

Supporting Information

Effects of Metal–Metal Bonding in Photosensitizers: Red-Shifted Absorption and Oscillator Strength Enhancement

Oshan J. Jinarathne and Malkanthi K. Karunananda*

Department of Chemistry, Saint Louis University, St. Louis, Missouri 63103, United States.

*E-mail: malkanthi.karunananda@slu.edu

Table of Contents

1. Benchmarking Data for DFT calculations.....	2
2. Calculated Absorption Spectra marked with Oscillator Strengths (Vertical Lines)	5
3. Comparison of [Ru-1] geometries.....	6
4. Visualized NTOs.....	8
5. Orbital Contributions for each NTO.....	12
6. Data Tables for the MVR analysis.....	14
7. MVR Plots.....	16
7.1 MVR analysis with Metal percentage in the <i>hole</i> (M_H) and Molecular Orbital Bond Order	16
7.2 MVR analysis with Metal percentage in the <i>hole</i> (M_H), Molecular Orbital Bond Order and HOMO-LUMO Energy gap	17
7.3 MVR analysis with Metal percentage in the <i>hole</i> (M_H), Molecular Orbital Bond Order, HOMO-LUMO Energy gap and Dielectric constant	18
7.4 Excluding one metal parameter at a time	19
8. Replacing M_H with difference between M_H and M_P	21
9. Calculated NBOs	22
10. Optimized Coordinates (Charge and Multiplicity added to the first line)	31
11. References.....	74

1. Benchmarking Data for DFT calculations

TD-DFT methods which have shown remarkable accuracy in predictions of absorption wavelengths and excited states in organic molecules were used here.¹⁻³ However, since most of the DFT functionals overestimate the excitation energies due to the underestimation of electronic correlation effects for transition metal complexes and also makes errors in the predictions of charge transfers,^{4,5} we performed benchmarking studies to identify the functional with the highest accuracy. A series of hybrid functionals (cam-B3LYP, B3PW91, BPV86, M06 and PBEPBE) were used with the Polarizable Continuum Model (PCM). The number of excited states was varied to match the best fit for the experimental wavelengths (Table S1, Column 2). While some functionals showed closer values for some of the absorption wavelengths (Table S1), the range separated hybrid functional cam-B3LYP which is known for minimizing the above mentioned errors was the most accurate in predicting all the peaks with reasonable accuracy.⁴⁻⁶ The functional cam-B3LYP was also the most accurate in predicting the experimental molar absorptivity in all the complexes (Table S2). UV-Vis plots were obtained from TD DFT output files using GaussView 6.¹⁶

Table S1: TD-DFT benchmarking Data for Absorption wavelength/nm

Complex	Number of Excited States	Wavelength/nm					
		Experimental nm	cam-B3LYP	B3PW91	BPV86	M06	PBEPBE
[Ag-1] ⁷	70	-	190	259	261	200	289
[Ag-2] ⁸	70	257* 351 364 467	228 304 - 438	252 320 - -	- 365 - -	255 333 - -	- 366 - -
[Ag-2-A] ⁸	70	254* 348 460	230 326 435	298 378 579	- - 428	272 354 405	- - 515
[Ru-1]	70	-	481	449	383	575	279
[Ru-2] ⁹	70	672* 880	591 868	629 821	668 812	607 -	665 -
[Mo-1]	30	-	289	343	776	392	781
[Mo-2] ¹⁰	30	521*	436	583	675	494	680
[Rh-2-A] ¹¹	70	330* 433 575	306 400 586	325 349 -	380 - 849	329 358 -	381 458 520

[Rh-2-B]¹²	70	258* 367 560 832	254 306 551 -	- 337 342	- - 481 886	- 341 - -	- - 470 -
[Rh-2-C]¹³	70	259* 366 554	272 331 515	- 339 523	- - 526	- 340 -	- - 527
[Rh-2-D]¹⁴	70	275* 371 531	256 312 -	- 330 496	- - 492	- 318 472	- - 492
[Rh-2-E]¹⁴	70	260* 315 419 525	285 341 430 -	- 339 449 522	- - 464 538	- 331 342 475	- - 464 -
[Rh-2-F]¹⁴	70	261* 314 418 553	285 340 482	- 355 455 588	- - 483 569	- 342 417 503	- - - 645
[Rh-2-G]¹³	70	251* 347 442 692	250 295 374 514	- 317 335 543	- - 431 689	- 310 414 529	- - 433 693
[Rh-2-H]¹³	70	235* 300 436 566	237 303 422 503	- 368 - 556	- - - 527	- - 351 490	- - - 523
[Mo-2-A]¹⁵	30	490*	396	493	572	485	575
[Mo-2-B]¹⁵	30	470*	409	555	613	545	413

* λ_{\max}

Table S2: TD DFT Benchmarking Data for ϵ

Complex	Experimental		Calculated $\epsilon / M^{-1}cm^{-1}$				
	Wavelength/nm	$\epsilon / M^{-1}cm^{-1}$	cam-B3LYP	B3PW91	BPV86	M06	PBEPBE
[Ag-2] in DCM	257	23000	22000	22000	-	22000	-
[Ag-2-A] in DCM	254	47000	45000	40000	-	30000	-
[Ru-2] in EtOAc	672	6729	6800	5600	6000	5600	5500
[Mo-2] in THF	521	46000	46000	40000	30000	45000	52000
[Rh-2-A] in DMF	330	18000	17000	19000	18000	19000	14000
[Rh-2-B] in Acetonitrile	258	124000	118000	-	-	-	-
[Rh-2-C] in Acetonitrile	259	83000	85000	-	-	-	-
[Rh2-D] in Acetonitrile	275	107000	110000	-	-	-	-
[Rh2-E] in Acetonitrile	260	92000	100000	-	-	-	-
[Rh2-F] in Acetonitrile	261	100000	100000	-	-	-	-
[Rh2-G] in Acetonitrile	251	67000	65000	-	-	-	-
[Rh2-H] in Acetonitrile	235	55000	56000	-	-	-	-
[Mo2-A] in THF	490	18600	20000	35000	12000	25000	12000
[Mo2-B] in THF	470	5600	5500	2000	5000	5000	6000

2. Calculated Absorption Spectra marked with Oscillator Strengths (Vertical Lines)

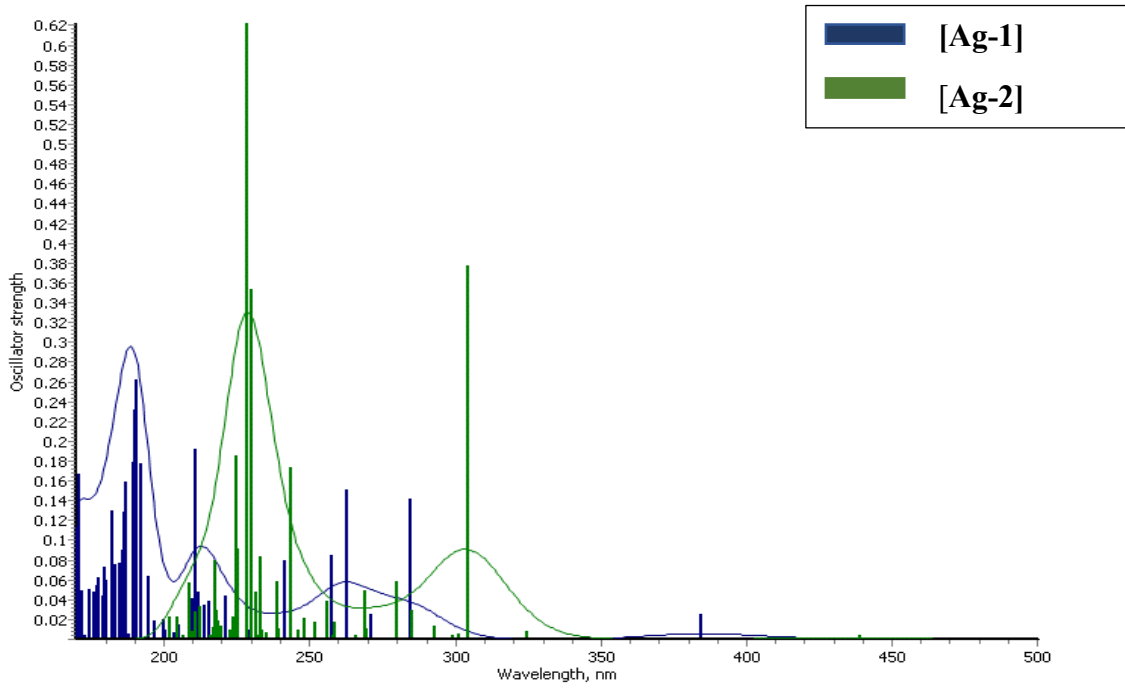


Figure S 1: Calculated Oscillator Strengths for [Ag-1] and [Ag-2]

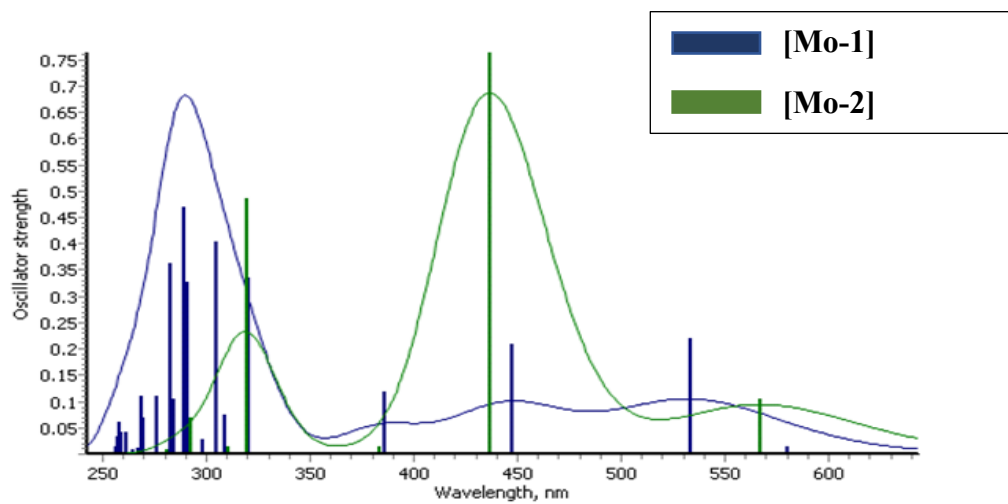


Figure S 2 : Calculated oscillator strengths of [Mo-1] and [Mo-2]

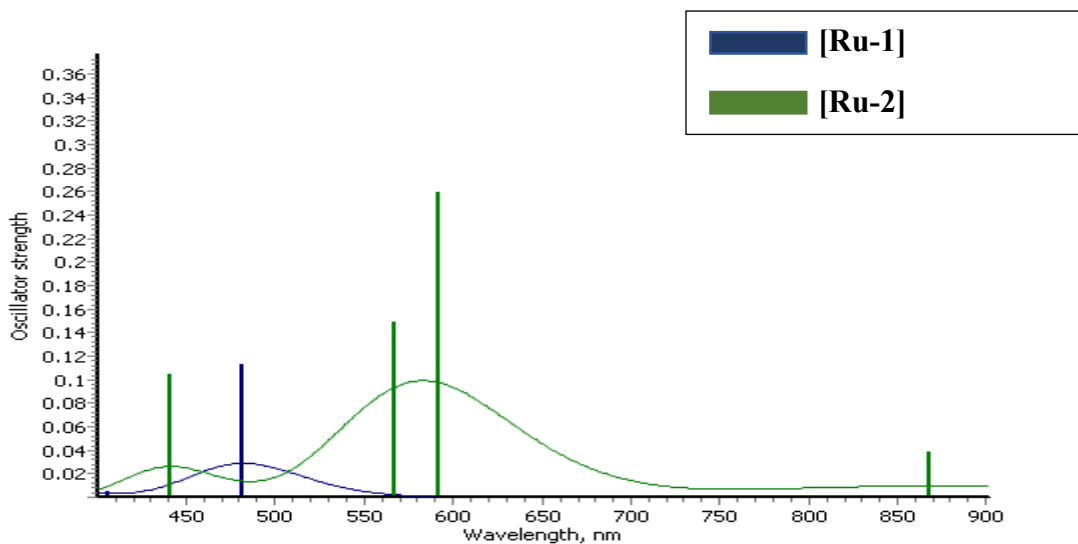


Figure S 4 : Calculated Oscillator Strengths for [Ru-1] and [Ru-2]

3. Comparison of [Ru-1] geometries

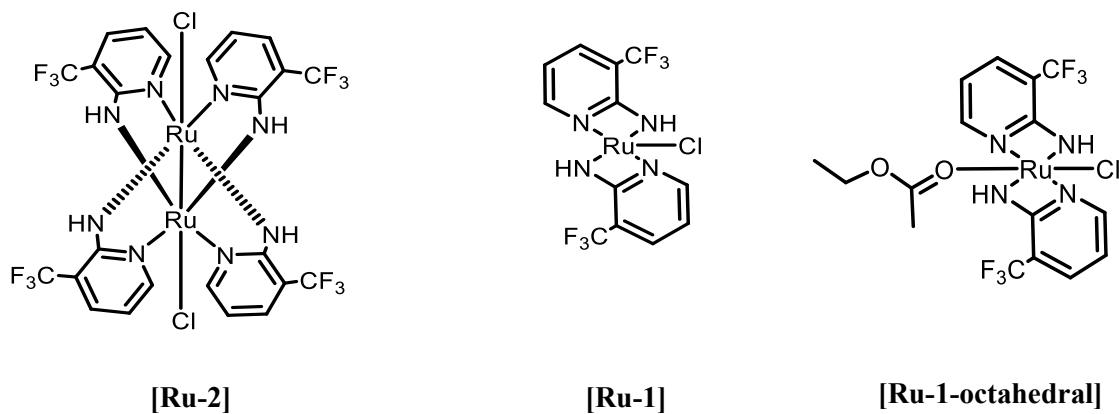


Figure S 5: [Ru-2], [Ru-1] and [Ru-1-octahedral] complexes

Since **[Ru-2]** exhibits a six-coordinate octahedral geometry which is favorable for photoreactivity, and **[Ru-1]** exhibits a square pyramidal geometry which is relatively unfavorable, we modeled a six-coordinate octahedral ruthenium analogue of the monomer, **[Ru-1-Octahedral]** to probe any geometrical effects that might skew our analysis. The empty coordination site of **[Ru-1]** was filled with a solvent molecule (ethyl acetate). The λ_{\max} (482nm in **[Ru-1]** vs. 496nm in **[Ru-1-Octahedral]**) and the oscillator strength (0.113 in **[Ru-1]** vs. 0.120 in **[Ru-1-Octahedral]**) values were comparable, and the trends remained the same.

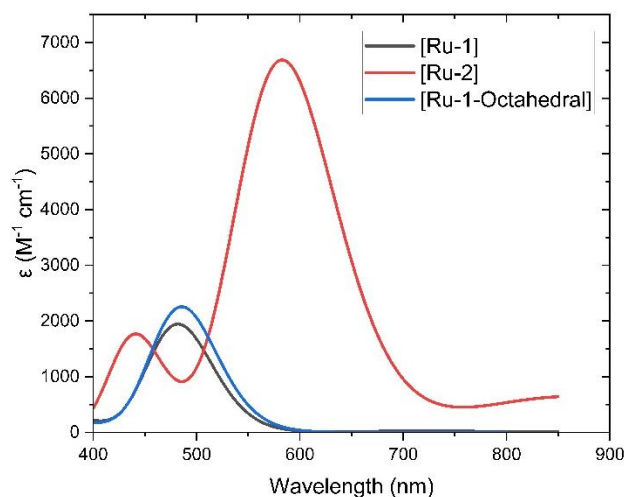


Figure S 6: Simulated UV-Vis spectra of **[Ru-1]**, **[Ru-1-Octahedral]** and **[Ru-2]**

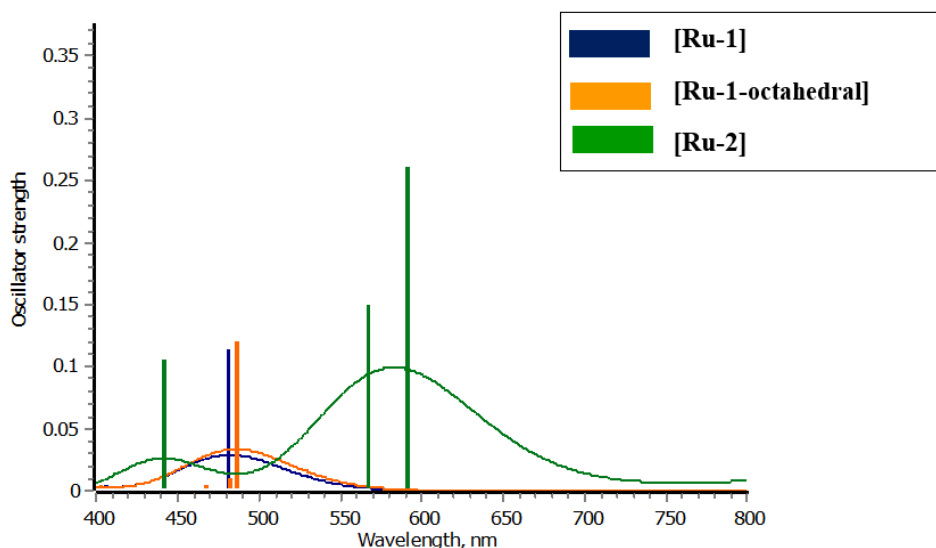


Figure S 7: Calculated Oscillator Strengths for **[Ru-1]**, **[Ru-1-Octahedral]** and **[Ru-2]**.

4. Visualized NTOs

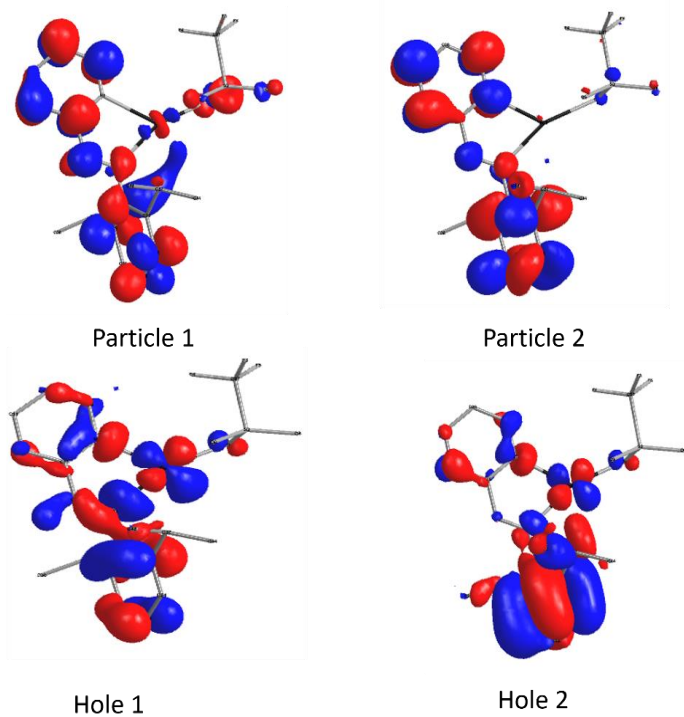


Figure S 8 : Particle 1 and 2 (Top) and Hole 2 (Bottom) for the maximum absorption transition for [Ag-1]

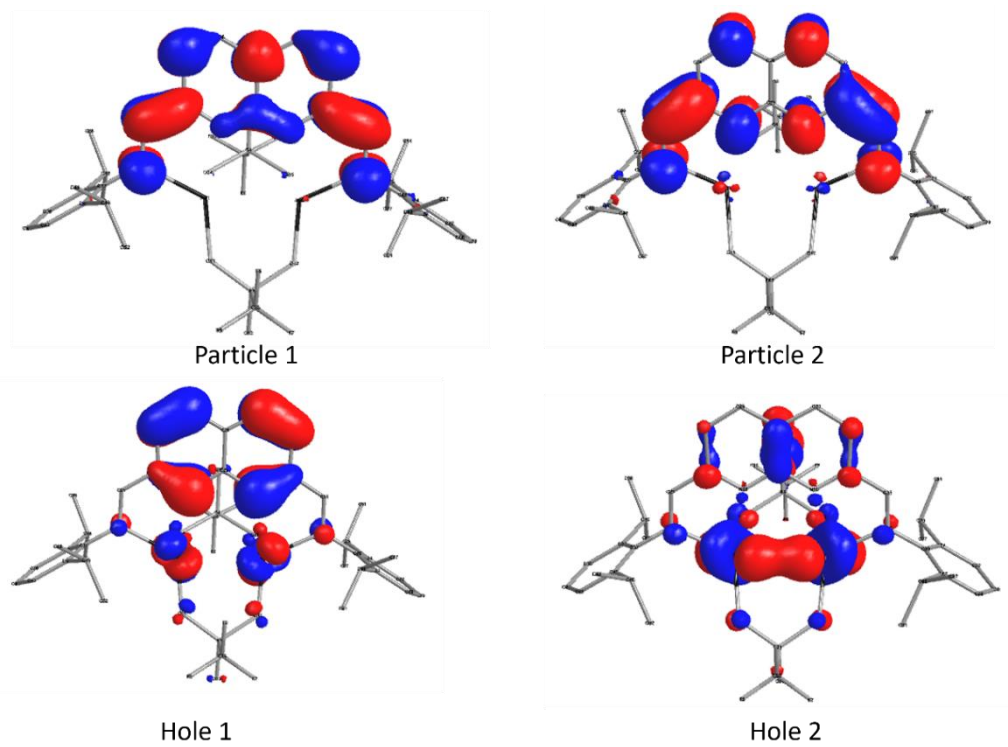


Figure S 9 : Particle 1 and 2 (Top) and Hole 2 (Bottom) for the maximum absorption transition for [Ag-2]

