000	17.119587000
C	15.763548000	7.912468000	18.096394000
C	16.385898000	6.673385000	17.965819000
C	16.069315000	5.907922000	16.820196000
N	15.069332000	6.225131000	15.965142000
C	18.171918000	3.172104000	15.248174000
C	17.167660000	4.125538000	15.369439000
C	16.988315000	4.787616000	16.576850000
N	17.817582000	4.541952000	17.622072000
C	18.773884000	3.613752000	17.515558000
C	18.979766000	2.897506000	16.343904000
Pd	17.633107000	5.805494000	19.211082000
Cl	17.305856000	7.382796000	20.903360000
C	19.632072000	4.240465000	21.265044000
N	18.937674000	4.762729000	20.504379000
C	20.503288000	3.588170000	22.217894000
H	11.725611000	6.476752000	16.757318000
H	10.978379000	6.324830000	19.118347000

H	11.774169000	4.386902000	20.511615000
H	13.225214000	2.678849000	19.455048000
H	15.139198000	2.431616000	13.717119000
H	15.757688000	0.160209000	14.489224000
H	15.291279000	-0.468354000	16.881824000
H	14.137982000	1.171831000	18.336617000
H	10.959409000	3.584784000	15.479792000
H	9.370731000	2.149186000	14.218972000
H	9.884060000	1.605386000	11.817366000
H	11.936472000	2.544368000	10.796315000
H	16.014990000	6.224488000	13.351484000
H	16.817573000	6.237678000	10.998754000
H	15.575159000	4.865687000	9.295216000
H	13.569326000	3.604241000	10.016469000
H	11.767083000	10.382476000	13.715255000
H	10.720093000	8.424575000	12.531615000
H	11.524685000	6.141343000	13.072440000
H	14.398017000	9.300911000	17.195830000
H	13.559705000	9.950940000	15.373639000
H	18.320746000	2.654741000	14.306002000
H	16.523103000	4.369651000	14.537011000
H	19.393900000	3.460666000	18.390393000
H	19.772428000	2.159903000	16.298640000
H	21.540956000	3.680286000	21.888414000
H	20.391776000	4.059296000	23.197315000
H	20.239913000	2.530529000	22.292639000
H	15.974099000	8.543237000	18.952976000

RuPd_2_³MC_{Ru}:

Ru	13.557407000	4.838347000	14.872846000
N	13.038839000	4.735424000	16.881439000
C	12.381625000	5.700566000	17.544676000
C	12.040236000	5.586165000	18.882767000
C	12.393071000	4.426724000	19.565934000
C	13.058801000	3.418425000	18.882519000
C	13.366116000	3.590797000	17.534438000
C	14.025470000	2.575464000	16.709094000
N	14.177015000	2.910181000	15.403754000
C	14.742508000	2.030540000	14.563382000
C	15.188542000	0.785459000	14.977102000
C	15.046660000	0.437092000	16.316622000
C	14.458190000	1.340856000	17.189953000
N	11.893695000	3.676406000	13.671339000
C	10.829174000	3.072329000	14.203928000

C	10.032767000	2.192261000	13.482303000
C	10.375925000	1.923718000	12.160953000
C	11.486027000	2.547374000	11.605758000
C	12.225539000	3.433160000	12.391365000
C	13.406864000	4.168012000	11.894555000
N	14.121032000	4.850047000	12.820153000
C	15.181804000	5.575238000	12.430010000
C	15.600810000	5.637357000	11.110502000
C	14.881317000	4.931127000	10.152520000
C	13.771551000	4.197850000	10.548478000
C	13.399517000	9.225303000	14.752489000
C	12.400356000	9.492065000	13.827586000
C	11.719716000	8.425795000	13.249137000
C	12.081760000	7.137621000	13.606703000
N	13.051714000	6.872670000	14.499856000
C	13.703440000	7.904157000	15.083457000
C	14.719890000	7.583709000	16.107756000
C	14.858464000	8.390389000	17.240607000
C	15.722499000	7.995596000	18.255963000
C	16.471327000	6.827791000	18.109333000
C	16.318571000	6.135047000	16.887405000
N	15.442746000	6.468690000	15.931061000
C	18.261258000	3.202855000	15.485024000
C	17.366042000	4.265620000	15.519324000
C	17.206789000	4.983715000	16.698850000
N	17.937128000	4.685508000	17.799720000
C	18.798745000	3.662629000	17.769382000
C	18.983281000	2.888819000	16.631236000
Pd	17.683375000	5.956959000	19.389379000
Cl	17.290977000	7.525592000	21.075099000
C	19.614054000	4.391124000	21.514036000
N	18.958158000	4.911755000	20.718645000
C	20.433229000	3.741336000	22.513871000
H	12.124311000	6.584514000	16.973323000
H	11.509768000	6.395256000	19.371120000
H	12.146563000	4.303802000	20.615063000
H	13.328130000	2.502794000	19.394190000
H	14.842633000	2.348529000	13.531979000
H	15.639768000	0.111053000	14.258681000
H	15.388512000	-0.526678000	16.678549000
H	14.338136000	1.085587000	18.235509000
H	10.613658000	3.306880000	15.242488000
H	9.172126000	1.728080000	13.950424000
H	9.788446000	1.231589000	11.566730000

