

Diarylethene-containing Carbon-Rich Ruthenium Organometallics: Tuning of Electrochromism

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Supporting Information

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1. ^{31}P and ^1H NMR data

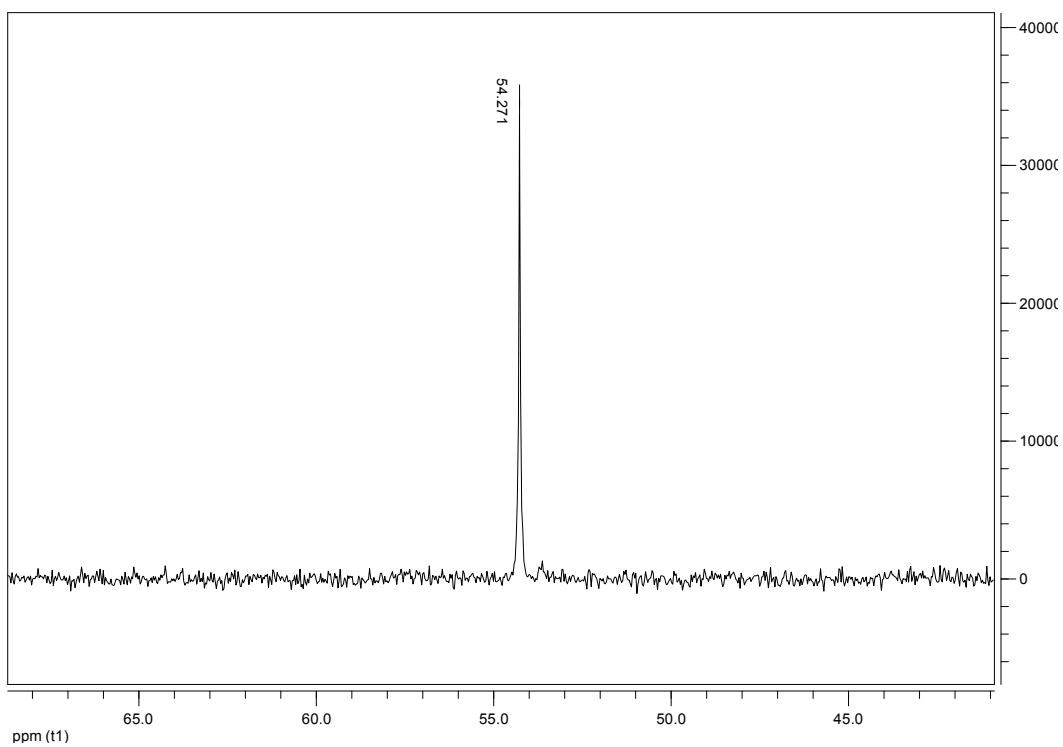
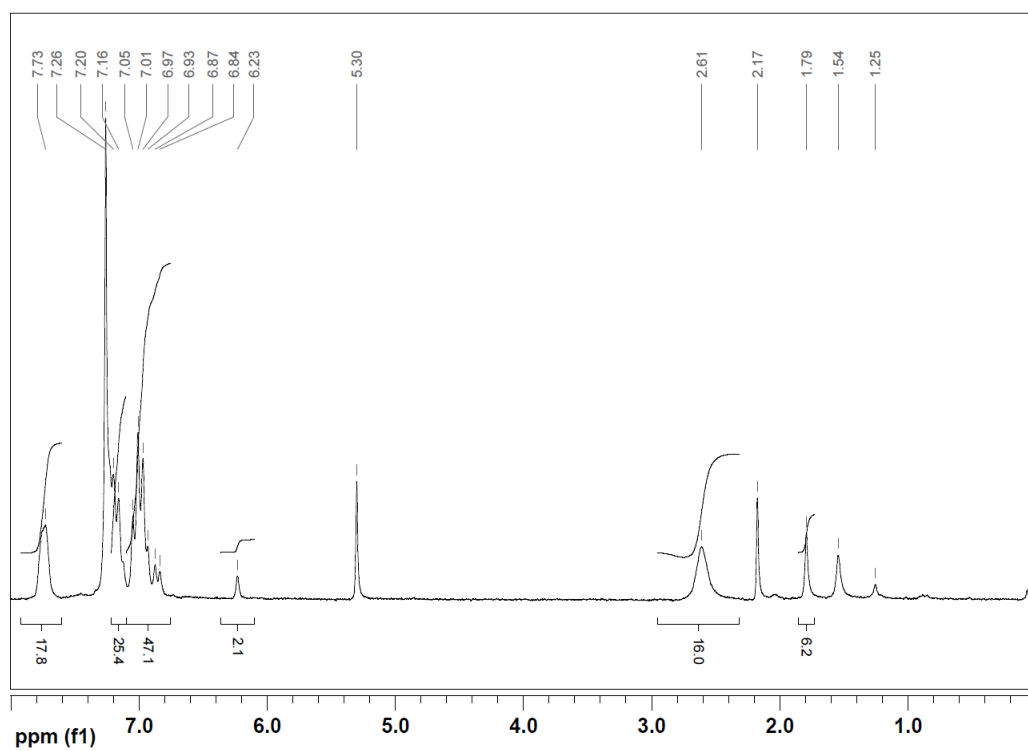