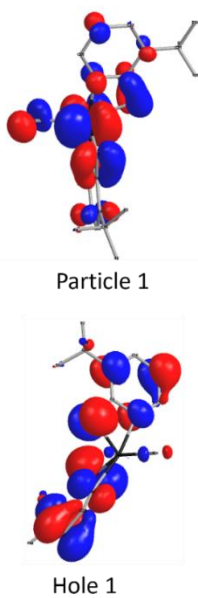
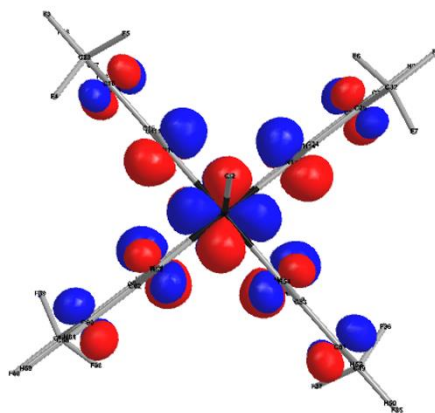
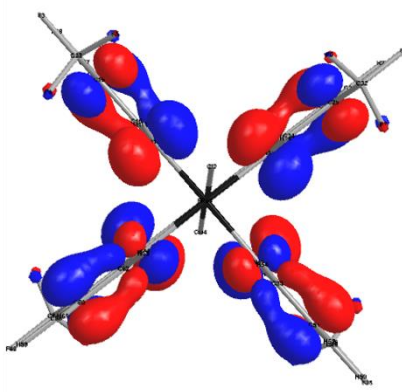


Figure S 10: Particle 1 (Top) and Hole (Bottom) for the maximum absorption transition for [Ru-1]



Particle 1



Hole 1

Figure S 11 : Particle 1 (Top) and Hole (Bottom) for the maximum absorption transition for **[Ru-2]**

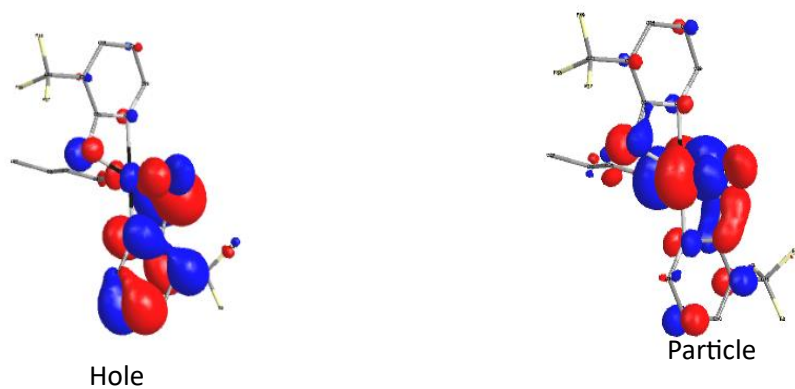


Figure S 12: Particle 1 (Top) and Hole (Bottom) for the maximum absorption transition for **[Ru-1-octahedral]**

5. Orbital Contributions for each NTO

Table S3 : Orbital contribution for the maximum absorption transition

Complex	Experimental Absorption Wavelength	Theoretical Absorption wavelength	Major Orbitals involved with the transition with metal percentage	% of the transition	Normalized Metal contribution to the NTOs associated with the transition
[Ag-1] ⁷	-	190.523 nm (OS0.232)	HOMO 21%→L+6 5%	21%	Hole 17% Particle 7%
			H-1 0% →L+5 3%	16%	
			HOMO 21%→ L+7 21%	9%	
			H-1 0%→ L+2 1%	8%	
			H-2 30%→L+2 1%	7%	
			HOMO 21%→ L+8 51%	7%	
[Ag-2] ⁸	257 nm (23000 M ⁻¹ cm ⁻¹)	228.539 nm (OS 0.622)	H-14 56% → LUMO 1%	21%	Hole 42% Particle 0%
			H-9 19%→ L+1 1%	18%	
			H-8 46%→ L+1 1%	18%	
			H-19 46%→ LUMO 1%	14%	
	351 nm (9700 M ⁻¹ cm ⁻¹)	304.579 nm (OS 0.378)	H-7 13%→ LUMO 1%	83%	Hole 6% Particle 1%
	364 nm (9500 M ⁻¹ cm ⁻¹)				
	467 nm (1800 M ⁻¹ cm ⁻¹)	438.869 nm (OS 0.004)	HOMO 22% → LUMO 1%	72%	Hole 29.2 % Particle 1%

[Ru-1]	-	481.775 nm (OS 0.113)	α HOMO 31% \rightarrow α LUMO 44%	85%	Hole 30% Particle 10%
[Ru-1- Octahedral]	-	496.217 nm (OS 0.057)	β HOMO 13% \rightarrow β LUMO 8%	49%	Hole 30% Particle 70%
			β HOMO-3 22% \rightarrow β LUMO+4 16%	18%	
[Ru-2]⁹	672 nm (6729 M ⁻¹ cm ⁻¹)	591.559 nm (OS 0.260)	H-2 0% \rightarrow LUMO 51%	97%	Hole 0% Particle 53%
	880 nm (6944 M ⁻¹ cm ⁻¹)	868.059 nm (OS 0.038)	HOMO 0% \rightarrow LUMO 65%	83%	Hole 35% Particle 3%
[Mo-1]	-	289.556 nm (OS 0.468)	H-4 2% \rightarrow L+1 1%	23%	Hole 32% Particle 2%
			H-4 2% \rightarrow LUMO 23%	17%	
			HOMO 88% \rightarrow L+4 1%	10%	
[Mo-2]¹⁰	521 nm (46000 M ⁻¹ cm ⁻¹)	436.520 nm (OS 0.763)	HOMO 64% \rightarrow LUMO 3%	67%	Hole 67% Particle 16%
			HOMO 64% \rightarrow L+6 51%	16%	

6. Data Tables for the MVR analysis

Table S4 : Data Table 1 for MVR analysis

Point #	Complex	Solvent	λ	M_H	M_P	$ M_H - M_P $
1	[Ag-2-A] ⁸	DCM	230.592	0.16	0.0077777778	0.1522222222
2	[Ag-2] ⁸	DCM	228.539	0.42	0.01	0.41
3	[Ru-2] ⁹	EtOAc	636.211	0	0.5	0.5
4	[Mo-2] ¹⁰	THF	436.459	0.67	0.16	0.51
5	[Rh-2-A] ¹¹	DMF	306.559	0.206666667	0.4544444444	0.2477777778
6	[Rh-2-B] ¹²	CH3CN	254.118	0.21	0.11	0.1
7	[Rh-2-C] ¹³	CH3CN	272.632	0.08	0.0277777778	0.0522222222
8	[Rh-2-D] ¹⁴	CH3CN	256.905	0.0244444444	0.1225	0.0980555556
9	[Rh-2-E] ¹⁴	CH3CN	285.292	0.308888889	0.216666667	0.0922222222
10	[Rh-2-F] ¹⁴	CH3CN	285.877	0.357	0.264	0.093
11	[Rh-2-G] ¹³	CH3CN	250.581	0.20125	0.305	0.10375
12	[Rh-2-H] ¹³	CH3CN	237.246	0.28	0.273	0.007
13	[Mo-2-A] ¹⁵	THF	396.434	0.69	0.04	0.65
14	[Mo-2-B] ¹⁵	THF	409.043	0.68	0.13	0.55

Table S5 : Data Table 2 for MVR analysis

Point #	New Name	M-M bond order Wiberg	M-M bond order NAO	M-M MO bond order	FSR	ϵ
1	[Ag-2-A]	0.1064	0.2736	0.4718	1.144884242	8.93
2	[Ag-2]	0.0832	0.2374	0.3084	1.144884242	8.93
3	[Ru-2]	0.8819	0.5793	1.1204	0.975020145	5.9867
4	[Mo-2]	3.093	1.4682	0.4104	0.814484895	7.4257
5	[Rh-2-A]	0.7691	0.4695	0.7714	0.947473937	37.219
6	[Rh-2-B]	0.6956	0.4484	0.6822	1.005613472	35.688
7	[Rh-2-C]	0.7178	0.4497	0.7423	0.993985565	35.688
8	[Rh-2-D]	0.7954	0.4294	1.3886	1.023656776	35.688
9	[Rh-2-E]	0.7948	0.4309	1.2399	1.023255814	35.688
10	[Rh-2-F]	0.786	0.4309	0.8587	1.023656776	35.688
11	[Rh-2-G]	0.6722	0.4486	0.9075	0.998396151	35.688
12	[Rh-2-H]	0.7734	0.4454	0.7799	0.977947073	35.688
13	[Mo-2-A]	3.28	1.583	0.1488	0.815863672	7.4257
14	[Mo-2-B]	3.2459	1.6375	-0.077	0.816034082	7.4257

Table S6 : Data Table 3 MVR analysis

Point #	New Name	Oxidation state	<i>d</i> electron count	NBO Charges	$\Delta E_{(\text{HOMO-LUMO})}$	Oscillator strength
1	[Ag-2-A]	1	10	0.667	5.265	0.45
2	[Ag-2]	1	10	0.7247	5.359	0.622
3	[Ru-2]	3	5	0.2836	1.976	0.226
4	[Mo-2]	2	4	0.6666	4.616	0.761
5	[Rh-2-A]	2	7	0.5231	4.656	0.556
6	[Rh2-B]	2	7	0.4047	4.373	0.139
7	[Rh2-C]	2	7	0.4334	4.304	0.238
8	[Rh-2-D]	2	7	0.6104	4.506	1.88
9	[Rh-2-E]	2	7	0.606	4.481	1.984
10	[Rh-2-F]	2	7	0.6074	4.337	1.685
11	[Rh-2-G]	2	7	0.3811	4.516	0.516
12	[Rh-2-H]	2	7	0.5701	4.744	0.223
13	[Mo-2-A]	2	4	0.8188	5.165	1.017
14	[Mo-2-B]	2	4	0.5283	4.887	0.919

7. MVR Plots

7.1 MVR analysis with Metal percentage in the *hole* (M_H) and Molecular Orbital Bond Order

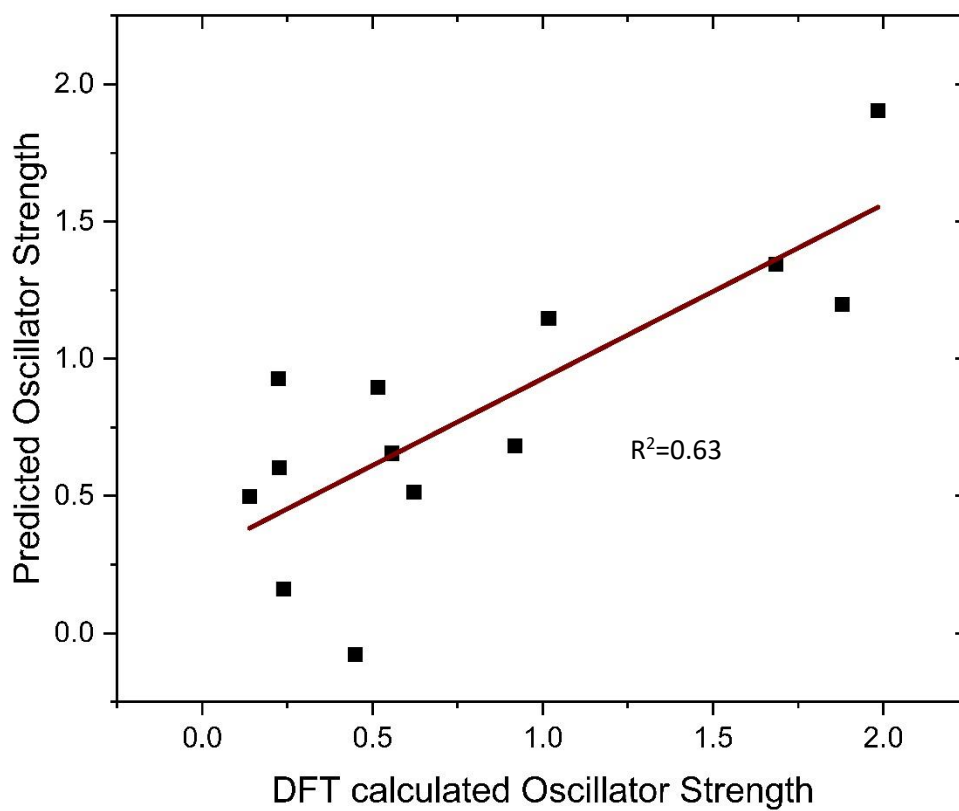


Figure S 13: MVR analysis with metal percentage in the *hole* (M_H) and Molecular Orbital Bond Order

$$\text{Oscillator Strength} = 3.47 M_H + 1.90 \text{BO}_{\text{MO}} - 1.53 \text{ (equation S1)}$$

7.2 MVR analysis with Metal percentage in the *hole* (M_H), Molecular Orbital Bond Order and HOMO-LUMO Energy gap ($\Delta E_{\text{HOMO-LUMO}}$)

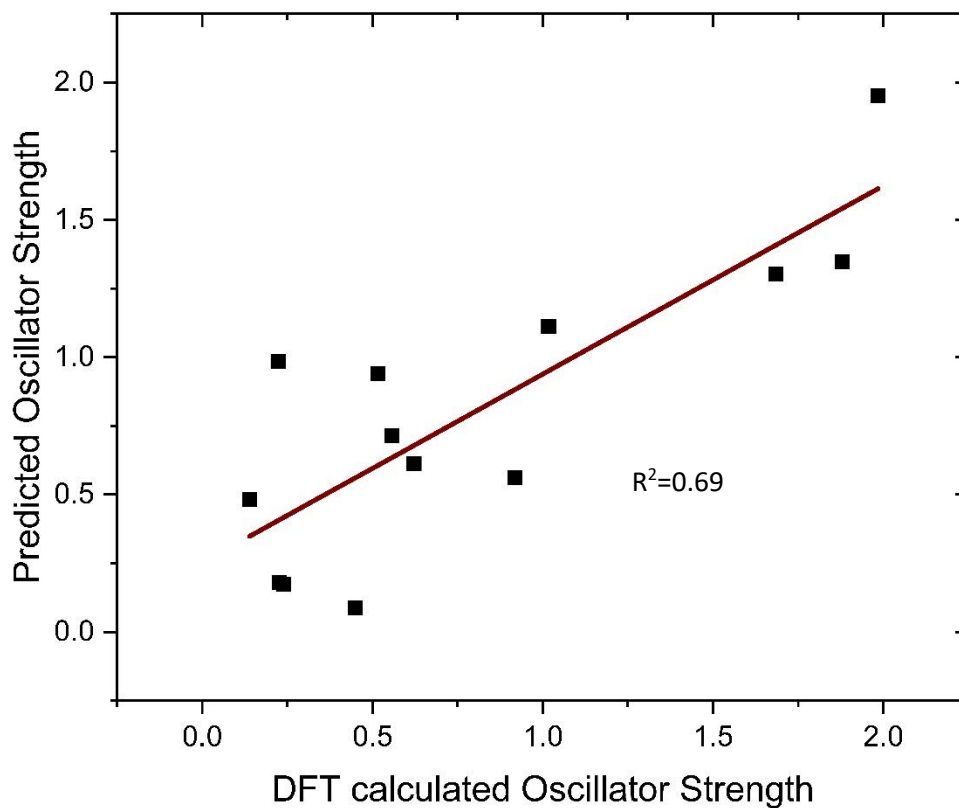


Figure S 14: MVR analysis with metal percentage in the *hole* (M_H), Molecular Orbital Bond Order and HOMO-LUMO Energy gap

$$\text{Oscillator Strength} = 3.20 M_H + 2.02 \text{BO}_{\text{MO}} + 0.21 \Delta E_{\text{LUMO-HOMO}} - 0.01 \varepsilon - 3.06 \text{ (equation S2)}$$

7.3 MVR analysis with Metal percentage in the *hole* (M_H), Molecular Orbital Bond Order, HOMO-LUMO Energy gap ($\Delta E_{\text{HOMO-LUMO}}$) and Dielectric constant (ϵ)

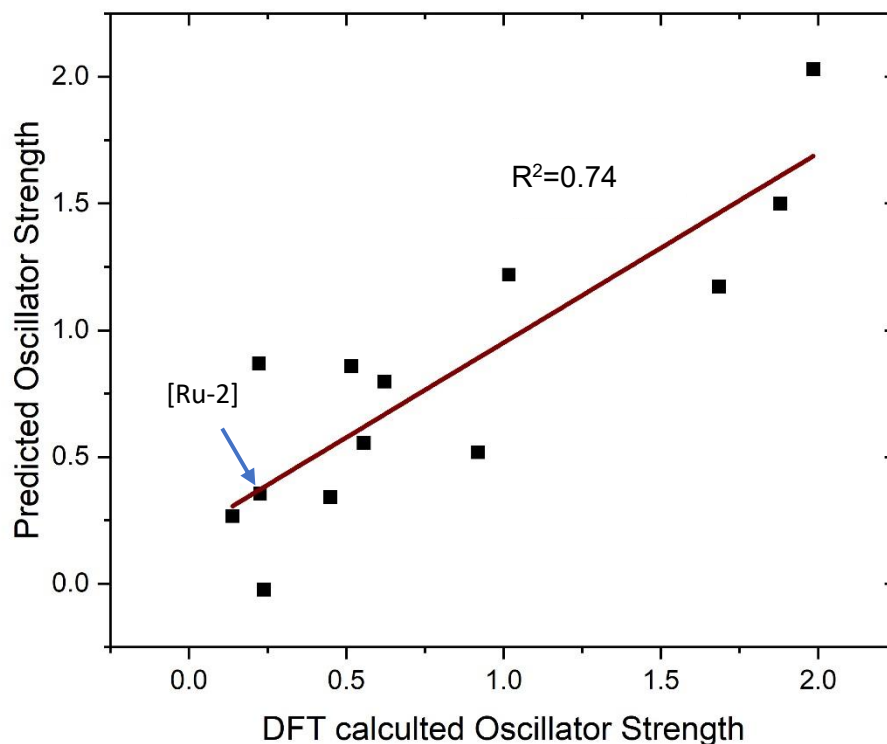


Figure S 15 : MVR analysis with metal percentage in the *hole* (M_H), Molecular Orbital Bond Order, HOMO-LUMO Energy gap and Dielectric constant

Only the outlier **[Ru-2]** is directly aligning with the plot line, all the relevant data are scattered giving a low R^2 value.

$$\text{Oscillator Strength} = 3.21 M_H + 2.52 B_{\text{MO}} + 0.35 \Delta E_{\text{LUMO-HOMO}} - 0.01 \epsilon - 3.06 \quad (\text{equation S3})$$

7.4 Excluding one metal parameter at a time

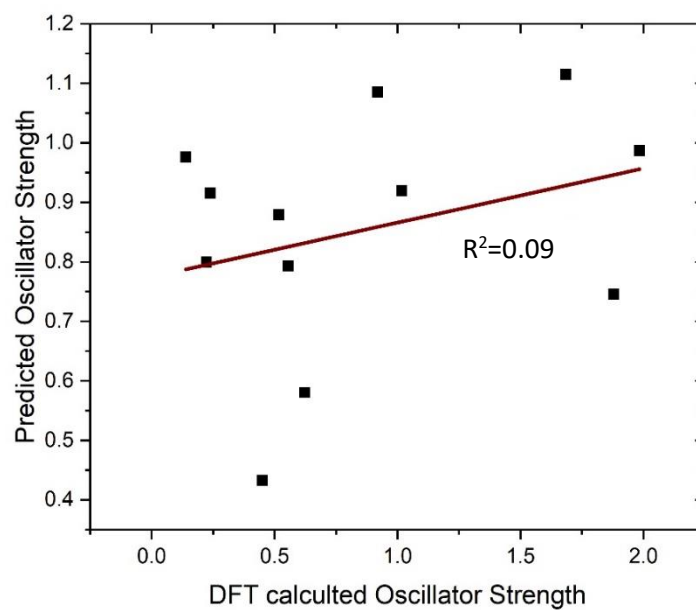


Figure S 16: MVR analysis without the Molecular Orbital Bond Order

$$\text{Oscillator Strength} = 0.79 M_H - 0.62 \Delta E_{\text{LUMO-HOMO}} - 0.002 \epsilon + 3.611 \text{ (equation S4)}$$

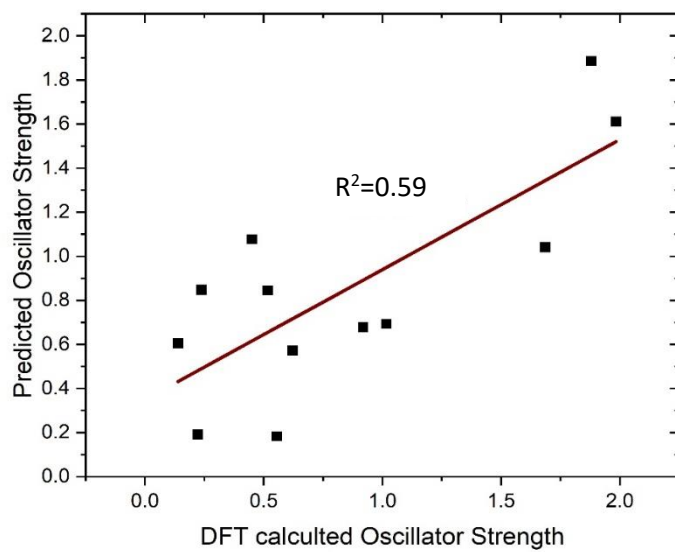


Figure S 17: MVR analysis without the metal percentage in the *hole* (M_H)

$$\text{Oscillator Strength} = 2.12B_{\text{OMO}} - 1.67\Delta E_{\text{LUMO-HOMO}} - 0.09\varepsilon + 9.69 \text{ (equation S5)}$$