H	11.770930000	2.335007000	10.582484000
H	15.695521000	6.119751000	13.216644000
H	16.467682000	6.232870000	10.848701000
H	15.171701000	4.958841000	9.107641000
H	13.184632000	3.665120000	9.810635000
H	12.160763000	10.515775000	13.559515000
H	10.926286000	8.579258000	12.526966000
H	11.582667000	6.274856000	13.179385000
H	14.254309000	9.284662000	17.353342000
H	13.961520000	10.032280000	15.208350000
H	18.397606000	2.632024000	14.572251000
H	16.804393000	4.558837000	14.641513000
H	19.351804000	3.472036000	18.681147000
H	19.691645000	2.068781000	16.651035000
H	21.445437000	3.602410000	22.126999000
H	20.471500000	4.360937000	23.412945000
H	20.004429000	2.767950000	22.763577000
H	15.799112000	8.582663000	19.164970000

RuPd_2_T_{ipy}:

Ru	13.617657000	4.990503000	14.974361000
N	12.861403000	4.940500000	16.900436000
C	12.049195000	5.878090000	17.414173000
C	11.620680000	5.840247000	18.731053000
C	12.061227000	4.802839000	19.546188000
C	12.896394000	3.828203000	19.015220000
C	13.279394000	3.910902000	17.679542000
C	14.101414000	2.907433000	16.994390000
N	14.352283000	3.168400000	15.688631000
C	15.007591000	2.261088000	14.952957000
C	15.470338000	1.066463000	15.484737000
C	15.250210000	0.805879000	16.831940000
C	14.552836000	1.734181000	17.594040000
N	12.221054000	3.717717000	13.921831000
C	11.188514000	3.101860000	14.511229000
C	10.413824000	2.162273000	13.847571000
C	10.739832000	1.837427000	12.534784000
C	11.813626000	2.472055000	11.924633000
C	12.536808000	3.422680000	12.641986000
C	13.665283000	4.187621000	12.090446000
N	14.326923000	4.965838000	12.979160000
C	15.313126000	5.767216000	12.550219000
C	15.718800000	5.797151000	11.225108000
C	15.066335000	4.980317000	10.308148000

C	14.023037000	4.174784000	10.744179000
C	13.246426000	9.212226000	14.667694000
C	12.227647000	9.461563000	13.763065000
C	11.545174000	8.389414000	13.183318000
C	11.913873000	7.102528000	13.530559000
N	12.894914000	6.859437000	14.415454000
C	13.565625000	7.889315000	14.986071000
C	14.577436000	7.482406000	15.954015000
C	14.801917000	8.213724000	17.105644000
C	15.558940000	7.668331000	18.152081000
C	16.210044000	6.453476000	17.946479000
C	16.084959000	5.839192000	16.682553000
N	15.155769000	6.240311000	15.733441000
C	18.411610000	3.403065000	14.975721000
C	17.372662000	4.308462000	15.120172000
C	17.080122000	4.837333000	16.382508000
N	17.835673000	4.478011000	17.460088000
C	18.834196000	3.600805000	17.318080000
C	19.152647000	3.027288000	16.095007000
Pd	17.398930000	5.488290000	19.182603000
Cl	16.737055000	6.728013000	21.060385000
C	19.360863000	3.788051000	21.180489000
N	18.687054000	4.360483000	20.437128000
C	20.204539000	3.072001000	22.112781000
H	11.743198000	6.669129000	16.740455000
H	10.961958000	6.616086000	19.102655000
H	11.754998000	4.747828000	20.585306000
H	13.239814000	3.010545000	19.636385000
H	15.167819000	2.507519000	13.909872000
H	15.997895000	0.366224000	14.847903000
H	15.605751000	-0.113393000	17.284716000
H	14.351932000	1.538062000	18.639803000
H	10.981547000	3.379418000	15.539315000
H	9.579834000	1.695481000	14.358459000
H	10.166401000	1.095073000	11.990090000
H	12.086232000	2.223495000	10.906316000
H	15.779186000	6.390110000	13.307187000
H	16.528192000	6.453592000	10.927862000
H	15.354196000	4.979862000	9.262375000
H	13.481891000	3.555940000	10.039226000
H	11.971182000	10.482474000	13.499609000
H	10.742078000	8.545168000	12.472736000
H	11.415343000	6.234312000	13.113904000
H	14.317644000	9.177951000	17.224022000