Figure S1. ^1H (up) and ^{31}P NMR spectra of **1o** in CDCl_3

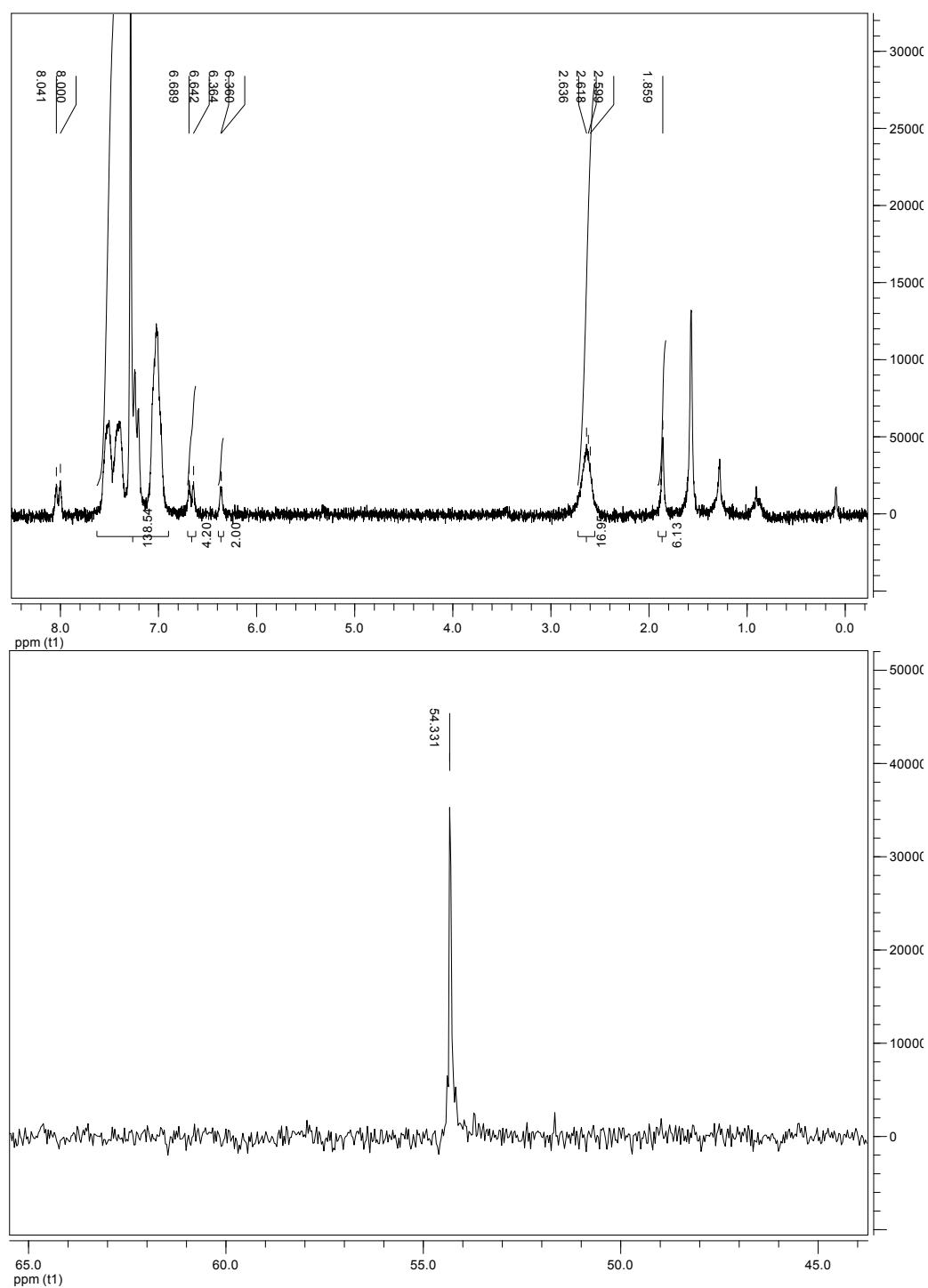


Figure S2. ^1H (up) and ^{31}P (bottom) NMR spectra of **2o** in CDCl_3

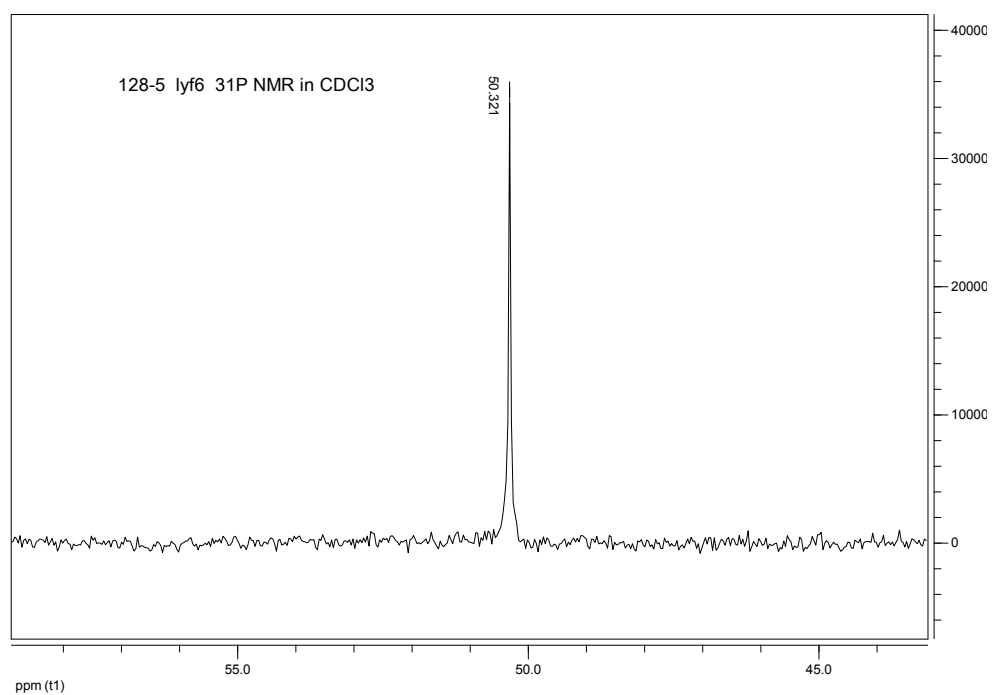
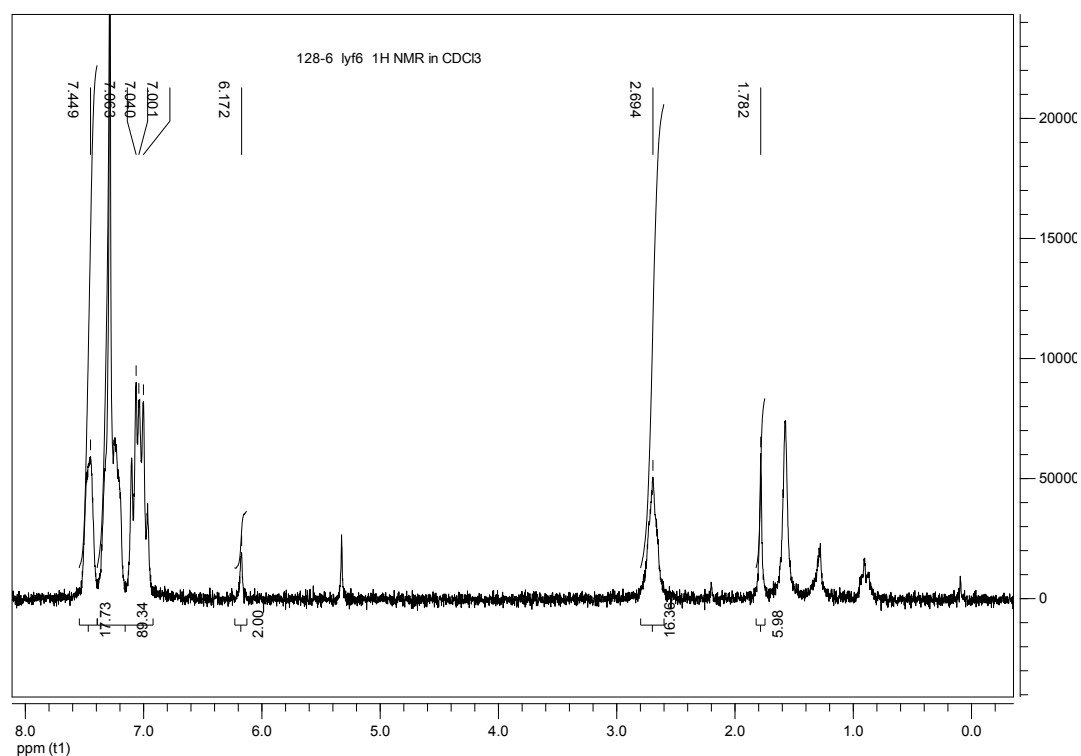