8. Replacing M_H with difference between M_H and M_P

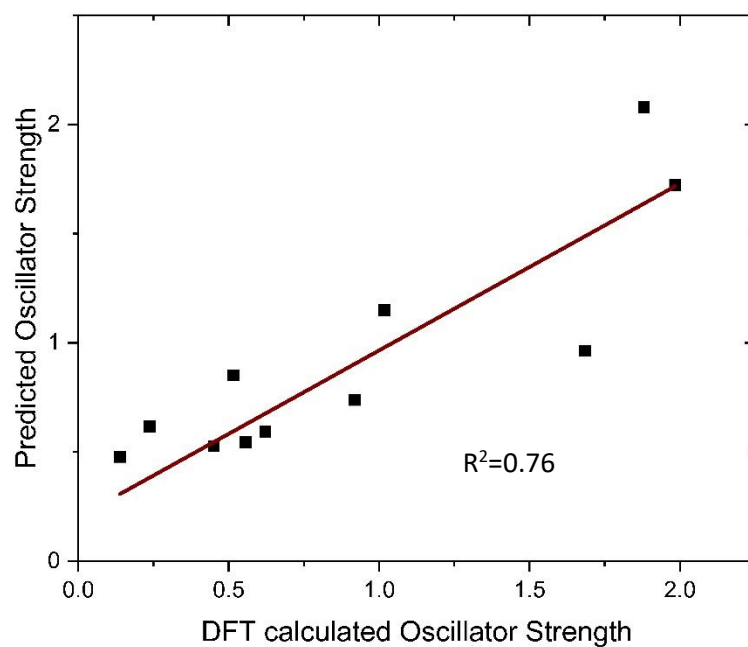


Figure S 18: Replacing M_H with difference between M_H and M_P

Oscillator strength = $2.40 \Delta(M_H - M_P) + 2.54 BO_{MO} - 0.06\epsilon - 1.46\Delta E_{LUMO-HOMO}$ (equation S6)

9. Calculated NBOs

Table S7 : Calculated NBOs of [Ag-1]

MO	Number	Energy/eV	Contribution (100% =1.00)		
HOMO-14	99	-10.614	0.93	(Other)	0.07 (Ag)
HOMO-13	100	-10.589	0.88	(Other)	0.12 (Ag)
HOMO-12	101	-10.523	0.79	(Other)	0.21 (Ag)
HOMO-11	102	-10.462	0.74	(Other)	0.26 (Ag)
HOMO-10	103	-10.44	0.98	(Other)	0.02 (Ag)
HOMO-9	104	-10.347	0.81	(Other)	0.19 (Ag)
HOMO-8	105	-10.251	0.96	(Other)	0.04 (Ag)
HOMO-7	106	-9.869	0.65	(Ag)	0.35 (Other)
HOMO-6	107	-9.843	0.58	(Ag)	0.42 (Other)
HOMO-5	108	-9.713	0.52	(Ag)	0.48 (Other)
HOMO-4	109	-9.355	0.91	(Other)	0.09 (Ag)
HOMO-3	110	-8.971	0.53	(Ag)	0.47 (Other)
HOMO-2	111	-8.657	0.7	(Other)	0.3 (Ag)
HOMO-1	112	-8.176	1	(Other)	0 (Ag)
HOMO	113	-7.725	0.79	(Other)	0.21 (Ag)
LUMO	114	-1.432	0.98	(Other)	0.02 (Ag)
LUMO+1	115	-0.706	0.88	(Other)	0.12 (Ag)
LUMO+2	116	-0.152	0.99	(Other)	0.01 (Ag)
LUMO+3	117	0.314	0.7	(Other)	0.3 (Ag)
LUMO+4	118	0.727	0.54	(Other)	0.46 (Ag)
LUMO+5	119	0.9	0.97	(Other)	0.03 (Ag)
LUMO+6	120	1.018	0.95	(Other)	0.05 (Ag)
LUMO+7	121	1.447	0.79	(Ag)	0.21 (Other)
LUMO+8	122	1.52	0.51	(Ag)	0.49 (Other)
LUMO+9	123	1.656	0.79	(Other)	0.21 (Ag)
LUMO+10	124	1.852	0.56	(Other)	0.44 (Ag)
LUMO+11	125	2.057	0.68	(Other)	0.32 (Ag)
LUMO+12	126	2.077	0.86	(Ag)	0.14 (Other)
LUMO+13	127	3.877	0.89	(Other)	0.11 (Ag)
LUMO+14	128	4.13	0.58	(Other)	0.42 (Ag)

Table S8 : Calculated NBOs of [Ag-2]

MO	Number	Energy/eV	Contribution			
HOMO-13	205	-9.753	0.65	(Ag)	0.35	(Other)
HOMO-12	206	-9.669	0.57	(Ag)	0.43	(Other)
HOMO-11	207	-9.4	0.56	(Other)	0.44	(Ag)
HOMO-10	208	-9.329	0.58	(Ag)	0.42	(Other)
HOMO-9	209	-9.314	0.81	(Other)	0.19	(Ag)
HOMO-8	210	-9.154	0.54	(Other)	0.46	(Ag)
HOMO-7	211	-9.066	0.87	(Other)	0.13	(Ag)
HOMO-6	212	-8.837	0.57	(Ag)	0.43	(Other)
HOMO-5	213	-8.707	0.51	(Other)	0.49	(Ag)
HOMO-4	214	-8.667	0.51	(Ag)	0.49	(Other)
HOMO-3	215	-8.091	1	(Other)	0	(Ag)
HOMO-2	216	-8.089	1	(Other)	0	(Ag)
HOMO-1	217	-7.783	0.9	(Other)	0.1	(Ag)
HOMO	218	-7.645	0.78	(Other)	0.22	(Ag)
LUMO	219	-2.286	0.99	(Other)	0.01	(Ag)
LUMO+1	220	-1.317	0.99	(Other)	0.01	(Ag)
LUMO+2	221	-0.97	0.74	(Other)	0.26	(Ag)
LUMO+3	222	-0.51	0.93	(Other)	0.07	(Ag)
LUMO+4	223	0.098	0.97	(Other)	0.03	(Ag)
LUMO+5	224	0.313	0.88	(Other)	0.12	(Ag)
LUMO+6	225	0.461	0.99	(Other)	0.01	(Ag)
LUMO+7	226	0.714	0.85	(Other)	0.15	(Ag)
LUMO+8	227	0.798	0.59	(Other)	0.41	(Ag)
LUMO+9	228	0.966	0.97	(Other)	0.03	(Ag)
LUMO+10	229	1.019	0.99	(Other)	0.01	(Ag)
LUMO+11	230	1.047	0.77	(Other)	0.23	(Ag)
LUMO+12	231	1.14	0.95	(Other)	0.05	(Ag)
LUMO+13	232	1.214	0.57	(Other)	0.43	(Ag)
LUMO+14	233	1.424	0.73	(Ag)	0.27	(Other)

Table S9 : Calculated NBOs of [Mo-1]

MO	Number	Energy/eV	Contribution			
HOMO-14	148	-9.097	0.97	(Other)	0.03	(Mo)
HOMO-13	149	-8.83	1	(Other)	0	(Mo)
HOMO-12	150	-8.828	1	(Other)	0	(Mo)
HOMO-11	151	-8.618	0.99	(Other)	0.01	(Mo)
HOMO-10	152	-8.583	0.99	(Other)	0.01	(Mo)
HOMO-9	153	-8.539	1	(Other)	0	(Mo)
HOMO-8	154	-8.454	1	(Other)	0	(Mo)
HOMO-7	155	-8.422	0.99	(Other)	0.01	(Mo)
HOMO-6	156	-8.324	1	(Other)	0	(Mo)
HOMO-5	157	-7.979	0.97	(Other)	0.03	(Mo)
HOMO-4	158	-7.891	0.98	(Other)	0.02	(Mo)
HOMO-3	159	-7.226	0.94	(Other)	0.06	(Mo)
HOMO-2	160	-6.959	0.97	(Other)	0.03	(Mo)
HOMO-1	161	-5.909	0.85	(Mo)	0.15	(Other)
HOMO	162	-5.841	0.88	(Mo)	0.12	(Other)
LUMO	163	-1.135	0.77	(Other)	0.23	(Mo)
LUMO+1	164	-1.035	0.9	(Other)	0.1	(Mo)
LUMO+2	165	-0.057	0.62	(Mo)	0.38	(Other)
LUMO+3	166	0.046	0.63	(Mo)	0.37	(Other)
LUMO+4	167	0.677	0.9	(Other)	0.1	(Mo)
LUMO+5	168	0.685	0.96	(Other)	0.04	(Mo)
LUMO+6	169	0.691	1	(Other)	0	(Mo)
LUMO+7	170	0.693	0.94	(Other)	0.06	(Mo)
LUMO+8	171	0.818	0.96	(Other)	0.04	(Mo)
LUMO+9	172	0.851	0.64	(Other)	0.36	(Mo)
LUMO+10	173	0.958	0.73	(Other)	0.27	(Mo)
LUMO+11	174	1.04	0.83	(Other)	0.17	(Mo)
LUMO+12	175	1.117	0.93	(Other)	0.07	(Mo)
LUMO+13	176	1.217	0.94	(Other)	0.06	(Mo)
LUMO+14	177	1.547	0.87	(Other)	0.13	(Mo)

Table S10 : Calculated NBOs of [Mo-2]

MO	Number	Energy/eV	Contribution			
HOMO-14	310	-8.249	0.95	(Other)	0.05	(Mo)
HOMO-13	311	-8.248	0.96	(Other)	0.04	(Mo)
HOMO-12	312	-8.24	1	(Other)	0	(Mo)
HOMO-11	313	-8.089	0.67	(Mo)	0.33	(Other)
HOMO-10	314	-8.088	0.68	(Mo)	0.32	(Other)
HOMO-9	315	-7.942	0.95	(Other)	0.05	(Mo)
HOMO-8	316	-7.743	0.92	(Other)	0.08	(Mo)
HOMO-7	317	-7.704	0.99	(Other)	0.01	(Mo)
HOMO-6	318	-7.627	0.94	(Other)	0.06	(Mo)
HOMO-5	319	-7.626	0.94	(Other)	0.06	(Mo)
HOMO-4	320	-7.516	0.74	(Mo)	0.26	(Other)
HOMO-3	321	-6.89	0.9	(Other)	0.1	(Mo)
HOMO-2	322	-6.801	0.82	(Other)	0.18	(Mo)
HOMO-1	323	-6.801	0.82	(Other)	0.18	(Mo)
HOMO	324	-5.421	0.64	(Mo)	0.36	(Other)
LUMO	325	-0.805	0.97	(Other)	0.03	(Mo)
LUMO+1	326	-0.805	0.97	(Other)	0.03	(Mo)
LUMO+2	327	-0.595	0.99	(Other)	0.01	(Mo)
LUMO+3	328	-0.223	0.89	(Other)	0.11	(Mo)
LUMO+4	329	0.156	0.75	(Mo)	0.25	(Other)
LUMO+5	330	0.393	0.76	(Other)	0.24	(Mo)
LUMO+6	331	0.632	0.51	(Mo)	0.49	(Other)
LUMO+7	332	0.632	0.51	(Mo)	0.49	(Other)
LUMO+8	333	0.64	0.95	(Other)	0.05	(Mo)
LUMO+9	334	0.653	0.95	(Other)	0.05	(Mo)
LUMO+10	335	0.731	0.98	(Other)	0.02	(Mo)
LUMO+11	336	0.735	0.93	(Other)	0.07	(Mo)
LUMO+12	337	0.75	0.98	(Other)	0.02	(Mo)
LUMO+13	338	0.752	1	(Other)	0	(Mo)
LUMO+14	339	0.752	1	(Other)	0	(Mo)

Table S11 : Calculated NBOs of [Ru-1]

MO	Number	Energy/eV	Contribution			
α HOMO-13	80	-12.255	0.68	(Other)	0.32	(Ru)
α HOMO-12	81	-11.674	0.92	(Other)	0.08	(Ru)
α HOMO-11	82	-11.292	0.96	(Other)	0.04	(Ru)
α HOMO-10	83	-10.938	0.86	(Other)	0.14	(Ru)
α HOMO-9	84	-10.838	0.9	(Other)	0.1	(Ru)
α HOMO-8	85	-10.67	0.97	(Other)	0.03	(Ru)
α HOMO-7	86	-10.541	0.82	(Other)	0.18	(Ru)
α HOMO-6	87	-9.926	0.71	(Other)	0.29	(Ru)
α HOMO-5	88	-9.487	0.85	(Other)	0.15	(Ru)
α HOMO-4	89	-9.222	0.56	(Other)	0.44	(Ru)
α HOMO-3	90	-8.698	0.51	(Other)	0.49	(Ru)
α HOMO-2	91	-8.207	0.5	(Ru)	0.5	(Other)
α HOMO-1	92	-7.96	0.98	(Other)	0.02	(Ru)
α HOMO	93	-7.448	0.76	(Other)	0.24	(Ru)
α LUMO	94	-1.229	0.52	(Ru)	0.48	(Other)
α LUMO+1	95	-0.663	0.99	(Other)	0.01	(Ru)
α LUMO+2	96	-0.533	0.87	(Other)	0.13	(Ru)
α LUMO+3	97	0.325	0.53	(Ru)	0.47	(Other)
α LUMO+4	98	0.339	0.86	(Other)	0.14	(Ru)
α LUMO+5	99	0.456	0.87	(Other)	0.13	(Ru)
α LUMO+6	100	1.251	0.93	(Ru)	0.07	(Other)
α LUMO+7	101	1.428	0.98	(Ru)	0.02	(Other)
α LUMO+8	102	1.641	1.06	(Ru)	-0.06	(Other)
α LUMO+9	103	2.26	1.28	(Ru)	-0.28	(Other)
α LUMO+10	104	3.234	0.98	(Other)	0.02	(Ru)
α LUMO+11	105	3.272	0.99	(Other)	0.01	(Ru)
α LUMO+12	106	3.365	0.99	(Other)	0.01	(Ru)
α LUMO+13	107	3.365	0.99	(Other)	0.01	(Ru)
α LUMO+14	108	4.152	0.95	(Other)	0.05	(Ru)

MO	Number	Energy/eV	Contribution			
β HOMO-14	78	-12.845	0.98	(Other)	0.02	(Ru)
β HOMO-13	79	-12.792	0.82	(Other)	0.18	(Ru)
β HOMO-12	80	-11.685	0.89	(Other)	0.11	(Ru)
β HOMO-11	81	-11.646	0.92	(Other)	0.08	(Ru)
β HOMO-10	82	-11.152	0.96	(Other)	0.04	(Ru)
β HOMO-9	83	-10.836	0.91	(Other)	0.09	(Ru)
β HOMO-8	84	-10.757	0.94	(Other)	0.06	(Ru)
β HOMO-7	85	-10.658	0.99	(Other)	0.01	(Ru)
β HOMO-6	86	-10.164	0.85	(Other)	0.15	(Ru)

βHOMO-5	87	-9.639	0.78	(Other)	0.22	(Ru)
βHOMO-4	88	-9.357	0.93	(Other)	0.07	(Ru)
βHOMO-3	89	-8.637	0.62	(Ru)	0.38	(Other)
βHOMO-2	90	-8.299	0.74	(Other)	0.26	(Ru)
βHOMO-1	91	-7.96	0.58	(Ru)	0.42	(Other)
βHOMO	92	-7.687	0.98	(Other)	0.02	(Ru)
βLUMO	93	-1.925	0.67	(Ru)	0.33	(Other)
βLUMO+1	94	-1.059	0.55	(Other)	0.45	(Ru)
βLUMO+2	95	-0.649	0.98	(Other)	0.02	(Ru)
βLUMO+3	96	-0.461	0.78	(Other)	0.22	(Ru)
βLUMO+4	97	0.451	0.89	(Other)	0.11	(Ru)
βLUMO+5	98	0.634	0.82	(Other)	0.18	(Ru)
βLUMO+6	99	0.727	0.66	(Ru)	0.34	(Other)
βLUMO+7	100	1.272	0.92	(Ru)	0.08	(Other)
βLUMO+8	101	1.449	0.96	(Ru)	0.04	(Other)
βLUMO+9	102	1.653	1.04	(Ru)	-0.04	(Other)
βLUMO+9	103	2.3	1.27	(Ru)	-0.27	(Other)
βLUMO+11	104	3.237	0.98	(Other)	0.02	(Ru)
βLUMO+12	105	3.279	0.99	(Other)	0.01	(Ru)
βLUMO+13	106	3.39	0.99	(Other)	0.01	(Ru)
βLUMO+14	107	3.401	0.99	(Other)	0.01	(Ru)

Table S 12: Calculated NBOs of [Ru-1-octahedral]

MO	Number	Energy	Contribution			
αHOMO-20	89	-13.166	0.73	(Other)	0.27	(Ru)
αHOMO-19	90	-12.777	0.99	(Other)	0.01	(Ru)
αHOMO-18	91	-12.688	1	(Other)	0	(Ru)
αHOMO-17	92	-12.648	0.93	(Other)	0.07	(Ru)
αHOMO-16	93	-11.902	0.77	(Other)	0.23	(Ru)
αHOMO-15	94	-11.605	0.84	(Other)	0.16	(Ru)
αHOMO-14	95	-11.428	0.87	(Other)	0.13	(Ru)
αHOMO-13	96	-11.394	0.91	(Other)	0.09	(Ru)
αHOMO-12	97	-11.07	0.97	(Other)	0.03	(Ru)
αHOMO-11	98	-10.934	0.94	(Other)	0.06	(Ru)
αHOMO-10	99	-10.703	0.96	(Other)	0.04	(Ru)
αHOMO-9	100	-10.56	0.96	(Other)	0.04	(Ru)
αHOMO-8	101	-10.19	0.92	(Other)	0.08	(Ru)
αHOMO-7	102	-10.139	0.96	(Other)	0.04	(Ru)
αHOMO-6	103	-9.937	0.77	(Other)	0.23	(Ru)
αHOMO-5	104	-9.302	0.81	(Other)	0.19	(Ru)
αHOMO-4	105	-8.963	0.94	(Ru)	0.06	(Other)
αHOMO-3	106	-8.585	0.78	(Other)	0.22	(Ru)
αHOMO-2	107	-8.161	0.51	(Ru)	0.49	(Other)

αHOMO-1	108	-7.761	0.99	(Other)	0.01	(Ru)
αHOMO	109	-7.295	0.87	(Other)	0.13	(Ru)
αLUMO	110	-0.632	0.92	(Other)	0.08	(Ru)
αLUMO+1	111	-0.381	0.96	(Other)	0.04	(Ru)
αLUMO+2	112	-0.309	0.66	(Other)	0.34	(Ru)
αLUMO+3	113	-0.122	0.79	(Other)	0.21	(Ru)
αLUMO+4	114	0.465	0.84	(Other)	0.16	(Ru)
αLUMO+5	115	0.756	0.96	(Other)	0.04	(Ru)
αLUMO+6	116	0.859	0.54	(Ru)	0.46	(Other)
αLUMO+7	117	1.254	0.99	(Ru)	0.01	(Other)
αLUMO+8	118	1.771	0.92	(Ru)	0.08	(Other)
αLUMO+9	119	1.779	1.07	(Ru)	-0.07	(Other)
αLUMO+10	120	2.69	1.01	(Ru)	-0.01	(Other)
αLUMO+11	121	3.259	0.78	(Other)	0.22	(Ru)
αLUMO+12	122	3.323	0.99	(Other)	0.01	(Ru)
αLUMO+13	123	3.391	0.99	(Other)	0.01	(Ru)
αLUMO+14	124	3.436	0.99	(Other)	0.01	(Ru)
αLUMO+15	125	3.54	0.99	(Other)	0.01	(Ru)
αLUMO+16	126	4.207	0.93	(Other)	0.07	(Ru)
αLUMO+17	127	4.289	0.95	(Other)	0.05	(Ru)
αLUMO+18	128	4.506	0.97	(Other)	0.03	(Ru)
αLUMO+19	129	4.915	0.9	(Other)	0.1	(Ru)
αLUMO+20	130	5.057	0.95	(Other)	0.05	(Ru)

MO	Number	Energy	Contribution			
βHOMO-20	89	-13.166	0.73	(Other)	0.27	(Ru)
βHOMO-19	90	-12.777	0.99	(Other)	0.01	(Ru)
βHOMO-18	91	-12.688	1	(Other)	0	(Ru)
βHOMO-17	92	-12.648	0.93	(Other)	0.07	(Ru)
βHOMO-16	93	-11.902	0.77	(Other)	0.23	(Ru)
βHOMO-15	94	-11.605	0.84	(Other)	0.16	(Ru)
βHOMO-14	95	-11.428	0.87	(Other)	0.13	(Ru)
βHOMO-13	96	-11.394	0.91	(Other)	0.09	(Ru)
βHOMO-12	97	-11.07	0.97	(Other)	0.03	(Ru)
βHOMO-11	98	-10.934	0.94	(Other)	0.06	(Ru)
βHOMO-10	99	-10.703	0.96	(Other)	0.04	(Ru)
βHOMO-9	100	-10.56	0.96	(Other)	0.04	(Ru)
βHOMO-8	101	-10.19	0.92	(Other)	0.08	(Ru)
βHOMO-7	102	-10.139	0.96	(Other)	0.04	(Ru)
βHOMO-6	103	-9.937	0.77	(Other)	0.23	(Ru)
βHOMO-5	104	-9.302	0.81	(Other)	0.19	(Ru)
βHOMO-4	105	-8.963	0.94	(Ru)	0.06	(Other)