H	13.810173000	10.024294000	15.112275000
H	18.645482000	2.996062000	13.996940000
H	16.797507000	4.633117000	14.263628000
H	19.391277000	3.362242000	18.216583000
H	19.968666000	2.317478000	16.029220000
H	21.245001000	3.127351000	21.784078000
H	20.114973000	3.519374000	23.105483000
H	19.895539000	2.025069000	22.158764000
H	15.636441000	8.185873000	19.100994000

RuPd_2_T_{py} (optimized by TD-PBE0) :

Ru	13.681801000	5.021894000	14.984491000
N	12.819521000	4.928764000	16.861772000
C	11.974194000	5.849226000	17.348689000
C	11.490158000	5.789616000	18.646466000
C	11.906042000	4.744833000	19.463491000
C	12.777167000	3.787104000	18.957116000
C	13.220807000	3.894929000	17.643219000
C	14.102413000	2.917388000	16.987392000
N	14.436685000	3.211202000	15.708199000
C	15.162962000	2.335094000	15.004941000
C	15.618679000	1.140302000	15.546091000
C	15.309811000	0.846229000	16.867677000
C	14.536641000	1.742877000	17.595496000
N	12.216823000	3.786393000	14.000234000
C	11.150889000	3.248030000	14.606013000
C	10.330177000	2.321618000	13.978884000
C	10.635735000	1.930310000	12.680651000
C	11.737714000	2.490774000	12.048293000
C	12.510699000	3.426672000	12.730863000
C	13.662929000	4.124329000	12.140011000
N	14.349280000	4.927080000	12.986249000
C	15.340782000	5.693417000	12.507775000
C	15.734059000	5.654323000	11.179096000
C	15.064979000	4.800327000	10.310231000
C	14.011165000	4.037152000	10.793995000
C	13.275669000	9.236419000	14.642070000
C	12.262456000	9.479250000	13.727659000
C	11.585782000	8.403726000	13.150967000
C	11.952586000	7.117683000	13.509761000
N	12.927572000	6.880090000	14.399821000
C	13.589376000	7.915763000	14.967184000
C	14.579973000	7.499768000	15.951594000
C	14.771673000	8.174459000	17.129397000