βHOMO-3	106	-8.585	0.78	(Other)	0.22	(Ru)
βHOMO-2	107	-8.161	0.51	(Ru)	0.49	(Other)
βHOMO-1	108	-7.761	0.99	(Other)	0.01	(Ru)
βHOMO	109	-7.295	0.87	(Other)	0.13	(Ru)
βLUMO	110	-0.632	0.92	(Other)	0.08	(Ru)
βLUMO+1	111	-0.381	0.96	(Other)	0.04	(Ru)
βLUMO+2	112	-0.309	0.66	(Other)	0.34	(Ru)
βLUMO+3	113	-0.122	0.79	(Other)	0.21	(Ru)
βLUMO+4	114	0.465	0.84	(Other)	0.16	(Ru)
βLUMO+5	115	0.756	0.96	(Other)	0.04	(Ru)
βLUMO+6	116	0.859	0.54	(Ru)	0.46	(Other)
βLUMO+7	117	1.254	0.99	(Ru)	0.01	(Other)
βLUMO+8	118	1.771	0.92	(Ru)	0.08	(Other)
βLUMO+9	119	1.779	1.07	(Ru)	-0.07	(Other)
βLUMO+9	120	2.69	1.01	(Ru)	-0.01	(Other)
βLUMO+11	121	3.259	0.78	(Other)	0.22	(Ru)
βLUMO+12	122	3.323	0.99	(Other)	0.01	(Ru)
βLUMO+13	123	3.391	0.99	(Other)	0.01	(Ru)
βLUMO+14	124	3.436	0.99	(Other)	0.01	(Ru)
βLUMO+15	125	3.54	0.99	(Other)	0.01	(Ru)
βLUMO+16	126	4.207	0.93	(Other)	0.07	(Ru)
βLUMO+17	127	4.289	0.95	(Other)	0.05	(Ru)
βLUMO+18	128	4.506	0.97	(Other)	0.03	(Ru)
βLUMO+19	129	4.915	0.9	(Other)	0.1	(Ru)
βLUMO+20	130	5.057	0.95	(Other)	0.05	(Ru)

Table S13 : Calculated NBOs of [Ru-2]

MO	Number	Energy/eV	Contribution			
HOMO-14	171	-10.597	0.98	(Other)	0.02	(Ru)
HOMO-13	172	-10.531	0.96	(Other)	0.04	(Ru)
HOMO-12	173	-10.248	0.87	(Other)	0.13	(Ru)
HOMO-11	174	-10.23	0.76	(Other)	0.24	(Ru)
HOMO-10	175	-10.105	0.76	(Other)	0.24	(Ru)
HOMO-9	176	-10.017	0.8	(Other)	0.2	(Ru)
HOMO-8	177	-9.337	0.79	(Other)	0.21	(Ru)
HOMO-7	178	-9.187	0.73	(Other)	0.27	(Ru)
HOMO-6	179	-8.96	0.56	(Other)	0.44	(Ru)
HOMO-5	180	-8.833	0.6	(Other)	0.4	(Ru)
HOMO-4	181	-8.547	0.55	(Other)	0.45	(Ru)
HOMO-3	182	-8.104	0.77	(Ru)	0.23	(Other)
HOMO-2	183	-7.858	1	(Other)	0	(Ru)
HOMO-1	184	-7.599	0.99	(Other)	0.01	(Ru)
HOMO	185	-7.533	0.75	(Other)	0.25	(Ru)
LUMO	186	-3.509	0.51	(Ru)	0.49	(Other)
LUMO+1	187	-2.999	0.77	(Ru)	0.23	(Other)
LUMO+2	188	-0.731	0.95	(Other)	0.05	(Ru)
LUMO+3	189	-0.721	0.98	(Other)	0.02	(Ru)
LUMO+4	190	-0.711	0.99	(Other)	0.01	(Ru)
LUMO+5	191	-0.616	1	(Other)	0	(Ru)
LUMO+6	192	-0.002	0.69	(Ru)	0.31	(Other)
LUMO+7	193	0.375	0.93	(Other)	0.07	(Ru)
LUMO+8	194	0.4	0.95	(Other)	0.05	(Ru)
LUMO+9	195	0.622	0.94	(Other)	0.06	(Ru)
LUMO+10	196	0.674	0.99	(Other)	0.01	(Ru)
LUMO+11	197	0.873	0.57	(Ru)	0.43	(Other)
LUMO+12	198	1.199	0.95	(Ru)	0.05	(Other)
LUMO+13	199	1.402	0.56	(Ru)	0.44	(Other)
LUMO+14	200	1.675	1.03	(Ru)	-0.03	(Other)
LUMO+15	201	1.688	1.07	(Ru)	-0.07	(Other)
LUMO+16	202	1.751	1.05	(Ru)	-0.05	(Other)
LUMO+17	203	2.023	0.98	(Ru)	0.02	(Other)
LUMO+18	204	2.031	0.98	(Ru)	0.02	(Other)
LUMO+19	205	3.158	0.67	(Other)	0.33	(Ru)
LUMO+20	206	3.167	0.98	(Other)	0.02	(Ru)

10. Optimized Coordinates (Charge and Multiplicity added to the first line)

[Ag-1]

0 1			
Ag	0.51665900	0.07531600	-0.55458500
S	3.13161000	-1.52114000	-0.44673300
F	5.40304200	-0.43780400	0.70412700
F	4.02938400	1.06581000	-0.22204200
F	5.32587800	-0.21622100	-1.51914300
O	2.31391700	-1.25514700	0.93956400
O	2.22261300	-0.90011800	-1.67534600
O	3.83787600	-2.93829500	-0.69167900
N	0.37988100	2.30605300	0.26932700
N	-1.64395100	0.38111100	0.22229600
C	-0.09445500	4.79270200	1.44013300
H	-0.27950000	5.76021200	1.89480500
C	-1.11514900	3.83364400	1.37273100
H	-2.10229700	4.03756500	1.77501900
C	-0.84037500	2.59470800	0.78027400
C	-1.88061100	1.54340600	0.71549800
H	-2.85865700	1.79930800	1.13278300
C	-2.65962100	-0.63764400	0.15956200
C	-3.80283600	-0.46251500	-0.65409500
C	-4.74929300	-1.50131500	-0.67811400
H	-5.63729100	-1.39640500	-1.29437400
C	-4.56225600	-2.66948500	0.06198000
H	-5.30748300	-3.45847100	0.02918400
C	-3.40474900	-2.83210000	0.83211600
H	-3.25566600	-3.75220500	1.38611000
C	-2.42936400	-1.82870300	0.89244200
C	4.57884800	-0.20048200	-0.36831600
C	1.16608800	4.48094100	0.91822300
H	1.98398800	5.19105700	0.95676500
C	1.36502700	3.21704400	0.33834300
H	2.32584300	2.92573800	-0.07100200
C	-1.18973300	-1.98788300	1.76639700
H	-0.37288400	-1.40533800	1.32463600
C	-4.02768600	0.75987100	-1.54365800
H	-3.15646900	1.41900800	-1.47683000
C	-5.26267800	1.56763700	-1.09204600
H	-5.39824200	2.45094200	-1.72723300
H	-6.17407700	0.96289300	-1.16107800
H	-5.17016700	1.90249300	-0.05158300
C	-4.15686200	0.35280800	-3.02674300
H	-5.03974900	-0.27355500	-3.19605700

H	-4.25427300	1.24361100	-3.65850300
H	-3.27802300	-0.20955800	-3.36022700
C	-0.68760000	-3.43794700	1.86490500
H	-1.36399300	-4.06910600	2.45432000
H	-0.56840400	-3.88948100	0.87404000
H	0.29169800	-3.44930500	2.35381900
C	-1.44835800	-1.41027800	3.17652800
H	-1.74826900	-0.35599200	3.13608700
H	-2.24615100	-1.96808500	3.68221200
H	-0.54020300	-1.48110800	3.78519500

[Ag-2]

0 1			
Ag	1.53454400	0.26201100	-0.19219500
Ag	-1.53329600	0.26012200	-0.19265600
S	-0.00082000	2.95609000	-1.75601600
S	0.00084500	-2.82179400	-0.65839200
F	1.10924000	5.40596600	-1.19904200
F	-0.02007500	4.49830500	0.50471500
F	-1.12782800	5.40180500	-1.21533800
F	-0.00488300	-3.65331100	-3.27127800
F	-1.11408600	-5.00712600	-1.87833100
F	1.12368900	-4.99878300	-1.88582100
O	1.34165900	2.28129600	-1.11431800
O	-1.34607800	2.27352500	-1.12864500
O	0.00676300	3.24712600	-3.32962600
O	1.35465100	-1.98080600	-0.99187500
O	-1.35756600	-1.98607600	-0.98652400
O	0.00508800	-3.58744500	0.76129900
N	3.62862800	-0.15653600	0.76366700
N	1.17239500	-0.78927000	2.01344400
N	-1.16921000	-0.78991100	2.01369400
N	-3.62636200	-0.15694100	0.76574400
C	3.60164000	-0.77491200	1.88370700
H	4.52051200	-1.03706900	2.41704600
C	2.33164700	-1.19974000	2.52516800
C	2.41221400	-2.05481600	3.66170800
H	3.38577900	-2.35674400	4.03141700
C	1.25065300	-2.49382200	4.25294500
H	1.27295200	-3.15918700	5.11058500
C	0.00217200	-2.07828800	3.71870200
C	0.00177300	-1.21228700	2.58289600
C	-1.24592500	-2.49441300	4.25334400
H	-1.26763400	-3.15974400	5.11102600
C	-2.40787800	-2.05600100	3.66242900

H	-3.38117800	-2.35835500	4.03248300
C	-2.32810400	-1.20092800	2.52582500
C	-3.59862000	-0.77679900	1.88490000
H	-4.51712100	-1.04068900	2.41802000
C	4.87394800	0.22809000	0.14206500
C	5.42986200	-0.64610900	-0.81855400
C	6.62871000	-0.25638700	-1.43293100
H	7.08444500	-0.90664900	-2.17223400
C	7.23464400	0.96588400	-1.12204400
H	8.16044200	1.25228800	-1.61202000
C	6.63706000	1.82858500	-0.19984400
H	7.09816000	2.78844900	0.01164300
C	5.44080800	1.48246300	0.44943500
C	4.75608700	2.48408600	1.37574000
H	3.94352200	1.97752700	1.90742800
C	5.71485500	3.05461300	2.43867900
H	6.18208200	2.25854400	3.03077800
H	5.16929400	3.71702600	3.12095600
H	6.51653300	3.64564400	1.98166100
C	4.11299500	3.61628400	0.54320600
H	4.87680800	4.16495300	-0.02119500
H	3.59990800	4.32924500	1.20025100
H	3.37971800	3.22278600	-0.16889800
C	4.75368400	-1.97092200	-1.16128800
H	3.68659100	-1.88905500	-0.92601200
C	5.33620000	-3.11966500	-0.30764700
H	6.40660900	-3.24951900	-0.50992400
H	4.82575800	-4.06163000	-0.53868100
H	5.22156000	-2.92807100	0.76646400
C	4.84810400	-2.32097600	-2.65724900
H	4.47975100	-1.49966500	-3.28119000
H	4.23485300	-3.20439900	-2.86677700
H	5.87573800	-2.55167200	-2.96341000
C	-4.87212200	0.22648600	0.14426200
C	-5.43614500	1.48325900	0.44678300
C	-6.63336000	1.82829500	-0.20122600
H	-7.09241400	2.78989100	0.00691800
C	-7.23447100	0.96219200	-1.11795400
H	-8.16100800	1.24767200	-1.60706600
C	-6.63102400	-0.26235400	-1.42465700
H	-7.08937600	-0.91523200	-2.16004700
C	-5.43133900	-0.65115700	-0.81125500
C	-4.75763200	-1.97812000	-1.15074300
H	-3.69049000	-1.89803300	-0.91514300
C	-4.85176800	-2.33052300	-2.64622400
H	-5.87976300	-2.55893000	-2.95285200

H	-4.24069900	-3.21591900	-2.85380700
H	-4.48069900	-1.51122000	-3.27117900
C	-5.34323900	-3.12405500	-0.29548300
H	-5.22876200	-2.93087100	0.77837000
H	-4.83493400	-4.06763500	-0.52466300
H	-6.41384800	-3.25177200	-0.49804400
C	-4.74807200	2.48766400	1.36753500
H	-3.93161900	1.98335100	1.89538200
C	-5.70235400	3.05779300	2.43477100
H	-6.50871100	3.64488200	1.98087600
H	-5.15502000	3.72369200	3.11222200
H	-6.16348800	2.26166000	3.03155600
C	-4.11171700	3.61980000	0.52984800
H	-3.38248100	3.22603900	-0.18621600
H	-3.59533800	4.33403800	1.18290700
H	-4.87958100	4.16703000	-0.03042500
C	-0.01048400	4.68925400	-0.85864000
C	0.00140900	-4.21675400	-2.02190600

[Ag-2-A]

2 1			
Ag	1.53349000	0.00015300	-0.00018500
Ag	-1.53319300	0.00007800	0.00015600
N	1.02912800	-2.19759700	0.55199900
N	1.02892100	2.19786300	-0.55217800
N	-1.02924800	2.19738600	0.55354200
N	-1.02924100	-2.19721700	-0.55337200
N	3.17592700	-0.78458200	1.65867900
N	-3.17583600	-0.78335300	-1.65923000
N	3.17544000	0.78485600	-1.65894500
N	-3.17558300	0.78339600	1.65947100
C	-0.00020700	2.90950300	0.00090600
C	4.24452600	-0.00919400	2.21315800
C	-1.05346000	5.00756700	0.68346200
H	-1.07019200	6.09258000	0.71422800
C	-0.00030500	4.33666400	0.00134800
C	2.00806600	-2.84567400	1.19113700
C	-2.00814600	2.84496300	1.19322700
C	-2.00821800	-2.84484200	-1.19290000
C	-0.00007300	-2.90928500	-0.00090000
C	3.10442500	2.05977500	-1.80208900
H	3.82578400	2.62514900	-2.39431600
C	2.00772400	2.84597600	-1.19146300
C	-4.88867100	1.96069800	-3.46738300
H	-4.62020300	2.84357700	-4.03944800

C	-3.10473400	2.05823700	1.80338500
H	-3.82623900	2.62318100	2.39584700
C	2.03751200	-4.26580400	1.29596900
H	2.84687400	-4.74257200	1.83709700
C	4.24386100	0.00925700	-2.21348200
C	-2.03772500	4.26502700	1.29893700
H	-2.84706100	4.74138000	1.84046800
C	-3.87621400	1.15906900	-2.92725100
C	-3.10492700	-2.05820900	-1.80298200
H	-3.82649300	-2.62325300	-2.39527500
C	1.05275500	5.00813400	-0.68035700
H	1.06933400	6.09316800	-0.71045600
C	3.10484800	-2.05950800	1.80169500
H	3.82633000	-2.62496300	2.39369900
C	-0.00011600	-4.33644700	-0.00133200
C	2.03711300	4.26610800	-1.29630300
H	2.84637800	4.74290300	-1.83755200
C	-4.24393200	0.00733800	2.21348000
C	-4.24434200	-0.00747300	-2.21318400
C	3.87556300	-1.15688800	-2.92809900
C	-5.60261500	0.35664700	2.01248700
C	5.60252300	0.35843500	-2.01210000
C	-6.23787800	1.62893100	-3.28836900
H	-7.01402500	2.25760400	-3.71260400
C	-2.03775300	-4.26490800	-1.29857700
H	-2.84715200	-4.74130400	-1.83997700
C	-1.05336300	-5.00740000	-0.68325100
H	-1.07005600	-6.09241400	-0.71400500
C	3.87656400	1.15701100	2.92785400
C	-4.88783000	-1.96112300	3.46744400
H	-4.61916600	-2.84406600	4.03931900
C	-5.60294800	-0.35693400	-2.01195900
C	5.60307100	-0.35876900	2.01176300
C	-6.58315300	0.48805100	-2.55869700
H	-7.63031100	0.24099000	-2.41104400
C	1.05308500	-5.00787100	0.68018900
H	1.06971000	-6.09290500	0.71029700
C	4.88914200	1.95817100	3.46845800
H	4.62080700	2.84078800	4.04099100
C	-6.58263200	-0.48855500	2.55922700
H	-7.62984300	-0.24161800	2.41174300
C	-3.87555600	-1.15927900	2.92729200
C	4.88789500	-1.95834400	-3.46871800
H	4.61929500	-2.84091400	-4.04119700
C	-6.23710600	-1.62949800	3.28867900
H	-7.01311000	-2.25834500	3.71291600

C	6.58340400	0.48574000	2.55900800
H	7.63052400	0.23858500	2.41124600
C	6.23829900	1.62626900	3.28931000
H	7.01453800	2.25457500	3.71391900
C	6.58259700	-0.48637800	-2.55934000
H	7.62979300	-0.23955100	-2.41156400
C	6.23714900	-1.62681300	-3.28962400
H	7.01319900	-2.25536200	-3.71422000
C	6.05311000	-1.56119100	1.20477000
H	7.04967900	-1.38147100	0.79330500
H	6.12713200	-2.46450700	1.82210500
H	5.38897900	-1.77947500	0.36212600
C	2.42486900	1.50578700	3.15957100
H	1.86774300	1.56511800	2.21602400
H	1.92308600	0.75138200	3.77663400
H	2.33841700	2.46736200	3.67321600
C	-6.05314900	1.55947000	1.20636800
H	-7.04970000	1.37968800	0.79488000
H	-6.12743700	2.46232300	1.82434800
H	-5.38918400	1.77858900	0.36381200
C	-2.42372900	-1.50777900	3.15858900
H	-1.86670200	-1.56624500	2.21493100
H	-1.92210900	-0.75366300	3.77613800
H	-2.33691700	-2.46969800	3.67152800
C	-6.05319400	-1.55973200	-1.20564400
H	-7.04973000	-1.38006900	-0.79406900
H	-6.12739300	-2.46267700	-1.82350100
H	-5.38909600	-1.77863100	-0.36313500
C	-2.42447000	1.50770000	-3.15887300
H	-1.86725600	1.56633500	-2.21533800
H	-1.92289300	0.75357000	-3.77643900
H	-2.33786800	2.46957100	-3.67194100
C	2.42375800	-1.50530300	-3.15967100
H	1.86673300	-1.56454500	-2.21605600
H	1.92208500	-0.75074900	-3.77663900
H	2.33701300	-2.46683600	-3.67334600
C	6.05298500	1.56062700	-1.20499800
H	7.04947500	1.38049500	-0.79351900
H	6.12738000	2.46395900	-1.82226500
H	5.38892100	1.77910200	-0.36235200

[Mo-1]

0 1			
C	-2.21972500	-2.37452800	-0.53984200
C	-2.98974800	-2.88550600	0.52114200
H	-3.21957500	-2.24977400	1.37045000
C	-3.42899400	-4.21478400	0.49608000
H	-4.01415700	-4.60087300	1.32605800
C	-3.10477700	-5.05107000	-0.58254900
H	-3.44385800	-6.08264100	-0.59699200
C	-2.33180200	-4.54520200	-1.63847600
H	-2.07396900	-5.18294300	-2.47926000
C	-1.89181900	-3.21617600	-1.61713900
H	-1.29868900	-2.81286500	-2.43274200
C	-2.49576600	0.05599500	-0.37547400
C	-3.91837800	0.05015500	-0.21662600
C	-5.12975900	0.03480100	-0.08677900
C	-6.55555400	0.02204500	0.06385500
C	-7.24811100	1.21388900	0.36214400
H	-6.68983700	2.13741100	0.48011100
C	-8.63869100	1.19838500	0.50737200
H	-9.16764100	2.11787200	0.73846400
C	-9.35030500	-0.00169800	0.35643400
H	-10.43030000	-0.01090700	0.46959600
C	-8.66519100	-1.19001600	0.05984800
H	-9.21492300	-2.11885600	-0.05724600
C	-7.27461700	-1.18191000	-0.08584900
H	-6.73712000	-2.09652500	-0.31611900
C	-2.14310100	2.48540700	-0.18418200
C	-1.48016300	3.32844900	0.72496100
H	-0.66539000	2.92255900	1.31512600
C	-1.87184900	4.66442800	0.86270700
H	-1.34916600	5.30347100	1.56850400
C	-2.92835900	5.17826100	0.09563000
H	-3.22970000	6.21606600	0.20272000
C	-3.58409400	4.34152900	-0.81964600
H	-4.39175500	4.73290300	-1.43222400
C	-3.19408700	3.00465700	-0.96502700
H	-3.68563500	2.37110400	-1.69629000
C	2.03767400	-2.40051600	0.76392900
C	3.10257800	-2.65329200	1.65125700
H	3.65281900	-1.82558500	2.08629100
C	3.43377500	-3.96855100	1.99695800
H	4.25399500	-4.14952200	2.68616300
C	2.70397000	-5.04682000	1.47555400
H	2.95907700	-6.06592100	1.75038900

C	1.63166400	-4.79333300	0.60668400
H	1.04822000	-5.61672800	0.20489100
C	1.30081600	-3.48194700	0.25257200
H	0.46936300	-3.28309100	-0.41294600
C	2.48153400	-0.01165500	0.29799800
C	3.88753200	-0.08641100	0.03883600
C	5.08312700	-0.13394700	-0.19442700
C	6.49184800	-0.18953200	-0.45372500
C	7.15486700	-1.43283000	-0.51665800
H	6.58604500	-2.34615300	-0.37261900
C	8.52985300	-1.48226000	-0.76555000
H	9.03548300	-2.44179800	-0.81421100
C	9.25585400	-0.29624800	-0.95424400
H	10.32350700	-0.33752600	-1.14844500
C	8.60024600	0.94307800	-0.89372400
H	9.16038000	1.86128400	-1.04165400
C	7.22556500	0.99983200	-0.64500500
H	6.71073300	1.95447300	-0.59905100
C	2.29352500	2.45076500	0.36848600
C	1.76540300	3.47621000	-0.43495900
H	0.97292800	3.23647700	-1.13657700
C	2.25802100	4.78129300	-0.32964200
H	1.83795400	5.56255500	-0.95640700
C	3.28668800	5.08191900	0.57577500
H	3.66826900	6.09545800	0.65565400
C	3.81182700	4.06172400	1.38345300
H	4.59850000	4.28489800	2.09890700
C	3.31839400	2.75579200	1.28623300
H	3.70950000	1.97683700	1.93316400
N	-1.72493800	-1.04379600	-0.53807800
N	-1.69953800	1.14683200	-0.31825300
N	1.64607100	-1.08300400	0.43196100
N	1.74717900	1.14974400	0.28117000
Mo	0.13296000	0.05518200	-0.40670500

[Mo-2]

0 1

C	2.39457800	-1.59405100	-2.34187200
C	3.76311300	-1.26146500	-2.36201900
H	4.23512700	-0.89854100	-1.45482100
C	4.50346200	-1.37192900	-3.54351700
H	5.55671000	-1.10602800	-3.54213700
C	3.88726800	-1.80477500	-4.72843100
H	4.46081300	-1.88485000	-5.64718300
C	2.52291700	-2.12730100	-4.71329900

H	2.03089100	-2.46502100	-5.62090100
C	1.78033600	-2.02547000	-3.52928000
H	0.73055000	-2.29072400	-3.52226300
C	2.01191100	-2.00978800	0.00028700
C	3.03202700	-3.02815900	0.00035600
C	3.89412500	-3.88853700	0.00025400
C	4.90930800	-4.90169800	0.00017400
C	5.54102400	-5.27637400	-1.20401900
H	5.24871600	-4.78900000	-2.12909600
C	6.53085700	-6.26433900	-1.20061800
H	7.01310700	-6.54802500	-2.13132200
C	6.90111700	-6.88945900	-0.00002000
H	7.66987300	-7.65664900	-0.00009400
C	6.27536100	-6.52059100	1.20067400
H	6.56012200	-7.00235200	2.13130400
C	5.28538300	-5.53277000	1.20426600
H	4.79751700	-5.24154000	2.12942300
C	1.59583000	-2.39266200	2.34252200
C	1.26700200	-3.76212100	2.36236200
H	0.90679000	-4.23531000	1.45470200
C	1.37760600	-4.50197500	3.54416300
H	1.11462900	-5.55595800	3.54250200
C	1.80677800	-3.88441900	4.72970000
H	1.88695900	-4.45760900	5.64866200
C	2.12547000	-2.51915900	4.71488700
H	2.46027700	-2.02604400	5.62297500
C	2.02351600	-1.77705500	3.53060000
H	2.28582600	-0.72652500	3.52388600
C	2.39323400	1.59596300	2.34182300
C	3.76201900	1.26442400	2.36200200
H	4.23432500	0.90184400	1.45481800
C	4.50223900	1.37543800	3.54352800
H	5.55568900	1.11033900	3.54218500
C	3.88566800	1.80779100	4.72842700
H	4.45911900	1.88828600	5.64720100
C	2.52107000	2.12927400	4.71325500
H	2.02875500	2.46659200	5.62084900
C	1.77861000	2.02690200	3.52920700
H	0.72863100	2.29138500	3.52211400
C	2.01024300	2.01141800	-0.00035200
C	3.02959500	3.03055200	-0.00044300
C	3.89103100	3.89159400	-0.00040300
C	4.90545900	4.90551200	-0.00019600
C	5.28112000	5.53693300	-1.20423500
H	4.79354500	5.24535900	-2.12943700
C	6.27031300	6.52553900	-1.20052900

H	6.55475400	7.00756900	-2.13111700
C	6.89569300	6.89484700	0.00022600
H	7.66383800	7.66265000	0.00038900
C	6.52585300	6.26937300	1.20076800
H	7.00781700	6.55339700	2.13151800
C	5.53680300	5.28062200	1.20405600
H	5.24482200	4.79297300	2.12909000
C	1.59383900	2.39394300	-2.34258600
C	2.02174200	1.77861700	-3.53073600
H	2.28464000	0.72823100	-3.52411200
C	2.12312500	2.52079500	-4.71502400
H	2.45813100	2.02788800	-5.62315100
C	1.80361700	3.88586200	-4.72978900
H	1.88335500	4.45911300	-5.64875200
C	1.37420300	4.50314100	-3.54419500
H	1.11059200	5.55696600	-3.54248800
C	1.26418100	3.76320700	-2.36238900
H	0.90381100	4.23619200	-1.45468600
C	-1.59584200	2.39266100	2.34247800
C	-1.26703100	3.76212400	2.36229100
H	-0.90681700	4.23529800	1.45462300
C	-1.37765300	4.50200200	3.54407600
H	-1.11468800	5.55598800	3.54239400
C	-1.80682900	3.88446600	4.72962200
H	-1.88702500	4.45767500	5.64857100
C	-2.12550800	2.51920300	4.71483500
H	-2.46031900	2.02610400	5.62293000
C	-2.02353700	1.77707500	3.53056400
H	-2.28583700	0.72654200	3.52386800
C	-2.01191600	2.00974000	0.00025300
C	-3.03203000	3.02811200	0.00030400
C	-3.89412100	3.88849700	0.00019200
C	-4.90921300	4.90175000	0.00018200
C	-5.28517600	5.53282800	1.20430700
H	-4.79729100	5.24153600	2.12943400
C	-6.27507000	6.52073400	1.20078300
H	-6.55974500	7.00249900	2.13143800
C	-6.90085200	6.88968100	0.00012700
H	-7.66954300	7.65693600	0.00010700
C	-6.53070400	6.26455400	-1.20050100
H	-7.01297600	6.54830100	-2.13117600
C	-5.54095500	5.27650400	-1.20397200
H	-5.24873500	4.78912400	-2.12907300
C	-2.39456600	1.59398100	-2.34190700
C	-3.76310300	1.26140800	-2.36207500
H	-4.23513600	0.89849400	-1.45488300

C	-4.50343000	1.37187100	-3.54358700
H	-5.55668100	1.10598000	-3.54222400
C	-3.88721100	1.80470400	-4.72849400
H	-4.46074000	1.88477800	-5.64725600
C	-2.52285700	2.12721700	-4.71334000
H	-2.03081300	2.46492600	-5.62093500
C	-1.78029800	2.02538600	-3.52930800
H	-0.73050900	2.29063000	-3.52227300
C	-2.39314100	-1.59600500	2.34192500
C	-3.76192900	-1.26448200	2.36218200
H	-4.23429000	-0.90189900	1.45502800
C	-4.50208100	-1.37551500	3.54374900
H	-5.55553500	-1.11042800	3.54246800
C	-3.88543900	-1.80787200	4.72861000
H	-4.45883700	-1.88838200	5.64741600
C	-2.52083700	-2.12933900	4.71335900
H	-2.02846800	-2.46665900	5.62092200
C	-1.77844600	-2.02694700	3.52927000
H	-0.72846300	-2.29141700	3.52211400
C	-2.01024600	-2.01145700	-0.00027000
C	-3.02958800	-3.03060300	-0.00031900
C	-3.89102100	-3.89164700	-0.00025500
C	-4.90556800	-4.90544600	-0.00009900
C	-5.53698100	-5.28051800	1.20412900
H	-5.24496700	-4.79292600	2.12918300
C	-6.52614000	-6.26916000	1.20079300
H	-7.00815600	-6.55315500	2.13152400
C	-6.89602100	-6.89456300	0.00022600
H	-7.66425000	-7.66228000	0.00035300
C	-6.27057200	-6.52529300	-1.20050400
H	-6.55504300	-7.00727000	-2.13111100
C	-5.28127000	-5.53679600	-1.20416200
H	-4.79364000	-5.24525400	-2.12934500
C	-1.59391300	-2.39402100	-2.34250800
C	-2.02184300	-1.77870600	-3.53065400
H	-2.28472000	-0.72831500	-3.52403700
C	-2.12327600	-2.52090100	-4.71492600
H	-2.45830100	-2.02800200	-5.62305100
C	-1.80379500	-3.88597500	-4.72967900
H	-1.88357300	-4.45923900	-5.64863000
C	-1.37435700	-4.50324300	-3.54408800
H	-1.11076800	-5.55707300	-3.54237300
C	-1.26428400	-3.76329200	-2.36229700
H	-0.90389700	-4.23627000	-1.45459800
N	1.42164000	-1.61854900	1.15060500
N	1.61997900	-1.42022900	-1.15015000

N	1.61879400	1.42155200	1.15008500
N	1.42026000	1.61970400	-1.15066500
N	-1.42163800	1.61852700	1.15057600
N	-1.61998500	1.42016000	-1.15017400
N	-1.61876600	-1.42157600	1.15014900
N	-1.42028900	-1.61976700	-1.15060400
Mo	0.00000800	-0.00000800	1.05170500
Mo	-0.00000600	-0.00003500	-1.05183800

[Ru-1]

0 2

Cl	-0.78014700	3.26380700	0.20652500
F	-4.99119800	-2.42384200	0.73183600
F	-2.90292200	-2.38652000	1.55002700
F	-4.34894800	-0.79280300	2.11045900
N	-1.80872600	0.59109900	-1.21708700
N	-1.17440900	-0.13455100	0.73388800
H	-1.11538500	-0.65225700	1.59957500
C	-2.20815700	-0.17792400	-0.14481900
C	-3.47912100	-0.78767300	-0.13946100
C	-4.31203600	-0.57772000	-1.24480600
H	-5.29258200	-1.04228000	-1.26514000
C	-3.89038700	0.22303400	-2.31465500
H	-4.53129700	0.39849800	-3.16855100
C	-2.61608300	0.80642100	-2.25933700
H	-2.24249500	1.44697800	-3.04944700
C	-3.92771400	-1.58179100	1.03159800
F	4.41245500	-1.22883600	-1.91296100
F	3.29799900	-2.69514300	-0.66940800
F	5.38240300	-2.10188400	-0.09976500
N	1.84452800	1.02927800	0.76803800
N	1.34321200	-0.34543700	-0.86697300
H	1.40725700	-1.14427300	-1.48526600
C	2.33105600	-0.01793100	0.00755600
C	3.63672100	-0.50272400	0.24791700
C	4.39476900	0.10477900	1.25574600
H	5.39688600	-0.26076400	1.45552900
C	3.87451300	1.17139600	2.00244200
H	4.45655000	1.64753800	2.78026400
C	2.57460100	1.61643600	1.72075500
H	2.11115000	2.43926000	2.25300700
C	4.17867600	-1.60663400	-0.58174400
Ru	0.01479700	1.05325200	-0.25988200

[Ru-1-octahedral]

0 2

Cl	-0.07311200	-2.87736800	0.75444900
F	-6.28658200	-0.79035900	-0.31910300
F	-4.96745400	0.41440100	-1.65801600
F	-4.66882600	-1.78230800	-1.50947100
N	-1.74953900	-0.24073300	1.19603600
N	-1.86237300	-0.80499300	-0.91234000
H	-2.25146700	-1.11987800	-1.79119900
C	-2.61973000	-0.51013800	0.14933800
C	-4.02362300	-0.44737900	0.38470900
C	-4.47209200	-0.16956100	1.67421200
H	-5.53957200	-0.13640200	1.86776000
C	-3.56051500	0.05453300	2.72149800
H	-3.90150100	0.24841900	3.72995600
C	-2.19244400	0.00865000	2.43301400
H	-1.44330300	0.15757300	3.20353500
C	-4.96764100	-0.65116800	-0.73823000
F	4.62405900	-0.92918600	1.91401500
F	4.87190300	1.01856700	0.87604700
F	6.20633700	-0.69388000	0.34641400
N	1.64256000	-1.00055700	-1.14528900
N	1.80485000	-0.29043900	0.92075400
H	2.22172900	-0.21092000	1.84029900
C	2.53485400	-0.68107300	-0.14061900
C	3.92854100	-0.80101600	-0.38775600
C	4.34725500	-1.27073700	-1.63390500
H	5.40923900	-1.37574300	-1.83214100
C	3.41006600	-1.60568400	-2.62409400
H	3.72404100	-1.97877800	-3.59002000
C	2.04800300	-1.44811500	-2.33643600
H	1.27719400	-1.69009800	-3.05934200
C	4.88999300	-0.37601900	0.65295600
Ru	-0.04377600	-0.61532200	0.02883200
O	0.02344300	1.38834100	-0.65497900
C	0.32368700	2.50814700	-0.20202100
O	0.37866800	3.51838100	-1.09373200
C	0.65820800	4.91892800	-0.72743600
H	1.34480300	4.95507200	0.12395200
H	1.16871800	5.31397700	-1.60660500
C	0.63784500	2.76365500	1.25026700
H	1.71516600	2.91275000	1.38017400
H	0.11273300	3.64483400	1.62752400
H	0.34806400	1.88694300	1.82590400
C	-0.64137500	5.66692800	-0.45890200

H	-0.42988600	6.73054000	-0.30180300
H	-1.31559100	5.57191200	-1.31444900
H	-1.15782800	5.28766300	0.42926800

[Ru-2]

0 1			
Ru	0.00006200	0.12394500	-1.20375400
Cl	-0.00014900	1.20204400	-3.37748800
F	4.63174500	4.35891200	-0.29259500
F	4.22995500	2.50864100	-1.47749500
F	2.70690500	4.12996300	-1.40256000
F	-2.70692300	4.13046900	-1.40209800
F	-4.22936800	2.50862600	-1.47807400
F	-4.63222200	4.35838900	-0.29273900
N	1.45020500	1.26721800	1.57245000
N	1.46563900	1.45490300	-0.75016900
H	1.81269200	1.93474600	-1.57970400
N	-1.45042200	1.26707700	1.57246000
N	-1.46568700	1.45478600	-0.75015100
H	-1.81283300	1.93449300	-1.57972900
C	1.97463300	1.84043000	0.42730100
C	3.02983400	2.81128700	0.58972100
C	3.48732500	3.14225700	1.84979000
H	4.28248800	3.87180700	1.95714500
C	2.92644800	2.52627900	2.99063300
H	3.27754600	2.75998700	3.98693000
C	1.92063100	1.59728700	2.80426000
H	1.46613900	1.06607700	3.63242300
C	3.63992900	3.44370200	-0.61359100
C	-1.97480400	1.84027100	0.42728100
C	-3.03006200	2.81106800	0.58965700
C	-3.48764100	3.14199200	1.84970500
H	-4.28284000	3.87150800	1.95702300
C	-2.92683000	2.52600200	2.99057600
H	-3.27801700	2.75966400	3.98685300
C	-1.92094000	1.59707600	2.80424900
H	-1.46646200	1.06587100	3.63242600
C	-3.63997200	3.44363900	-0.61366800
Ru	-0.00006200	-0.12394500	1.20375400
Cl	0.00015000	-1.20204400	3.37748800
F	-4.63174600	-4.35891100	0.29259600
F	-4.22995400	-2.50864100	1.47749600
F	-2.70690500	-4.12996400	1.40255900
F	2.70692300	-4.13046700	1.40210000
F	4.22937000	-2.50862500	1.47807300

F	4.63222100	-4.35839000	0.29274000
N	-1.45020500	-1.26721800	-1.57245000
N	-1.46563800	-1.45490400	0.75016900
H	-1.81269000	-1.93474700	1.57970300
N	1.45042200	-1.26707700	-1.57246100
N	1.46568800	-1.45478600	0.75015000
H	1.81283300	-1.93449300	1.57972900
C	-1.97463300	-1.84043000	-0.42730100
C	-3.02983400	-2.81128700	-0.58972100
C	-3.48732600	-3.14225600	-1.84978900
H	-4.28248900	-3.87180600	-1.95714400
C	-2.92644900	-2.52627900	-2.99063300
H	-3.27754800	-2.75998700	-3.98693000
C	-1.92063100	-1.59728700	-2.80426000
H	-1.46613900	-1.06607700	-3.63242300
C	-3.63992900	-3.44370100	0.61359100
C	1.97480400	-1.84027100	-0.42728100
C	3.03006100	-2.81106900	-0.58965700
C	3.48764100	-3.14199300	-1.84970500
H	4.28284000	-3.87150900	-1.95702200
C	2.92683000	-2.52600300	-2.99057600
H	3.27801700	-2.75966600	-3.98685200
C	1.92093900	-1.59707700	-2.80425000
H	1.46646200	-1.06587300	-3.63242700
C	3.63997300	-3.44363800	0.61366900

[Rh-2-A]

2 1			
Rh	-1.08785300	-0.46186500	0.09698000
Rh	1.08778900	0.46195500	0.09689100
N	-0.02870700	-1.55912000	-1.37560500
N	1.20449800	-1.10954000	-1.28751900
N	-1.20483500	1.11007100	-1.28688900
N	0.02835600	1.55966700	-1.37507100
N	-1.61252700	0.84479700	1.54870500
N	0.44110500	1.76856300	1.52672400
N	-0.44081900	-1.76902000	1.52618000
N	1.61281700	-0.84523500	1.54802300
C	-0.36769500	-2.57695300	-2.24256600
C	-1.73066800	-2.96129500	-2.34057900
H	-2.47603600	-2.43847300	-1.75036200
C	-2.09099600	-3.97550900	-3.20236600
H	-3.12903700	-4.27639000	-3.29136000
C	-1.09942100	-4.63315900	-3.98397600
H	-1.39543200	-5.43365000	-4.65356500

C	0.23031600	-4.25912900	-3.90422600
H	0.96254800	-4.77092600	-4.51646000
C	0.63413700	-3.21401400	-3.03373600
C	1.99203900	-2.75342000	-2.89840600
C	2.24097300	-1.66991700	-2.00278700
C	3.55245000	-1.16190100	-1.81126000
H	3.72054700	-0.36550200	-1.09442400
C	4.60261400	-1.72040700	-2.50896200
H	5.61216900	-1.35243300	-2.36377000
C	4.36899700	-2.79563000	-3.41191300
H	5.20540600	-3.22636200	-3.95212600
C	3.09463700	-3.30209900	-3.60091800
H	2.94808000	-4.12597200	-4.28843500
C	-2.24141500	1.67059200	-2.00189200
C	-3.55287300	1.16258700	-1.81021700
H	-3.72087600	0.36610500	-1.09345000
C	-4.60313600	1.72121300	-2.50767700
H	-5.61267900	1.35325100	-2.36236500
C	-4.36963500	2.79654300	-3.41053000
H	-5.20611900	3.22736200	-3.95055800
C	-3.09529300	3.30301300	-3.59966300
H	-2.94882500	4.12697500	-4.28709100
C	-1.99260000	2.75422300	-2.89738800
C	-0.63471600	3.21484300	-3.03282800
C	0.36722200	2.57766700	-2.24188500
C	1.73017500	2.96206200	-2.33997200
H	2.47561900	2.43917000	-1.74991100
C	2.09038400	3.97643000	-3.20163000
H	3.12840700	4.27735700	-3.29067900
C	1.09870900	4.63417900	-3.98302800
H	1.39462600	5.43478900	-4.65251600
C	-0.23101200	4.26010700	-3.90319300
H	-0.96332200	4.77199500	-4.51525700
C	-2.96992200	0.95364000	1.99539100
C	-3.46421500	2.12601900	2.59075200
H	-2.80269400	2.96802500	2.75538000
C	-4.80798700	2.18709900	2.97319400
H	-5.18841800	3.08891800	3.44219600
C	-5.66614300	1.09750800	2.75337200
H	-6.70662000	1.15350000	3.05531300
C	-5.16656300	-0.06707300	2.15505600
H	-5.81622400	-0.92364100	2.00528700
C	-3.81988300	-0.14253300	1.78027000
H	-3.42885500	-1.07855000	1.38771600
C	1.32776200	2.68894800	2.18489800
C	1.35448700	2.77899200	3.58416100

H	0.68405900	2.16639900	4.17717000
C	2.24937600	3.66142400	4.19945900
H	2.27015600	3.73595000	5.28183700
C	3.12358900	4.44117800	3.42682200
H	3.81732400	5.12095500	3.91015300
C	3.09027200	4.34600900	2.02802700
H	3.74952300	4.96478000	1.42725600
C	2.18965700	3.47386500	1.40457400
H	2.12458700	3.44216200	0.32146900
C	-1.32727100	-2.68970800	2.18420500
C	-2.18956500	-3.47410600	1.40380300
H	-2.12500800	-3.44173800	0.32068600
C	-3.08997100	-4.34655600	2.02712900
H	-3.74952400	-4.96492300	1.42627400
C	-3.12269500	-4.44254400	3.42588000
H	-3.81626900	-5.12255500	3.90911300
C	-2.24810900	-3.66328500	4.19859600
H	-2.26844600	-3.73842200	5.28094000
C	-1.35342100	-2.78056100	3.58343000
H	-0.68270700	-2.16835400	4.17651200
C	2.97029700	-0.95417800	1.99442900
C	3.46473200	-2.12670700	2.58937800
H	2.80327000	-2.96878100	2.75388200
C	4.80857100	-2.18785100	2.97157100
H	5.18911300	-3.08979000	3.44025200
C	5.66665200	-1.09816500	2.75191700
H	6.70718100	-1.15420800	3.05366800
C	5.16692800	0.06657100	2.15402500
H	5.81653200	0.92320600	2.00439100
C	3.82018200	0.14208800	1.77948400
H	3.42906100	1.07820700	1.38726400
N	-0.77412100	1.73260800	2.01399700
N	0.77452700	-1.73322900	2.01317100