C	15.487099000	7.575426000	18.201617000
C	16.141615000	6.370846000	17.981334000
C	16.075238000	5.800692000	16.687489000
N	15.099586000	6.206001000	15.746499000
C	18.563204000	3.595714000	14.909942000
C	17.472267000	4.431485000	15.073569000
C	17.127156000	4.890123000	16.354952000
N	17.884859000	4.517959000	17.433892000
C	18.931097000	3.705585000	17.269613000
C	19.305473000	3.210067000	16.026641000
Pd	17.343246000	5.399395000	19.197213000
Cl	16.550488000	6.488959000	21.116723000
C	19.344941000	3.688566000	21.147405000
N	18.658888000	4.270691000	20.423009000
C	20.204128000	2.959968000	22.055522000
H	11.686891000	6.642007000	16.668920000
H	10.807134000	6.552634000	19.000084000
H	11.554253000	4.669957000	20.486829000
H	13.104269000	2.966652000	19.583302000
H	15.387514000	2.606051000	13.980219000
H	16.206887000	0.466126000	14.934708000
H	15.654166000	-0.073933000	17.327251000
H	14.266238000	1.520391000	18.620091000
H	10.952023000	3.575306000	15.619960000
H	9.475094000	1.918313000	14.508498000
H	10.024397000	1.199027000	12.163006000
H	11.991933000	2.197736000	11.037254000
H	15.819782000	6.353077000	13.222927000
H	16.546768000	6.287603000	10.843484000
H	15.345486000	4.741177000	9.264196000
H	13.453338000	3.394351000	10.124606000
H	12.006042000	10.498281000	13.456792000
H	10.788384000	8.554396000	12.432855000
H	11.455958000	6.247766000	13.094624000
H	14.292960000	9.138871000	17.268622000
H	13.834225000	10.050241000	15.090266000
H	18.836048000	3.246967000	13.918899000
H	16.889993000	4.755180000	14.222701000
H	19.483073000	3.452005000	18.167295000
H	20.160453000	2.549594000	15.945880000
H	21.240015000	3.027041000	21.714783000
H	20.124890000	3.388154000	23.057488000
H	19.901118000	1.910700000	22.085801000
H	15.532192000	8.066941000	19.165906000

RuPd_2_T_{bpy} :

Ru	13.696932000	4.883881000	14.886045000
N	12.896584000	4.768176000	16.789536000
C	12.076601000	5.656320000	17.368894000
C	11.709409000	5.586561000	18.701401000
C	12.231768000	4.539388000	19.491377000
C	13.065959000	3.612942000	18.917958000
C	13.404222000	3.716926000	17.540196000
C	14.213442000	2.806937000	16.831231000
N	14.411509000	3.108493000	15.461123000
C	14.903814000	2.133533000	14.651272000
C	15.358635000	0.930900000	15.120468000
C	15.316312000	0.674756000	16.531006000
C	14.750530000	1.600610000	17.362035000
N	12.258353000	3.810578000	13.904091000
C	11.176892000	3.285997000	14.499413000
C	10.262917000	2.507339000	13.807196000
C	10.484298000	2.255884000	12.457531000
C	11.605173000	2.796696000	11.841158000
C	12.483713000	3.578938000	12.585093000
C	13.679022000	4.230335000	12.031878000
N	14.423948000	4.916565000	12.933645000
C	15.485322000	5.617493000	12.511096000
C	15.883269000	5.632715000	11.182372000
C	15.146580000	4.903477000	10.256272000
C	14.026814000	4.202016000	10.683892000
C	13.082369000	9.118834000	14.829532000
C	12.085345000	9.360780000	13.895303000
C	11.500679000	8.286267000	13.232355000
C	11.946676000	7.007255000	13.520705000
N	12.908720000	6.770511000	14.425539000
C	13.473233000	7.805395000	15.086082000
C	14.508612000	7.447971000	16.065358000
C	14.842569000	8.307358000	17.109225000
C	15.710430000	7.874991000	18.101118000
C	16.335943000	6.637177000	17.972948000
C	16.052185000	5.887344000	16.807994000
N	15.074709000	6.222280000	15.935526000
C	18.178917000	3.150884000	15.265454000
C	17.193660000	4.127600000	15.359762000
C	16.972391000	4.766779000	16.572707000
N	17.754225000	4.489911000	17.646129000
C	18.694043000	3.543213000	17.563778000

C	18.929984000	2.838275000	16.390377000
Pd	17.542914000	5.745868000	19.239714000
Cl	17.202847000	7.322190000	20.928291000
C	19.459461000	4.138985000	21.335393000
N	18.796960000	4.676805000	20.557419000
C	20.289057000	3.466966000	22.311246000
H	11.693097000	6.443422000	16.728441000
H	11.033010000	6.326617000	19.111371000
H	11.968897000	4.461476000	20.541114000
H	13.464329000	2.795273000	19.506764000
H	14.975882000	2.383937000	13.598478000
H	15.770455000	0.205084000	14.429716000
H	15.712408000	-0.253216000	16.928713000
H	14.672511000	1.407187000	18.425773000
H	11.058590000	3.506001000	15.553273000
H	9.400820000	2.106216000	14.326700000
H	9.793039000	1.644498000	11.887698000
H	11.792258000	2.608179000	10.791502000
H	16.019238000	6.183109000	13.266850000
H	16.752242000	6.210596000	10.890536000
H	15.429815000	4.890342000	9.209400000
H	13.426523000	3.650554000	9.971112000
H	11.772814000	10.377842000	13.683983000
H	10.717626000	8.428266000	12.496998000
H	11.522446000	6.142511000	13.024915000
H	14.368289000	9.278494000	17.186428000
H	13.564337000	9.943214000	15.340390000
H	18.356519000	2.647356000	14.321203000
H	16.605545000	4.400554000	14.495994000
H	19.276545000	3.365059000	18.459327000
H	19.705104000	2.081247000	16.366985000
H	21.327067000	3.463825000	21.970319000
H	20.224144000	3.990413000	23.268053000
H	19.946503000	2.437287000	22.437659000
H	15.900011000	8.494692000	18.970625000