[Rh-2-B]

2 1			
Rh	1.25274700	0.04691000	0.03483200
N	-1.05358400	-2.02985800	0.58795200
N	1.30636900	-1.95637700	0.61662400
N	1.35115800	-0.66713900	-1.86291900
N	-1.00208400	-0.54566400	-2.05605600
N	3.60021500	0.03345800	-0.45256200
C	2.47615400	-2.79316100	0.63735300
C	3.74245800	-0.80465800	-1.48618600

C	0.22069300	-0.82731000	-2.62369500
C	2.55222200	-1.02602500	-2.34289100
C	3.49568100	-2.61086800	1.58397900
H	3.40126400	-1.82968200	2.32968300
C	0.14100200	-2.58801600	0.74558800
H	0.16924200	-3.64580100	1.01665300
C	-2.17315800	-2.92081600	0.76991400
C	0.31480400	-1.25956000	-3.97664900
C	2.69552000	-1.52345200	-3.66790100
H	3.67439900	-1.78078200	-4.04535800
C	-2.08083400	-0.56167600	-2.84312800
H	-3.01609600	-0.29476800	-2.37848900
C	1.59392800	-1.61597400	-4.48244500
H	1.68768200	-1.95197700	-5.51020000
C	7.13470700	0.22352400	0.75352600
H	8.08960500	-0.25967700	0.56935000
C	2.60248800	-3.84972300	-0.28334600
H	1.82099800	-4.00933200	-1.02270000
C	4.60739000	-3.45878000	1.60625900
H	5.37730100	-3.30717800	2.35847200
C	-2.37324800	-3.99025300	-0.11675000
H	-1.69482900	-4.12304500	-0.95638100
C	-0.86010900	-1.30434700	-4.77261900
H	-0.79595200	-1.62122200	-5.80877600
C	5.99876100	-0.18139200	-0.00251800
C	-2.05787100	-0.92525400	-4.20799900
H	-2.98191000	-0.91483700	-4.77264100
C	4.73541100	-4.52539300	0.69671500
C	4.97732000	-1.43552700	-1.79643200
H	5.04034900	-2.16376700	-2.59309200
C	4.72749800	0.42774700	0.24260100
C	3.71199700	-4.70324200	-0.24903900
H	3.77739000	-5.52418500	-0.95819200
C	-3.04758300	-2.77348100	1.85762100
H	-2.87984600	-1.97199500	2.56988200
C	7.02725800	1.23575200	1.68474800
H	7.89501500	1.55517800	2.25201300
C	-3.43206000	-4.88924100	0.07645300
H	-3.56291200	-5.71782700	-0.61407300
C	4.65539500	1.49997200	1.17506500
H	3.72970100	2.05185200	1.26335900
C	5.77847500	1.89452200	1.87374200
H	5.72036200	2.73660300	2.55642700
C	5.91231300	-5.47061800	0.76576300
H	6.82531700	-4.95773700	1.08522900
H	6.10901500	-5.94321300	-0.20152200

H	5.72422300	-6.27481700	1.48751900
C	-4.10513000	-3.66773900	2.04065900
H	-4.76715300	-3.54582800	2.89427000
C	-4.31863900	-4.74292000	1.15493900
C	-5.45153900	-5.71661800	1.38190300
H	-6.41013700	-5.19733000	1.49184100
H	-5.29236100	-6.29932500	2.29682600
H	-5.54643400	-6.42433800	0.55344900
Rh	-1.25283000	-0.04680800	-0.03496200
N	1.05348800	2.02991500	-0.58824900
N	-1.30646600	1.95655000	-0.61653100
N	-1.35124600	0.66708500	1.86283800
N	1.00204300	0.54613700	2.05581400
N	-3.60007300	-0.03353900	0.45227000
C	-2.47623100	2.79336600	-0.63681800
C	-3.74255900	0.80422000	1.48615700
C	-0.22075500	0.82756800	2.62351400
C	-2.55235300	1.02578100	2.34285100
C	-3.49589600	2.61141800	-1.58336300
H	-3.40158100	1.83051400	-2.32937600
C	-0.14109100	2.58815500	-0.74562600
H	-0.16933300	3.64597200	-1.01657200
C	2.17310300	2.92079900	-0.77026600
C	-0.31485500	1.25999300	3.97641300
C	-2.69566400	1.52325800	3.66783900
H	-3.67456100	1.78041400	4.04536000
C	2.08088200	0.56266900	2.84275400
H	3.01617700	0.29597300	2.37805500
C	-1.59402700	1.61612600	4.48228200
H	-1.68777800	1.95222700	5.51000500
C	-7.13456100	-0.22454500	-0.75367900
H	-8.08962200	0.25825700	-0.56930500
C	-2.60243300	3.84959900	0.28427600
H	-1.82082100	4.00895900	1.02355600
C	-4.60761500	3.45932900	-1.60517100
H	-5.37763200	3.30800000	-2.35733000
C	2.37322900	3.99031600	0.11629900
H	1.69478800	4.12324300	0.95589100
C	0.86012700	1.30526700	4.77225400
H	0.79597900	1.62228400	5.80836800
C	-5.99871800	0.18056100	0.00242000
C	2.05795500	0.92649400	4.20755900
H	2.98206300	0.91649100	4.77209600
C	-4.73551200	4.52560600	-0.69521600
C	-4.97763700	1.43453500	1.79665100
H	-5.04092200	2.16248900	2.59354700

C	-4.72724400	-0.42804000	-0.24294900
C	-3.71195400	4.70312200	0.25044700
H	-3.77724200	5.52381300	0.95990200
C	3.04757000	2.77328500	-1.85791400
H	2.87982700	1.97171500	-2.57007800
C	-7.02679700	-1.23646000	-1.68520400
H	-7.89447000	-1.55603700	-2.25251300
C	3.43210500	4.88921800	-0.07695900
H	3.56298200	5.71786900	0.61348300
C	-4.65480900	-1.49996200	-1.17573400
H	-3.72891700	-2.05146300	-1.26426500
C	-5.77778300	-1.89471700	-1.87446100
H	-5.71939800	-2.73657200	-2.55740100
C	-5.91242500	5.47085500	-0.76374000
H	-6.82538000	4.95817800	-1.08366700
H	-6.10924600	5.94277600	0.20385000
H	-5.72426400	6.27556000	-1.48491400
C	4.10518200	3.66745400	-2.04100000
H	4.76724500	3.54539800	-2.89456000
C	4.31871600	4.74272500	-1.15539500
C	5.45166200	5.71635000	-1.38243800
H	6.41016800	5.19698600	-1.49279800
H	5.29227400	6.29931300	-2.29716300
H	5.54687700	6.42385100	-0.55383200
N	6.08485300	-1.15817100	-1.02898000
N	-6.08511300	1.15699400	1.02918100

[Rh-2-C]

2 1			
Rh	-1.23945700	-0.01894700	0.50540800
Rh	1.23945600	0.01897600	0.50541800
N	1.16835200	1.26690900	-1.11282500
N	-1.12018800	1.66976100	-0.70655800
N	1.12019300	-1.66980000	-0.70645600
N	-1.16834900	-1.26698400	-1.11275800
N	1.16667300	-1.23133800	2.17821900
N	-1.12135800	-1.67060200	1.78190000
N	-3.58388000	-0.77745800	0.83337100
N	-5.66749700	-2.67624700	0.57945700
N	-1.16669900	1.23146100	2.17813500
N	1.12134800	1.67067700	1.78185600
N	3.58386700	0.77750600	0.83334200
N	5.66749700	2.67628900	0.57944500
C	5.69108200	2.97614600	-4.30031800
H	6.39080900	2.15831100	-4.49691700

H	6.24793600	3.79306500	-3.82987100
H	5.33533800	3.34263400	-5.27096500
C	4.53527900	2.52415600	-3.43917800
C	4.18314900	1.16670600	-3.34183000
H	4.76500600	0.42562500	-3.88332200
C	3.08923800	0.75050100	-2.57446900
H	2.82830600	-0.29678800	-2.51797300
C	2.31684100	1.68458700	-1.87540100
C	2.67071300	3.04502800	-1.94704000
H	2.09342000	3.78544600	-1.39799300
C	3.76052000	3.45428400	-2.72246300
H	4.01461000	4.50975400	-2.77099400
C	-5.14074500	5.68843300	-1.86485900
H	-4.64495200	6.61678700	-2.17360600
H	-5.75833200	5.92435000	-0.99274000
H	-5.80596900	5.39201300	-2.68197200
C	-4.12374800	4.61437600	-1.55594300
C	-3.60222600	3.79303800	-2.57175200
H	-3.94942600	3.92245300	-3.59320300
C	-2.63754200	2.81835800	-2.29624800
H	-2.24204700	2.21301600	-3.10683400
C	-2.16060700	2.62941500	-0.98674800
C	-2.65660700	3.46377400	0.02811000
H	-2.26695100	3.37612300	1.03537000
C	-3.63108100	4.43000600	-0.25165200
H	-3.99776900	5.06565100	0.54999000
C	0.02857800	1.90100800	-1.34647300
H	0.03633100	2.68994300	-2.10033000
C	5.14076100	-5.68849500	-1.86463800
H	5.80604100	-5.39207500	-2.68170600
H	4.64495000	-6.61682200	-2.17345100
H	5.75828400	-5.92446500	-0.99249300
C	4.12377600	-4.61442100	-1.55574700
C	3.63117600	-4.42994800	-0.25144500
H	3.99792500	-5.06551300	0.55023000
C	2.65669600	-3.46371300	0.02828600
H	2.26709400	-3.37598200	1.03555900
C	2.16062500	-2.62945000	-0.98661500
C	2.63750000	-2.81849000	-2.29612300
H	2.24195800	-2.21322000	-3.10674000
C	3.60218800	-3.79317400	-2.57159700
H	3.94934200	-3.92266000	-3.59305500
C	-5.69108600	-2.97639500	-4.30015900
H	-5.33525000	-3.34464600	-5.27010100
H	-6.38989900	-2.15814400	-4.49825400
H	-6.24898900	-3.79208400	-3.82880500

C	-4.53525300	-2.52433600	-3.43909300
C	-3.76041400	-3.45445100	-2.72243400
H	-4.01443800	-4.50993600	-2.77100900
C	-2.67062300	-3.04516400	-1.94701700
H	-2.09328000	-3.78557200	-1.39800800
C	-2.31682600	-1.68469900	-1.87533000
C	-3.08929200	-0.75063600	-2.57434000
H	-2.82842200	0.29666700	-2.51781600
C	-4.18319900	-1.16687700	-3.34170200
H	-4.76510200	-0.42580700	-3.88315700
C	-0.02856700	-1.90108100	-1.34637000
H	-0.03630500	-2.69004800	-2.10019200
C	2.27772800	-1.43295300	2.89585000
H	3.13562800	-0.83547000	2.61550400
C	2.36882900	-2.38838000	3.93232000
H	3.30092500	-2.49999100	4.47215200
C	1.26821100	-3.17433500	4.20585600
H	1.30013800	-3.94111400	4.97363000
C	0.07075400	-2.96998700	3.46935400
C	0.03673400	-1.95735400	2.47031000
C	-1.10863500	-3.73050200	3.69873500
H	-1.10685400	-4.51107300	4.45284100
C	-2.24007700	-3.45281000	2.97343100
H	-3.15281500	-4.00280900	3.15480500
C	-2.22678800	-2.39420500	2.01868300
C	-3.46909000	-2.02379300	1.31171000
C	-4.52162600	-2.97819600	1.16315600
H	-4.40157600	-4.00282200	1.49258300
C	-5.83999500	-1.39095600	0.13533900
C	-4.78687400	-0.42079000	0.25913900
C	-7.08079000	-1.02533700	-0.44686100
H	-7.84605600	-1.78886000	-0.52693500
C	-7.27967700	0.27160500	-0.87471600
H	-8.22849800	0.56308200	-1.31271000
C	-6.24188300	1.23990300	-0.73634100
H	-6.41441100	2.25810000	-1.06898000
C	-5.02076200	0.90345100	-0.18836700
H	-4.23696500	1.63919100	-0.09211800
C	-2.27777300	1.43312300	2.89572500
H	-3.13567900	0.83565600	2.61536600
C	-2.36888000	2.38856800	3.93217700
H	-3.30099200	2.50021700	4.47197300
C	-1.26824400	3.17448500	4.20574700
H	-1.30016900	3.94127000	4.97351500
C	-0.07077000	2.97009100	3.46928600
C	-0.03675100	1.95745300	2.47024500

C	1.10863700	3.73056400	3.69870900
H	1.10686100	4.51112900	4.45282200
C	2.24009000	3.45284100	2.97343500
H	3.15284200	4.00280500	3.15484300
C	2.22679000	2.39425400	2.01866800
C	3.46908900	2.02383600	1.31169500
C	4.52162700	2.97823800	1.16314600
H	4.40159000	4.00285500	1.49260100
C	5.83998400	1.39100500	0.13530700
C	4.78685700	0.42084100	0.25909700
C	7.08077300	1.02539000	-0.44690700
H	7.84603900	1.78891400	-0.52697400
C	7.27965700	-0.27154800	-0.87477500
H	8.22847800	-0.56302300	-1.31277100
C	6.24186100	-1.23984300	-0.73640700
H	6.41438300	-2.25803900	-1.06905300
C	5.02074200	-0.90339400	-0.18842700
H	4.23694700	-1.63913400	-0.09218200

[Rh-2-D]

2 1

Rh	-1.32485700	1.27333400	-0.09111300
Rh	-1.32499400	-1.27332700	0.09105000
N	-2.95333200	1.02207400	-1.28796400
N	0.44129000	1.68397400	0.95006900
N	-0.00059200	-1.46163600	1.69105100
N	-0.00041700	1.46156700	-1.69106200
N	-2.55598500	1.25488300	1.53577400
F	-6.24985800	5.45995500	-2.11247700
N	0.44113900	-1.68405500	-0.95007300
N	-2.95347600	-1.02195200	1.28787800
N	-2.55610000	-1.25478900	-1.53585400
F	-3.16797400	-5.94508800	-4.52385200
F	-3.16731700	5.94538800	4.52358900
N	5.08953800	2.75621300	0.14641400
C	1.51476600	1.87822100	0.12488400
C	1.51460300	-1.87834100	-0.12487800
C	-3.24867100	-0.15641300	-1.82293300
H	-4.07849900	-0.21806100	-2.52979700
C	-3.81205000	2.14622600	-1.50427000
C	1.27501000	-1.76030200	1.30251500
C	2.78266300	2.22269500	0.61255100
C	-0.28736500	1.39272100	-3.00276300
H	-1.31339800	1.17148900	-3.26396300
C	2.30459900	1.98902400	-2.22619600

N	4.62047200	-2.52973200	2.62915100
C	1.27518500	1.76019600	-1.30251400
N	5.08933800	-2.75645600	-0.14637000
C	-5.19978500	2.05162200	-1.29501100
H	-5.63331100	1.11690200	-0.95278000
C	2.94148700	2.37136500	2.00612900
H	3.91567200	2.64729700	2.39307300
C	3.88230400	2.44009500	-0.33017400
C	-2.68679800	-3.69969200	-1.67428700
H	-2.58390900	-3.76059300	-0.59627600
C	0.59927500	1.83658800	2.27552100
H	-0.27963200	1.70049300	2.89060600
C	1.84113700	-2.18019900	-2.83694600
H	1.92105900	-2.30616300	-3.90983100
C	2.30440200	-1.98917000	2.22620700
C	-2.74303300	-2.44456600	-2.30652300
C	-3.25473100	3.37091900	-1.91845500
H	-2.18809500	3.44596400	-2.10902000
C	3.64419500	-2.32531000	1.74069000
N	4.62068800	2.52952500	-2.62911300
C	2.94130200	-2.37160500	-2.00610800
H	3.91547400	-2.64760100	-2.39303700
C	-0.28754800	-1.39279400	3.00274100
H	-1.31357300	-1.17152400	3.26395400
C	1.99688600	1.90888000	-3.60000800
H	2.78406600	2.09478100	-4.32166600
C	-4.06859100	4.48996300	-2.11914000
H	-3.66360800	5.44114900	-2.44639500
C	6.09808800	2.97614600	-0.74457200
C	3.64440100	2.32511600	-1.74066300
C	0.59911900	-1.83671200	-2.27552000
H	-0.27977400	-1.70057700	-2.89061600
C	1.84130900	2.17998700	2.83695900
H	1.92124100	2.30591400	3.90984800
C	-3.81225900	-2.14602600	1.50431200
C	-2.68606900	3.69979700	1.67419100
H	-2.58291000	3.76065200	0.59620100
C	2.78248200	-2.22288400	-0.61253300
C	3.88211000	-2.44030900	0.33020100
F	-6.25028000	-5.45955300	2.11280100
C	-3.24863400	0.15655900	1.82289100
H	-4.07841200	0.21828200	2.52979800
C	1.99667500	-1.90903400	3.60002400
H	2.78384700	-2.09497500	4.32167900
C	-5.44015100	4.35740800	-1.91102100
C	-2.74279900	2.44469100	2.30642900

C	0.69209800	-1.61238500	3.98590700
H	0.41602200	-1.56011400	5.03224300
C	-2.93694300	-2.38571400	-3.70162900
H	-2.95933900	-1.42850500	-4.21445400
C	-2.93703600	2.38593000	3.70149300
H	-2.95978700	1.42875900	4.21437000
C	-3.02869000	-4.78157800	-3.78785800
C	-2.82187700	-4.87774400	-2.41365600
H	-2.79207200	-5.85321400	-1.94105600
C	6.92369900	-3.09854100	3.07681800
H	6.72069800	-3.01009200	4.13781200
C	-3.09695900	-3.55751900	-4.44888500
H	-3.26202000	-3.53153600	-5.52036300
C	-6.02654400	3.15929400	-1.50796800
H	-7.09918600	3.10813400	-1.35774300
C	0.69229900	1.61226900	-3.98591000
H	0.41625400	1.56000200	-5.03225400
C	-5.20003800	-2.05126200	1.29538200
H	-5.63354500	-1.11646900	0.95333000
C	-3.02816500	4.78183400	3.78764300
C	5.85838700	-2.86029900	2.16319700
C	8.40689300	-3.55575700	1.18808900
H	9.39776800	-3.83074600	0.84197700
C	7.39634800	3.32818800	-0.27900700
H	7.55284100	3.41583200	0.78990900
C	-3.25497900	-3.37080700	1.91828400
H	-2.18830800	-3.44597900	2.10861000
C	6.09787900	-2.97640100	0.74462400
C	-2.82099700	4.87791100	2.41349100
H	-2.79080500	5.85335800	1.94086900
C	7.39613600	-3.32847100	0.27906900
H	7.55264000	-3.41610300	-0.78984600
C	5.85860500	2.86005700	-2.16314900
C	-3.09691000	3.55780200	4.44867200
H	-3.26220900	3.53188500	5.52011500
C	8.40712200	3.55544200	-1.18801400
H	9.39800000	3.83040700	-0.84188900
C	-5.44050000	-4.35707500	1.91126600
C	8.16957900	3.43944500	-2.59577300
H	8.98567800	3.62830400	-3.28534000
C	-6.02686100	-3.15886400	1.50844500
H	-7.09953300	-3.10758900	1.35847700
C	6.92393300	3.09827200	-3.07676000
H	6.72093300	3.00984800	-4.13775600
C	-4.06891200	-4.48978100	2.11908100
H	-3.66395700	-5.44102300	2.44620600

C	8.16933900	-3.43975500	2.59584300
H	8.98542300	-3.62865400	3.28541700

[Rh-2-E]

2 1			
Rh	2.11536100	-1.26956200	-0.12891800
Rh	2.11531000	1.26957700	0.12890000
N	3.34777200	0.97225800	1.72863700
N	3.74510400	-1.22847100	1.09334200
N	3.74503900	1.22852700	-1.09338700
N	3.34783600	-0.97223400	-1.72863300
N	0.79171800	-1.72881400	1.41440700
N	0.34908700	-1.49003300	-1.22329200
N	0.34902800	1.49004700	1.22328800
N	0.79166400	1.72884900	-1.41440600
N	-3.82758100	-2.91949700	2.16288000
N	-4.29894600	-2.66208200	-0.61832300
N	-4.29902800	2.66197600	0.61830200
N	-3.82764800	2.91944600	-2.16289300
C	6.23310500	-4.62011800	1.13937200
C	6.81975500	-3.37018000	0.95216900
H	7.89288900	-3.29330900	0.81720100
C	5.99258200	-2.24268100	0.93081100
H	6.42627100	-1.26267200	0.75681800
C	4.60409400	-2.37250200	1.11482400
C	4.04656500	-3.65071700	1.30812600
H	2.97920400	-3.75789600	1.47806600
C	4.86088800	-4.78724900	1.31549200
H	4.45546900	-5.78086100	1.47114400
C	4.04007000	-0.15920300	1.82278100
H	4.86971000	-0.21986700	2.52998700
C	3.73071000	1.71354300	4.05640500
H	3.75250900	0.68238800	4.39689200
C	3.53545300	2.01144000	2.69240200
C	3.47874800	3.35668700	2.28581600
H	3.37389300	3.60213000	1.23458300
C	3.61499300	4.38994400	3.21664700
H	3.58457800	5.43213900	2.91885700
C	3.82325600	4.05875400	4.55352400
C	3.89164400	2.73928100	4.99401800
H	4.05715800	2.52920900	6.04494500
C	3.89174200	-2.73922000	-4.99403200
H	4.05716600	-2.52916000	-6.04497500
C	3.73071600	-1.71350200	-4.05642200
H	3.75233000	-0.68232700	-4.39687700

C	3.53559500	-2.01141700	-2.69239700
C	3.47909800	-3.35665900	-2.28577700
H	3.37432800	-3.60208900	-1.23452900
C	3.61543600	-4.38990500	-3.21661300
H	3.58519100	-5.43210300	-2.91882300
C	3.82357400	-4.05869600	-4.55350000
C	4.04006600	0.15926400	-1.82280300
H	4.86967800	0.21996900	-2.53004500
C	4.60397500	2.37258700	-1.11483200
C	4.04640400	3.65079600	-1.30807100
H	2.97903500	3.75795200	-1.47798400
C	4.86068400	4.78735600	-1.31538100
H	4.45521900	5.78095900	-1.47097900
C	6.23291100	4.62027100	-1.13927600
C	6.81960300	3.37034400	-0.95214600
H	7.89274300	3.29349100	-0.81720400
C	5.99247000	2.24281300	-0.93083900
H	6.42620500	1.26281100	-0.75690800
C	1.08241800	-1.88864200	2.71808100
H	2.10983900	-1.71932100	3.01048400
C	0.10382200	-2.27060600	3.64999300
H	0.38133900	-2.40118500	4.68910000
C	-1.20313700	-2.48998900	3.22114100
H	-1.99057700	-2.79401400	3.90116900
C	-1.51432500	-2.33033400	1.85562600
C	-0.48505900	-1.95037600	0.98323800
C	-0.72569100	-1.81879600	-0.44480300
C	-1.99466300	-2.06733300	-0.98457500
C	-2.15184400	-1.97091300	-2.38238300
H	-3.12737400	-2.17016500	-2.81072000
C	-1.04985700	-1.64365900	-3.16792000
H	-1.12991200	-1.58047300	-4.24632100
C	0.19261700	-1.40917300	-2.55587500
H	1.07285300	-1.17172800	-3.13709300
C	-2.85932300	-2.57211700	1.32509500
C	-3.09994400	-2.43997300	-0.09570900
C	-5.07902200	-3.16277000	1.65004400
C	-5.32061600	-3.03136600	0.22365900
C	-6.59800900	-3.28974500	-0.28965000
H	-6.75644200	-3.19095100	-1.35824800
C	-6.12582700	-3.54532600	2.49868700
H	-5.92344700	-3.64148100	3.56009100
C	-7.40240700	-3.80657500	1.98410800
C	-7.64357100	-3.67649100	0.55908200
C	-8.95915400	-3.95525000	0.05183100
H	-9.13924800	-3.86229800	-1.01478100

C	-9.96777200	-4.33736500	0.89932100
H	-10.95832400	-4.55035400	0.51098300
C	-9.72898000	-4.46559200	2.31125900
H	-10.54444200	-4.77209700	2.95809500
C	-8.48803500	-4.20854700	2.83603400
H	-8.30734600	-4.30902300	3.90184900
C	1.08237500	1.88869900	-2.71807600
H	2.10980500	1.71941400	-3.01046700
C	0.10377700	2.27065000	-3.64999200
H	0.38129300	2.40124900	-4.68909600
C	-1.20319000	2.48999800	-3.22114700
H	-1.99063300	2.79401400	-3.90117700
C	-1.51438400	2.33032800	-1.85563600
C	-0.48511600	1.95038500	-0.98324300
C	-0.72575000	1.81878600	0.44479800
C	0.19256000	1.40916600	2.55587100
H	1.07280400	1.17174700	3.13708900
C	-1.04992800	1.64360100	3.16790900
H	-1.12998900	1.58040200	4.24630800
C	-2.15192200	1.97082900	2.38236900
H	-3.12746000	2.17004100	2.81070500
C	-1.99473600	2.06727500	0.98456400
C	-3.10002000	2.43989400	0.09569300
C	-2.85938700	2.57207600	-1.32510700
C	-5.32069800	3.03125900	-0.22368100
C	-5.07909600	3.16268700	-1.65006300
C	-6.12590100	3.54524500	-2.49870500
H	-5.92351800	3.64141800	-3.56010700
C	-6.59809900	3.28960500	0.28962400
H	-6.75653700	3.19078400	1.35821900
C	-7.64366100	3.67635000	-0.55910900
C	-7.40248900	3.80646700	-1.98413100
C	-8.48811500	4.20843900	-2.83605700
H	-8.30741900	4.30894100	-3.90186800
C	-9.72906800	4.46545800	-2.31128700
H	-10.54452700	4.77196800	-2.95812400
C	-9.96786800	4.33719800	-0.89935300
H	-10.95842500	4.55016500	-0.51101500
C	-8.95925100	3.95508000	-0.05186300
H	-9.13935500	3.86210600	1.01474500
F	3.96411100	-5.07844600	-5.47879200
F	7.04320900	5.74103300	-1.15026500
F	7.04344700	-5.74085200	1.15041600
F	3.96370000	5.07850900	5.47882000

[Rh-2-F]

2 1			
Rh	-2.14450300	1.26640900	0.24754400
Rh	-2.14949300	-1.25834500	-0.13123300
N	-0.86154200	1.82080600	-1.30922800
N	-0.82906600	-1.81618100	1.38779600
N	-3.28982000	0.88069000	1.88226400
N	-0.37808100	-1.42500600	-1.23252600
N	-0.33592200	1.40094800	1.29260900
N	-3.36842500	-0.88612100	-1.70948600
N	-3.77283700	-1.25097400	1.09520500
N	-3.80759700	1.27129600	-0.95156300
C	0.43162000	1.99704800	-0.90543400
N	3.75310900	2.98492000	-2.13088600
C	-3.36347600	1.83128000	2.94524100
C	-4.02108500	-0.23381000	1.90671600
H	-4.84329900	-0.32357100	2.61918600
C	2.80648600	2.59874200	-1.28576500
C	0.69561000	-1.78719800	-0.46853400
C	0.71725800	1.76398400	0.50138200
C	-1.18643500	2.07368400	-2.58814700
H	-2.22315200	1.94017100	-2.85889300
N	4.31398200	2.51937400	0.60602800
C	-0.14608400	-2.48873300	3.58907700
H	-0.42710800	-2.68276600	4.61724000
N	3.79801200	-3.00626700	2.08618900
C	-0.23245000	2.50459700	-3.52407700
H	-0.54093300	2.70933600	-4.54221400
C	1.16389300	-2.67244100	3.15346300
H	1.95116800	-3.01019000	3.81743000
C	2.01010500	1.94692500	1.01124400
C	-4.05982000	0.24957700	-1.76069200
H	-4.87476700	0.33825900	-2.48060200
C	-4.58099800	2.47632800	-1.08644400
C	3.09289700	2.36054200	0.11274100
C	-0.13236800	1.21600000	2.60840300
H	-0.99492400	0.95151000	3.20343200
C	1.97046100	-1.98791900	-1.01498100
C	1.09000000	2.67540800	-3.12456600
H	1.86139800	3.01209200	-3.80738300
C	1.43925700	2.41900300	-1.78371700
C	0.44991300	-2.00496800	0.94885400
C	-3.65820900	1.45020000	4.26843500
H	-3.84791900	0.40903900	4.51448900
C	1.47865300	-2.42816500	1.80168200
N	4.28119900	-2.57242200	-0.67072500

C	5.02724500	3.16457700	-1.64714100
C	2.21592400	1.74284800	2.39028500
H	3.21071500	1.88926800	2.79476100
C	3.07627300	-2.39969200	-0.14369100
C	2.82948600	-2.62198400	1.26542600
C	-4.75325800	3.08995800	-2.34155800
H	-4.29811200	2.65993300	-3.23075100
C	1.13608200	1.37765900	3.18918200
H	1.25252400	1.22879200	4.25571800
C	1.03290900	-1.44455600	-3.17405700
H	1.11781700	-1.31474000	-4.24607100
C	-0.21581800	-1.26341700	-2.55680900
H	-1.09710400	-1.00532000	-3.12762900
C	-1.12340200	-2.05643800	2.67774000
H	-2.15256400	-1.90890600	2.97559900
C	2.13462800	-1.80479700	-2.40278800
H	3.11517900	-1.96475700	-2.83591200
C	5.31465700	2.92620500	-0.24462700
C	-4.67946600	-2.35923000	1.03704100
C	-3.53086200	-1.88326000	-2.71885100
C	-5.52544700	4.24987200	-2.46562200
H	-5.65581200	4.70177000	-3.44476300
C	6.10388000	-3.61719500	2.39801000
H	5.89644100	-3.78101200	3.45013100
C	5.05623500	-3.19948600	1.56717200
C	-3.66847300	-1.53715800	-4.07699600
H	-3.66887400	-0.49259700	-4.37892500
C	-3.40970500	3.76011800	5.04031600
C	-5.95622500	4.21917300	-0.09616600
H	-6.43197000	4.64439100	0.78345200
C	-6.13485600	4.84198500	-1.34558000
C	-3.69389200	2.40587100	5.29024300
H	-3.93600800	2.09076900	6.30158700
C	-5.19669900	3.05349100	0.03617900
H	-5.10590300	2.57277900	1.00171900
C	-4.19445500	-3.66695900	1.20103000
H	-3.13891100	-3.83490600	1.39990400
C	5.30377700	-2.97746900	0.15440500
C	-3.06997900	3.18296400	2.68872100
H	-2.85608000	3.51180000	1.67421500
C	-6.95105900	6.10632500	-1.47285700
H	-6.39871200	6.97200700	-1.08752600
H	-7.88391900	6.03731200	-0.90366400
H	-7.20838900	6.31660800	-2.51474700
C	6.61514000	3.11867100	0.23895900
H	6.80779600	2.93941000	1.29136400

C	-3.79709700	-2.53240700	-5.05151700
H	-3.91646000	-2.24574600	-6.09280700
C	6.05292900	3.58398100	-2.50416300
H	5.81577100	3.76016900	-3.54797200
C	-3.49959800	-3.24375200	-2.36944100
H	-3.44621200	-3.53263400	-1.32445100
C	7.38763500	-3.82627900	1.87742000
C	-3.08423200	4.12437900	3.72123300
H	-2.85590300	5.16259700	3.49628500
C	7.64003800	3.54170400	-0.61759300
C	7.35280700	3.77912300	-2.01952200
C	-6.05060700	-2.16079100	0.80340000
H	-6.42995000	-1.15516100	0.64327000
C	8.97944800	3.75329800	-0.14047500
H	9.19400500	3.57958800	0.90960000
C	-3.76469700	-3.89742900	-4.71179300
C	8.41815700	4.21651500	-2.87992100
H	8.20271600	4.39714800	-3.92862500
C	-3.60268600	-4.23010800	-3.35495600
H	-3.58162000	-5.27656600	-3.06306600
C	-5.07131400	-4.75649100	1.13591200
H	-4.68377600	-5.76228500	1.27115800
C	-3.47228200	4.78920400	6.14433600
H	-4.47958100	5.21607900	6.22406700
H	-2.78078200	5.61771300	5.96279900
H	-3.22745700	4.35141200	7.11695500
C	-3.92757700	-4.96829300	-5.76455100
H	-4.98000000	-5.26158800	-5.86265300
H	-3.36058600	-5.86994700	-5.51297600
H	-3.59350500	-4.62173200	-6.74722400
C	-6.44771000	-4.57192700	0.91701800
C	-6.91882700	-3.25485700	0.75347800
H	-7.97764700	-3.08687300	0.57588400
C	8.47494700	-4.26216700	2.71063900
H	8.28935200	-4.43052300	3.76706300
C	9.96742300	4.17207900	-0.99481200
H	10.97606200	4.33373100	-0.62877500
C	9.68283100	4.40683700	-2.38436800
H	10.48270000	4.74016900	-3.03744200
C	6.58808500	-3.18390200	-0.36518300
H	6.75083600	-3.01670200	-1.42459900
C	7.63497800	-3.60524300	0.46525500
C	-7.39999400	-5.74335800	0.86658100
H	-8.01605300	-5.71700300	-0.03886600
H	-8.08365700	-5.73168000	1.72353100
H	-6.86661000	-6.69791800	0.88206400

C	9.72318600	-4.46632200	2.18009700
H	10.53973600	-4.79846600	2.81281500
C	8.95827400	-3.83097400	-0.04883300
H	9.14293200	-3.66949400	-1.10651300
C	9.96822800	-4.24780800	0.78041300
H	10.96454400	-4.42016200	0.38657400

[Rh-2-G]

2 1

Rh	-1.19319400	-0.35647200	-0.31746100
Rh	1.19320900	0.35645500	-0.31744900
N	-0.69102700	-1.62498800	1.21538300
N	1.60736300	-1.17736400	0.98322500
N	-1.60739300	1.17730700	0.98325800
N	0.69099400	1.62493800	1.21542400
N	-1.62548800	0.98554600	-1.82969500
N	0.57184800	1.85311800	-1.70992400
N	-0.57179600	-1.85305700	-1.71000500
N	1.62552900	-0.98546100	-1.82974300
N	-3.39605400	-0.74684000	-0.73854300
N	3.39608600	0.74685600	-0.73847500
C	-1.98531900	-3.69471500	1.57643700
H	-1.48817600	-4.13832800	0.71745600
C	-2.91834900	-4.43935900	2.31120400
H	-3.14379300	-5.45962000	2.01319900
C	-3.55089500	-3.89585300	3.44394600
C	-3.21606900	-2.57975200	3.81806300
H	-3.67709000	-2.14447300	4.70075600
C	-2.28320200	-1.83190000	3.09021600
H	-2.01209400	-0.82891100	3.40376300
C	-1.66492900	-2.38099900	1.95612700
C	-4.52347800	-4.71082900	4.26407400
H	-4.02716100	-5.13549500	5.14503700
H	-4.93799000	-5.54483100	3.68999600
H	-5.35685000	-4.10029800	4.62639500
C	0.58321500	-1.84464800	1.51194300
H	0.80966200	-2.62968400	2.23746600
C	2.91140200	-1.76270900	1.15208500
C	3.15334600	-3.07028300	0.69430700
H	2.35356500	-3.62147200	0.20440600
C	4.40609300	-3.67266300	0.87184400
H	4.56508400	-4.69013500	0.52479100
C	5.45610400	-2.98700600	1.50406100
C	5.20712400	-1.67356700	1.94751800
H	5.99936400	-1.12525600	2.45117600

C	3.95761700	-1.06991300	1.78110600
H	3.78358700	-0.06950800	2.15723100
C	6.79658100	-3.64484300	1.73575400
H	7.62233000	-2.93918600	1.59721400
H	6.95498100	-4.48896600	1.05789200
H	6.86930200	-4.03061800	2.75988500
C	-3.95763400	1.06976900	1.78112600
H	-3.78360300	0.06934300	2.15719700
C	-5.20717100	1.67338000	1.94755800
H	-5.99938200	1.12499600	2.45118400
C	-5.45618700	2.98682200	1.50417400
C	-4.40617300	3.67255400	0.87201400
H	-4.56519900	4.69004600	0.52503800
C	-3.15341600	3.07022500	0.69445600
H	-2.35364100	3.62145700	0.20459300
C	-2.91143600	1.76261800	1.15216500
C	-6.79668500	3.64462200	1.73585700
H	-7.62235000	2.93861900	1.59858200
H	-6.95563600	4.48792900	1.05711300
H	-6.86895200	4.03154800	2.75958800
C	-0.58324500	1.84460700	1.51196200
H	-0.80969900	2.62965800	2.23746900
C	1.66490500	2.38093200	1.95616400
C	2.28321100	1.83179500	3.09021900
H	2.01209900	0.82880000	3.40374000
C	3.21610000	2.57961700	3.81806600
H	3.67714200	2.14430800	4.70073200
C	3.55092200	3.89573000	3.44398200
C	2.91834800	4.43927300	2.31127500
H	3.14378900	5.45954200	2.01329300
C	1.98529300	3.69465800	1.57650900
H	1.48814000	4.13830600	0.71755000
C	4.52353300	4.71068100	4.26410200
H	4.93822700	5.54454400	3.68995200
H	5.35677800	4.10008300	4.62659900
H	4.02718100	5.13554300	5.14495100
C	1.45448900	2.78753200	-2.08091900
H	2.42569900	2.73885000	-1.61315700
C	1.18288800	3.79992900	-3.02907600
H	1.95768900	4.51521600	-3.27592900
C	-0.06398000	3.84457000	-3.61377900
H	-0.31750900	4.59952500	-4.35130600
C	-1.03661400	2.88662500	-3.22439700
C	-0.69326100	1.89879300	-2.25788900
C	-2.35769100	2.88635900	-3.75003700
H	-2.63540100	3.62293200	-4.49724800

C	-3.27098700	1.97013700	-3.29140000
H	-4.28215800	1.97965900	-3.67100800
C	-2.88402300	1.02682300	-2.29946300
C	-3.86210800	0.07556500	-1.71582500
C	-5.20483600	0.03729400	-2.11533400
H	-5.58198900	0.69211600	-2.88915900
C	-6.08135900	-0.86036900	-1.49488600
H	-7.12371100	-0.89925100	-1.79183800
C	-5.59285800	-1.69643700	-0.48650700
H	-6.23656600	-2.40141100	0.02627800
C	-4.24063800	-1.60682500	-0.13616900
H	-3.82304000	-2.23144900	0.64240400
C	-1.45443300	-2.78744800	-2.08105800
H	-2.42561100	-2.73886700	-1.61321200
C	-1.18287500	-3.79969800	-3.02938800
H	-1.95767200	-4.51497500	-3.27627800
C	0.06394200	-3.84419900	-3.61421100
H	0.31743300	-4.59902100	-4.35188700
C	1.03658200	-2.88628800	-3.22475300
C	0.69328200	-1.89862800	-2.25805400
C	2.35761800	-2.88589100	-3.75050100
H	2.63527500	-3.62229700	-4.49789600
C	3.27093800	-1.96975100	-3.29174400
H	4.28206900	-1.97914900	-3.67146500
C	2.88404500	-1.02665900	-2.29956900
C	3.86215900	-0.07552400	-1.71577400
C	5.20492800	-0.03734800	-2.11514600
H	5.58211800	-0.69220400	-2.88892500
C	6.08145600	0.86024300	-1.49459700
H	7.12384000	0.89905000	-1.79144800
C	5.59291900	1.69633600	-0.48625900
H	6.23662300	2.40126700	0.02659100
C	4.24066600	1.60678700	-0.13602300
H	3.82305000	2.23140800	0.64254300

[Rh-2-H]

2 1			
Rh	-1.21952800	0.02200100	0.48166900
Rh	1.21948800	0.02198200	0.48171300
N	-1.16859000	1.81604800	-0.47356400
N	1.16860900	1.81601100	-0.47354200
N	-1.16649200	-0.97193300	-1.28524600
N	1.16647500	-0.97194200	-1.28521200
N	-1.18348300	-1.86138400	1.42649700
N	1.18338700	-1.86139000	1.42657600

N	-1.18325900	0.99472400	2.34014000
N	1.18322100	0.99472600	2.34015900
C	-3.33161000	2.94636600	-0.12024700
H	-3.12940000	2.98313500	0.94536100
C	-4.51358800	3.50097300	-0.62753500
H	-5.23902200	3.93271100	0.05629800
C	-4.76519200	3.53870400	-2.01067800
C	-3.79538600	2.99088200	-2.87297800
H	-3.96709000	3.00672900	-3.94564400
C	-2.62052300	2.42177900	-2.37454600
H	-1.89708100	1.97861600	-3.05303100
C	-2.37582500	2.39782900	-0.98985700
C	-6.02002400	4.17299800	-2.56163600
H	-6.43490400	3.58922600	-3.38964700
H	-5.81054100	5.17796400	-2.94753100
H	-6.79415500	4.27109900	-1.79521400
C	0.00002200	2.33678000	-0.83002700
H	0.00004400	3.25150700	-1.42508800
C	2.37587400	2.39771900	-0.98985500
C	2.62062600	2.42151000	-2.37452500
H	1.89721000	1.97828100	-3.05299600
C	3.79554000	2.99051900	-2.87297300
H	3.96728600	3.00623300	-3.94563300
C	4.76531900	3.53839800	-2.01069700
C	4.51365800	3.50081700	-0.62754800
H	5.23908900	3.93260000	0.05626200
C	3.33164900	2.94630900	-0.12025400
H	3.12939200	2.98318000	0.94534300
C	6.02017300	4.17267300	-2.56162600
H	6.43406900	3.58987200	-3.39080400
H	6.79491900	4.26913900	-1.79561300
H	5.81106800	5.17835800	-2.94585600
C	-3.59774200	-0.87370400	-1.45595700
H	-3.57224700	0.14248900	-1.07550200
C	-4.83043600	-1.45553800	-1.77771900
H	-5.74399600	-0.89813000	-1.59094000
C	-4.90718500	-2.72540300	-2.37241500
C	-3.69784400	-3.41003900	-2.60835800
H	-3.72714300	-4.39966500	-3.05642200
C	-2.46369800	-2.85244400	-2.26772500
H	-1.56114800	-3.43464800	-2.42916900
C	-2.39594800	-1.56174900	-1.70313600
C	-6.23173300	-3.33098400	-2.77129300
H	-7.06642400	-2.86069100	-2.24350700
H	-6.26234600	-4.40574300	-2.56457700
H	-6.41007100	-3.20354400	-3.84588600