RuPd_2_Q:

Ru	13.662307369	4.949695441	14.933940196
N	12.938824860	4.874022279	16.870734325
C	12.154951691	5.819275263	17.412894991
C	11.773854852	5.781954668	18.744715379
C	12.236352117	4.740880913	19.542477864
C	13.046356058	3.761421499	18.981354131
C	13.379080911	3.841023129	17.632003476

C	14.179172146	2.838060821	16.919102925
N	14.422032964	3.118310525	15.615967647
C	15.064918391	2.220227284	14.858666002
C	15.519882235	1.011709386	15.365763648
C	15.303176638	0.727754822	16.708577376
C	14.620592280	1.648741542	17.493288551
N	12.257689443	3.710626240	13.945628657
C	11.237845925	3.099278967	14.563328475
C	10.392568615	2.224078160	13.898499443
C	10.626132054	1.963547209	12.552604263
C	11.687029090	2.591810167	11.913592889
C	12.490626759	3.471235766	12.634139523
C	13.621562468	4.213476344	12.061165660
N	14.320875388	4.965823647	12.943981904
C	15.317486755	5.749538539	12.506820112
C	15.696775342	5.783403819	11.174003653
C	15.008306268	4.990668751	10.262374713
C	13.953997860	4.205090520	10.709040476
C	13.091202666	9.171021198	14.796025545
C	11.998898908	9.384689107	13.993658160
C	11.352827463	8.286708864	13.386413773
C	11.833925148	7.013096809	13.639346422
N	12.884743157	6.782459667	14.435078876
C	13.568772804	7.847106347	15.008059884
C	14.692286325	7.501027760	15.774402310
C	15.287884474	8.416700885	16.752606987
C	15.915060957	7.892444772	17.870558009
C	16.243337915	6.535723737	17.904014976
C	16.098175018	5.816770350	16.615643479
N	15.136107495	6.187242791	15.683667410
C	18.472712664	3.371267627	15.052812668
C	17.438291847	4.278759417	15.127748188
C	17.097106827	4.857990696	16.373389469
N	17.818661226	4.522330593	17.505814600
C	18.809303843	3.637062977	17.418157341
C	19.168042149	3.026223831	16.219556214
Pd	17.272604916	5.534780367	19.204039749
Cl	16.505889631	6.829533635	21.000655195
C	19.093198759	3.809984608	21.321164626
N	18.468093370	4.387024870	20.539503788
C	19.874883093	3.087536545	22.301264604
H	11.832969190	6.613559466	16.750855516
H	11.134984504	6.562347015	19.140593990
H	11.968653729	4.687614815	20.592255880

H	13.411142173	2.944033137	19.590582457
H	15.219753696	2.483929691	13.818843926
H	16.037173634	0.318478708	14.713118340
H	15.650093283	-0.204359850	17.141364248
H	14.421580994	1.433125631	18.535518912
H	11.100028166	3.328665509	15.613925976
H	9.574679615	1.757809635	14.434946265
H	9.991167616	1.276499844	12.003794961
H	11.885970313	2.395001650	10.867493395
H	15.810303706	6.355311602	13.259700322
H	16.514562370	6.424631652	10.866961572
H	15.278003782	4.992727082	9.211832723
H	13.388927417	3.603011961	10.008510871
H	11.640197803	10.393847213	13.819870054
H	10.490034650	8.416582878	12.744635278
H	11.351256917	6.138780474	13.215278803
H	15.057378356	9.472836595	16.691433409
H	13.610720314	10.006773953	15.248672069
H	18.748752260	2.934846747	14.098394932
H	16.900908012	4.584966155	14.239512851
H	19.335361010	3.414555157	18.339622257
H	19.980811466	2.309863529	16.207159866
H	20.930513492	3.112752947	22.020517129
H	19.750856169	3.551606916	23.282547822
H	19.538012983	2.049234219	22.347211106
H	16.148888772	8.532980018	18.715147230