C	-0.00000100	-1.31162200	-1.82919200
H	0.00000100	-1.88614600	-2.75476900
C	2.39596200	-1.56169700	-1.70309600
C	2.46378100	-2.85226100	-2.26796500
H	1.56126200	-3.43443700	-2.42967600
C	3.69797000	-3.40978500	-2.60855800
H	3.72731100	-4.39931300	-3.05683900
C	4.90728600	-2.72521600	-2.37230000
C	4.83046600	-1.45547700	-1.77734600
H	5.74400600	-0.89811400	-1.59034300
C	3.59773200	-0.87370900	-1.45562200
H	3.57219300	0.14241800	-1.07498800
C	6.23187300	-3.33075400	-2.77111500
H	6.26291400	-4.40530600	-2.56336000
H	7.06661400	-2.85968100	-2.24411500
H	6.40974000	-3.20432200	-3.84590400
C	-2.33928700	-2.48247400	1.68277200
H	-3.24676100	-1.96065300	1.40020300
C	-2.41786500	-3.76609100	2.27124300
H	-3.38967500	-4.20867700	2.45051800
C	-1.24811800	-4.42241600	2.59085700
H	-1.26341300	-5.41067500	3.04003300
C	-0.00008200	-3.79617500	2.31514000
C	-0.00005900	-2.49974600	1.72659900
C	1.24793000	-4.42242200	2.59094000
H	1.26319200	-5.41068200	3.04011500
C	2.41770400	-3.76610100	2.27141100
H	3.38949800	-4.20869100	2.45075300
C	2.33917100	-2.48248200	1.68293600
H	3.24666700	-1.96066100	1.40043800
C	-2.33744600	1.29949900	2.94039100
H	-3.24560000	1.01832500	2.41877200
C	-2.41723000	1.96058300	4.18768600
H	-3.38889300	2.17878200	4.61308100
C	-1.24713000	2.31554900	4.82537300
H	-1.26203900	2.82819800	5.78219200
C	-0.00003700	1.99868800	4.21785000
C	-0.00002700	1.33104800	2.95952100
C	1.24704700	2.31556700	4.82538600
H	1.26193700	2.82821900	5.78220400
C	2.41715600	1.96061900	4.18771100
H	3.38881300	2.17883600	4.61311100
C	2.33739400	1.29952300	2.94041900
H	3.24555900	1.01836000	2.41881100

[Mo-2-A]

0 1			
C	-0.15807300	2.80714600	0.21096600
C	-0.26979200	4.22735100	0.37159900
C	-0.37599600	5.42968500	0.53488600
C	-0.49744200	6.84951300	0.70017700
C	-0.65430500	7.68258600	-0.42716000
H	-0.68499500	7.23629800	-1.41631900
C	-0.77163100	9.06672100	-0.26642800
H	-0.89342900	9.70282200	-1.13787600
C	-0.73377600	9.63405500	1.01646500
H	-0.82548000	10.70920500	1.13875500
C	-0.57830800	8.80955700	2.14124000
H	-0.54955500	9.24652000	3.13476100
C	-0.46081000	7.42470100	1.98709900
H	-0.34121500	6.78139900	2.85315900
C	-0.22987700	2.92706400	-2.21683100
C	-1.29487100	2.66083200	-3.09340900
H	-2.05681200	1.94457000	-2.79897000
C	-1.36684400	3.32513100	-4.32436400
H	-2.19340400	3.11822300	-4.99774000
C	-0.37949200	4.25261900	-4.68684400
H	-0.43520200	4.76409300	-5.64317500
C	0.68713100	4.50874200	-3.81165100
H	1.46346500	5.21471600	-4.09224600
C	0.76681100	3.84665300	-2.58089300
H	1.60236700	4.02546300	-1.91149200
C	0.15316200	-2.74550100	-0.16297200
C	0.26467600	-4.16571900	-0.32361400
C	0.37063600	-5.36808000	-0.48687200
C	0.49183200	-6.78794000	-0.65207600
C	0.64853200	-7.62096500	0.47532000
H	0.67931600	-7.17461400	1.46444800
C	0.76560600	-9.00513100	0.31468500
H	0.88727000	-9.64119500	1.18617800
C	0.72766200	-9.57254900	-0.96817000
H	0.81918000	-10.64772300	-1.09038400
C	0.57235900	-8.74809900	-2.09300200
H	0.54354500	-9.18512500	-3.08649400
C	0.45510800	-7.36321000	-1.93895900
H	0.33562700	-6.71995000	-2.80506600
C	0.22520900	-2.86531200	2.26487700
C	1.29006700	-2.59869800	3.14151300
H	2.05185800	-1.88227600	2.84706700
C	1.36213800	-3.26287900	4.37252400
H	2.18859900	-3.05569700	5.04593600

C	0.37502100	-4.19061300	4.73502100
H	0.43082100	-4.70200000	5.69139300
C	-0.69147200	-4.44710000	3.85978200
H	-1.46764300	-5.15325000	4.14038300
C	-0.77125100	-3.78513900	2.62895800
H	-1.60673800	-3.96423500	1.95955800
C	2.76904400	0.20018800	-0.04172900
C	4.25275800	0.31914500	-0.06599600
C	4.86609100	1.37288400	0.64490200
C	6.26879300	1.45355500	0.63347100
H	6.75722100	2.25981100	1.17383600
C	7.05829400	0.53197900	-0.05855800
C	6.41785100	-0.49970900	-0.76499800
H	7.02060000	-1.21838000	-1.30930900
C	5.02601900	-0.62908400	-0.78722700
C	4.06879300	2.42542900	1.41402700
H	3.00963700	2.32573300	1.16222100
C	4.49198800	3.86157200	1.04563300
H	5.51767700	4.08017300	1.36442600
H	3.83154300	4.58316900	1.54090600
H	4.43306300	4.02948800	-0.03614700
C	4.18767900	2.18871500	2.93405500
H	3.81567300	1.19325900	3.19630500
H	3.59767600	2.93193600	3.48358400
H	5.23068100	2.26764600	3.26526600
C	8.57626100	0.65005300	-0.04858800
H	8.83629800	1.52458300	0.56306200
C	9.13566400	0.88833000	-1.46633400
H	10.22418100	1.01833800	-1.43404900
H	8.69513600	1.78263000	-1.92090400
H	8.91913100	0.03747900	-2.12319600
C	9.23707800	-0.58511100	0.59746900
H	8.86810800	-0.74438800	1.61678800
H	10.32591100	-0.46104100	0.64039900
H	9.02604600	-1.49230800	0.01884500
C	4.36240100	-1.80885400	-1.49905400
H	3.42952000	-1.45141000	-1.94332900
C	5.20780300	-2.40774300	-2.63501000
H	6.10249400	-2.91749700	-2.25682100
H	5.52497900	-1.64062700	-3.35066400
H	4.61508700	-3.15307900	-3.17758300
C	4.00529600	-2.90886000	-0.47148200
H	4.91492800	-3.31322800	-0.00987600
H	3.47206600	-3.73201100	-0.96095000
H	3.36497000	-2.52562200	0.33082700
C	-2.77384200	-0.13641500	0.08982600

C	-4.25792800	-0.25107500	0.11418300
C	-4.87537900	-1.30696600	-0.59610300
C	-6.27498300	-1.38546700	-0.58882900
H	-6.75663800	-2.19499200	-1.12944800
C	-7.06374900	-0.45668900	0.10058800
C	-6.42187700	0.57253600	0.80320100
H	-7.03118100	1.29103100	1.34147100
C	-5.02679000	0.70010400	0.82971800
C	-4.07531500	-2.36082000	-1.36126400
H	-3.01897300	-2.27038900	-1.09405600
C	-4.17115000	-2.11287300	-2.88119900
H	-5.21017100	-2.18227500	-3.22691200
H	-3.57872700	-2.85640000	-3.42774700
H	-3.78863500	-1.11834000	-3.13114700
C	-4.51211600	-3.79695900	-1.00969700
H	-4.47477100	-3.97198600	0.07187200
H	-3.84579300	-4.51856800	-1.49701000
H	-5.53230900	-4.00931100	-1.34988300
C	-8.58310900	-0.55824300	0.09862400
H	-8.97165800	0.27997900	0.69252900
C	-9.15975800	-0.42832900	-1.32612500
H	-8.84872000	0.51159400	-1.79545700
H	-10.25586700	-0.45544800	-1.30187200
H	-8.81867500	-1.25116800	-1.96568100
C	-9.06397000	-1.86440900	0.76404500
H	-10.15962700	-1.89869700	0.79852800
H	-8.68423200	-1.95025300	1.78818800
H	-8.71844300	-2.74147400	0.20383500
C	-4.36466300	1.88132000	1.54007200
H	-3.42824000	1.52713400	1.97940200
C	-5.20774900	2.47417400	2.68106100
H	-4.61580200	3.22072000	3.22282800
H	-5.51867700	1.70396400	3.39608300
H	-6.10633300	2.98054300	2.30787900
C	-4.01731800	2.98415600	0.51224700
H	-3.37760500	2.60457200	-0.29234500
H	-3.48700800	3.80986800	1.00060200
H	-4.93065600	3.38396700	0.05400700
Mo	-0.03174600	0.07867600	-1.02780400
Mo	0.02704200	-0.01706300	1.07575900
N	-0.15759600	2.19651300	-0.98236500
N	0.15285200	-2.13485300	1.03035600
O	-0.07631400	2.05923500	1.28641400
O	0.07142600	-1.99758600	-1.23841400
O	2.07238000	0.20296600	-1.13862400
O	2.13508400	0.09957400	1.09239100

O	-2.13989600	-0.03701800	-1.04439300
O	-2.07711500	-0.14055600	1.18662900

[Mo-2-B]

0 1

C	-2.12812700	-2.14788300	-0.33376800
C	-3.15362100	-3.13835300	-0.39629300
C	-4.03607700	-3.97598500	-0.48413400
C	-5.07038400	-4.96495300	-0.56693500
C	-5.50756900	-5.43785900	-1.82174600
H	-5.05339700	-5.04356800	-2.72531200
C	-6.51563600	-6.40394800	-1.89611800
H	-6.84806700	-6.76399300	-2.86497600
C	-7.09806600	-6.90782300	-0.72306900
H	-7.88126100	-7.65766700	-0.78351400
C	-6.66740600	-6.44051400	0.52810600
H	-7.11792700	-6.82839300	1.43665400
C	-5.65952900	-5.47485400	0.60918500
H	-5.32228200	-5.10717000	1.57339800
C	-2.14221400	-2.18516000	2.08491400
C	-2.82176700	-1.31208100	2.94918400
H	-3.00755200	-0.28941100	2.63429900
C	-3.25535700	-1.77495400	4.19877200
H	-3.78462700	-1.10072000	4.86543400
C	-3.00731800	-3.09878400	4.58805600
H	-3.34032000	-3.45322900	5.55900300
C	-2.31715500	-3.96211000	3.72253200
H	-2.10954200	-4.98432800	4.02483700
C	-1.88114700	-3.50863800	2.47254600
H	-1.33031500	-4.16402700	1.80555000
C	1.98094500	-1.94822200	-0.00617200
C	3.04236600	-2.99267800	-0.01674700
C	4.16805300	-2.85882900	0.83587700
C	5.15656600	-3.84681200	0.78387700
H	6.02427600	-3.75504200	1.42853500
C	5.05927300	-4.95049800	-0.07925400
C	3.93527700	-5.05403700	-0.90376400
H	3.85057600	-5.90886400	-1.56918100
C	2.91257600	-4.09130200	-0.89188100
C	4.34733700	-1.62201800	1.71563900
H	3.35803000	-1.28032500	2.03222900
C	5.16475200	-1.88124600	2.99226100
H	4.76098600	-2.72447000	3.56413800
H	5.13666800	-0.99181300	3.63204800
H	6.21874000	-2.08887800	2.77078800

C	4.99332900	-0.48478900	0.88997700
H	6.00256000	-0.76844700	0.56573200
H	5.06663100	0.42930200	1.49031400
H	4.40498400	-0.25173500	-0.00481500
C	6.14866300	-6.01362800	-0.11837200
H	5.85229600	-6.76407500	-0.86371300
C	6.28748500	-6.73292800	1.23921300
H	7.04255900	-7.52611600	1.17951500
H	5.33768000	-7.18383100	1.54748400
H	6.59702600	-6.03384500	2.02520000
C	7.50259500	-5.42303700	-0.56299100
H	7.42058400	-4.93613100	-1.54111800
H	8.26221000	-6.21102300	-0.63274900
H	7.86076900	-4.67542600	0.15473600
C	1.70933000	-4.26329500	-1.81675900
H	0.93633800	-3.54184600	-1.53631500
C	2.10132000	-3.95025600	-3.27594000
H	2.48243400	-2.92735900	-3.35971500
H	1.22955600	-4.04705100	-3.93388500
H	2.87748400	-4.63908700	-3.63228200
C	1.08116900	-5.66652700	-1.70578000
H	1.75942200	-6.44756700	-2.06868700
H	0.16809300	-5.71414900	-2.31060800
H	0.81729000	-5.90444200	-0.66879300
Mo	-0.18336300	-0.18919400	1.02046100
N	-1.66173600	-1.67679400	0.82088600
O	1.29085800	-1.69992700	1.06583700
O	1.72101000	-1.26133000	-1.08151100
S	-1.49710400	-1.52292400	-1.86510300
C	2.12806300	2.14778600	0.33375700
C	3.15356400	3.13825200	0.39628300
C	4.03602200	3.97588200	0.48412700
C	5.07032800	4.96485100	0.56694300
C	5.50750000	5.43775400	1.82175900
H	5.05332100	5.04345700	2.72532000
C	6.51556100	6.40384600	1.89614400
H	6.84798300	6.76388800	2.86500700
C	7.09799800	6.90773100	0.72310200
H	7.88118800	7.65757900	0.78355700
C	6.66734800	6.44042700	-0.52807900
H	7.11787400	6.82831400	-1.43662100
C	5.65947700	5.47476200	-0.60917000
H	5.32223800	5.10708300	-1.57338700
C	2.14214300	2.18506400	-2.08492300
C	2.82165500	1.31196700	-2.94920800
H	3.00741200	0.28929000	-2.63432900

C	3.25524500	1.77483200	-4.19879900
H	3.78448300	1.10058300	-4.86547100
C	3.00724800	3.09867300	-4.58807200
H	3.34025000	3.45311400	-5.55902000
C	2.31713000	3.96201900	-3.72253100
H	2.10955200	4.98424600	-4.02482600
C	1.88112300	3.50855500	-2.47254100
H	1.33032700	4.16396100	-1.80553600
C	-1.98099500	1.94817500	0.00620100
C	-3.04235300	2.99269900	0.01679000
C	-4.16800500	2.85898700	-0.83591300
C	-5.15641400	3.84707200	-0.78395500
H	-6.02407900	3.75542300	-1.42869000
C	-5.05907900	4.95071800	0.07923000
C	-3.93514000	5.05410800	0.90382800
H	-3.85039300	5.90890500	1.56927900
C	-2.91252800	4.09127100	0.89198000
C	-4.34732200	1.62222600	-1.71574300
H	-3.35802400	1.28062300	-2.03246600
C	-5.16491600	1.88146800	-2.99224400
H	-4.76130600	2.72476500	-3.56412400
H	-5.13683100	0.99208000	-3.63209100
H	-6.21889600	2.08898400	-2.77061900
C	-4.99315400	0.48490400	-0.89008300
H	-6.00237100	0.76848600	-0.56572600
H	-5.06645800	-0.42915500	-1.49046900
H	-4.40471700	0.25182400	0.00463800
C	-6.14836000	6.01395900	0.11829300
H	-5.85197700	6.76434800	0.86368500
C	-6.28698900	6.73332100	-1.23927900
H	-7.04198200	7.52658800	-1.17961800
H	-5.33710800	7.18413400	-1.54745400
H	-6.59653900	6.03429900	-2.02531700
C	-7.50239300	5.42349600	0.56277400
H	-7.42051900	4.93655300	1.54089500
H	-8.26193100	6.21156100	0.63248900
H	-7.86058300	4.67594500	-0.15500500
C	-1.70931000	4.26319700	1.81690200
H	-0.93634400	3.54170400	1.53650700
C	-2.10137600	3.95021300	3.27607300
H	-2.48254200	2.92733500	3.35986000
H	-1.22963600	4.04698400	3.93405100
H	-2.87752400	4.63908300	3.63237500
C	-1.08108100	5.66640000	1.70591600
H	-1.75930900	6.44747400	2.06880200
H	-0.16801100	5.71398500	2.31075700

H	-0.81717800	5.90428700	0.66893100
Mo	0.18327800	0.18910500	-1.02045500
N	1.66166600	1.67670600	-0.82089300
O	-1.29093400	1.69986200	-1.06582100
O	-1.72107600	1.26126700	1.08153100
S	1.49704200	1.52284300	1.86510300

11. References

- (1) Adamo, C.; Jacquemin, D. The calculations of excited-state properties with Time-Dependent Density Functional Theory. *Chemical Society Reviews* **2013**, 42 (3), 845-856.
- (2) Brémond, É. A. G.; Kieffer, J.; Adamo, C. A reliable method for fitting TD-DFT transitions to experimental UV–visible spectra. *Journal of Molecular Structure: THEOCHEM* **2010**, 954 (1), 52-56.
- (3) Guillaumont, D.; Nakamura, S. Calculation of the absorption wavelength of dyes using time-dependent density-functional theory (TD-DFT). *Dyes and Pigments* **2000**, 46 (2), 85-92.
- (4) Martynov, A. G.; Mack, J.; May, A. K.; Nyokong, T.; Gorbunova, Y. G.; Tsivadze, A. Y. Methodological Survey of Simplified TD-DFT Methods for Fast and Accurate Interpretation of UV–Vis–NIR Spectra of Phthalocyanines. *ACS Omega* **2019**, 4 (4), 7265-7284. DOI: 10.1021/acsomega.8b03500.
- (5) Latouche, C.; Skouteris, D.; Palazzetti, F.; Barone, V. TD-DFT Benchmark on Inorganic Pt(II) and Ir(III) Complexes. *Journal of Chemical Theory and Computation* **2015**, 11 (7), 3281-3289. DOI: 10.1021/acs.jctc.5b00257.
- (6) Farshad, M.; Perera, D. C.; Rasaiah, J. C. Theoretical study of the stability, structure, and optical spectra of small silver clusters and their formation using density functional theory. *Physical Chemistry Chemical Physics* **2021**, 23 (45), 25507-25517, 10.1039/D1CP04070G. DOI: 10.1039/D1CP04070G.
- (7) Powers, I. G.; Andjaba, J. M.; Luo, X.; Mei, J.; Uyeda, C. Catalytic Azoarene Synthesis from Aryl Azides Enabled by a Dinuclear Ni Complex. *Journal of the American Chemical Society* **2018**, 140 (11), 4110-4118.
- (8) Shields, D. J.; Elkoush, T.; Miura-Stempel, E.; Mak, C. L.; Niu, G.-H.; Gudmundsdottir, A. D.; Campbell, M. G. Visible Light Absorption and Long-Lived Excited States in Dinuclear Silver(I) Complexes with Redox-Active Ligands. *Inorganic Chemistry* **2020**, 59 (24), 18338-18344.
- (9) Kataoka, Y.; Imasaki, N.; Yano, N.; Mitsumi, M.; Handa, M. Redox-triggered reversible modulation of intense near-infrared and visible absorption using a paddlewheel-type diruthenium(III) complex. *Dalton Transactions* **2021**, 50 (27), 9547-9553, 10.1039/D1DT01681D.
- (10) Jiang, C.; Young, P. J.; Durr, C. B.; Spilker, T. F.; Chisholm, M. H. Synthesis, Structure, and Photophysical Properties of Mo₂(NN)₄ and Mo₂(NN)₂(TiPB)₂, Where NN = N,N'-Diphenylphenylpropiolamidinate and TiPB = 2,4,6-Triisopropylbenzoate. *Inorganic Chemistry* **2016**, 55 (12), 5836-5844.

- (11) Huang, J.; Gallucci, J. C.; Turro, C. Panchromatic dirhodium photocatalysts for dihydrogen generation with red light. *Chemical Science* **2020**, 11 (36), 9775-9783.
- (12) Millet, A.; Xue, C.; Song, E.; Turro, C.; Dunbar, K. R. Synthetic Strategies for Trapping the Elusive trans-Dirhodium(II,II) Formamidinate Isomer: Effects of Cis versus Trans Geometry on the Photophysical Properties. *Inorganic Chemistry* **2020**, 59 (4), 2255-2265.
- (13) Whittemore, T. J.; Millet, A.; Sayre, H. J.; Xue, C.; Dolinar, B. S.; White, E. G.; Dunbar, K. R.; Turro, C. Tunable Rh₂ (II, II) light absorbers as excited-state electron donors and acceptors accessible with red/near-infrared irradiation. *Journal of the American Chemical Society* **2018**, 140 (15), 5161-5170.
- (14) Li, Z.; Leed, N. A.; Dickson-Karn, N. M.; Dunbar, K. R.; Turro, C. Directional charge transfer and highly reducing and oxidizing excited states of new dirhodium(ii,ii) complexes: potential applications in solar energy conversion. *Chemical Science* **2014**, 5 (2), 727-737, 10.1039/C3SC52366G.
- (15) Jiang, C.; Young, P. J.; Brown-Xu, S.; Gallucci, J. C.; Chisholm, M. H. Femtosecond Study of Dimolybdenum Paddlewheel Compounds with Amide/Thioamide Ligands: Symmetry, Electronic Structure, and Charge Distribution in the 1MLCT S₁ State. *Inorganic Chemistry* **2017**, 56 (3), 1433-1445. DOI: 10.1021/acs.inorgchem.6b02517.
- (16) GaussView, Version 6, Dennington, Roy; Keith, Todd A.; Millam, John M. Semichem Inc., Shawnee Mission, KS, 2016.