RuPd_2_S_{tpy}:

Ru	13.634591000	4.953114000	14.934863000
N	12.881562000	4.889486000	16.863522000
C	12.086525000	5.829936000	17.395562000
C	11.672959000	5.785310000	18.717596000
C	12.110039000	4.737083000	19.520187000
C	12.925864000	3.757441000	18.970059000
C	13.293591000	3.849459000	17.630376000
C	14.093057000	2.841286000	16.926849000
N	14.330677000	3.110845000	15.620347000
C	14.955534000	2.199745000	14.862295000
C	15.402653000	0.991165000	15.373117000
C	15.198806000	0.721202000	16.721541000
C	14.531979000	1.653026000	17.505840000
N	12.228528000	3.764238000	13.906284000
C	11.167807000	3.184482000	14.484087000
C	10.352066000	2.295006000	13.801952000

C	10.664356000	1.979653000	12.483243000
C	11.766448000	2.575074000	11.884639000
C	12.532588000	3.478752000	12.617197000
C	13.689670000	4.205193000	12.077656000
N	14.363456000	4.962160000	12.977892000
C	15.371733000	5.744954000	12.566408000
C	15.793102000	5.769765000	11.246404000
C	15.132044000	4.970798000	10.318756000
C	14.063706000	4.188449000	10.736100000
C	13.165291000	9.172388000	14.739924000
C	12.154589000	9.414104000	13.828688000
C	11.514951000	8.336164000	13.203723000
C	11.922077000	7.055817000	13.518131000
N	12.895980000	6.816130000	14.415502000
C	13.529150000	7.850907000	15.029962000
C	14.551054000	7.460779000	15.985496000
C	14.814198000	8.232910000	17.107345000
C	15.599078000	7.722955000	18.143322000
C	16.239973000	6.496847000	17.960015000
C	16.070309000	5.833509000	16.727368000
N	15.128486000	6.218623000	15.787037000
C	18.333446000	3.304452000	15.071764000
C	17.316604000	4.235787000	15.199229000
C	17.042176000	4.804829000	16.449660000
N	17.805987000	4.462559000	17.529241000
C	18.783992000	3.560464000	17.402535000
C	19.075666000	2.941150000	16.195535000
Pd	17.452887000	5.574075000	19.205356000
Cl	16.922296000	6.953854000	21.029720000
C	19.446522000	3.936215000	21.226688000
N	18.755924000	4.481214000	20.478168000
C	20.313000000	3.255390000	22.164461000
H	11.776490000	6.629084000	16.733757000
H	11.025717000	6.564687000	19.101789000
H	11.815033000	4.677097000	20.562195000
H	13.266693000	2.929199000	19.578448000
H	15.105308000	2.456145000	13.820034000
H	15.906643000	0.287826000	14.721025000
H	15.543628000	-0.209840000	17.158324000
H	14.343655000	1.447876000	18.552085000
H	10.974671000	3.451893000	15.516947000
H	9.496633000	1.858469000	14.303764000
H	10.057676000	1.274904000	11.924915000
H	12.027274000	2.333914000	10.861526000

H	15.839617000	6.354590000	13.332740000
H	16.620849000	6.407718000	10.959948000
H	15.432932000	4.968114000	9.276677000
H	13.517211000	3.586758000	10.020646000
H	11.870336000	10.433637000	13.589519000
H	10.718131000	8.486996000	12.485289000
H	11.459865000	6.185639000	13.065872000
H	14.337360000	9.202380000	17.210195000
H	13.695803000	9.992118000	15.210189000
H	18.551426000	2.867837000	14.102038000
H	16.747987000	4.554522000	14.336372000
H	19.347913000	3.339256000	18.301272000
H	19.873772000	2.210361000	16.143297000
H	21.350996000	3.342587000	21.834720000
H	20.209110000	3.707388000	23.153659000
H	20.038825000	2.199235000	22.218777000
H	15.709479000	8.271996000	19.070799000