Figure S3. ^1H (up) and ^{31}P (bottom) NMR spectra of **3o** in CDCl_3

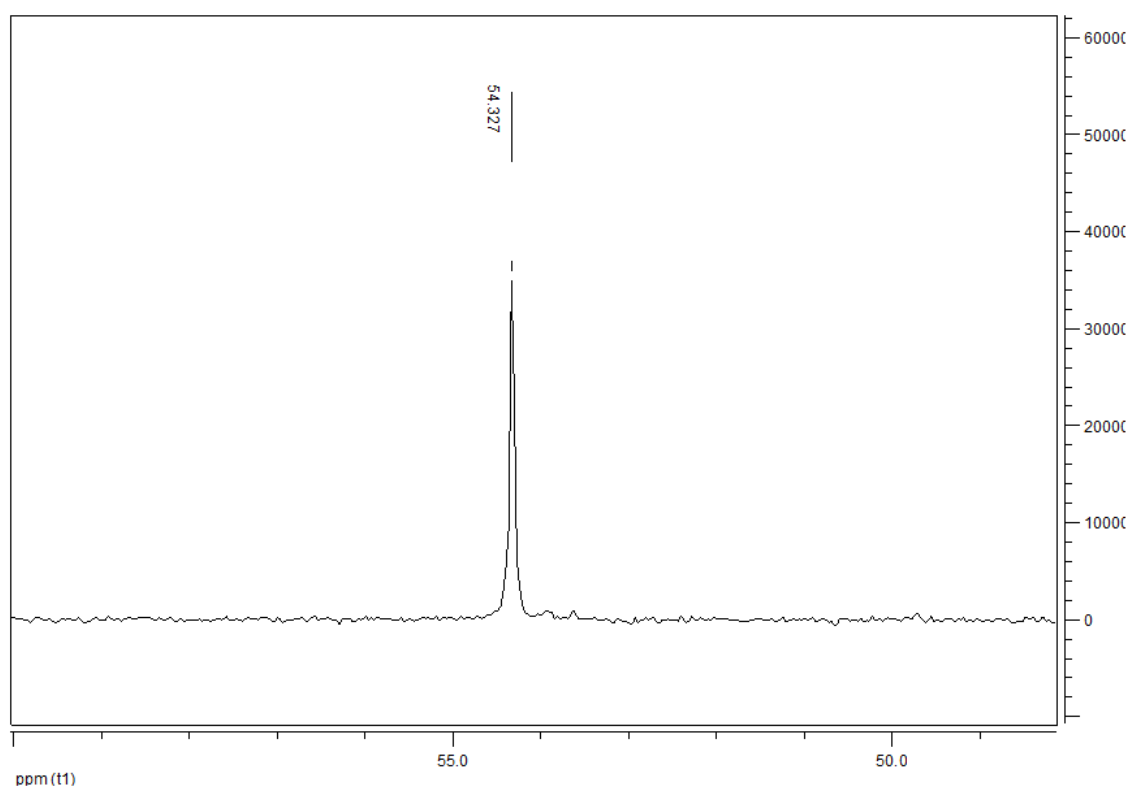


Figure S4. ^1H (up) and ^{31}P (bottom) NMR spectra of **4o** in CD_2Cl_2

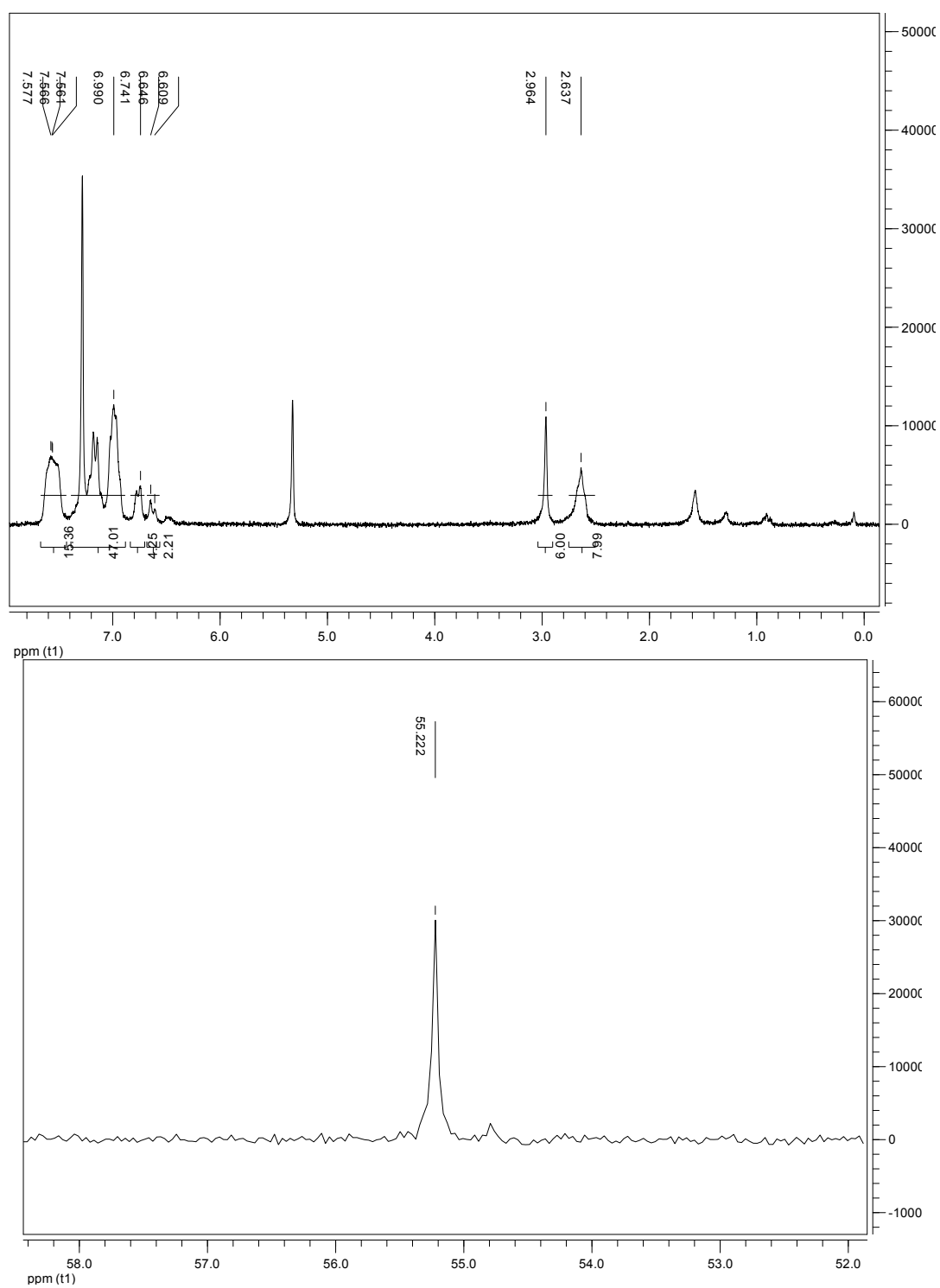


Figure S6. ^1H (up) and ^{31}P (bottom) NMR spectra of **6** in CDCl_3

2. UV-vis data.

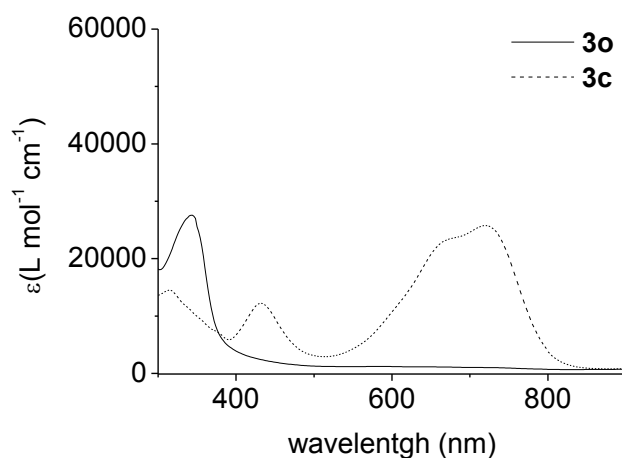


Fig.S7 UV-Vis absorption spectra of **3o** and spectral changes upon 350 nm irradiation (CH_2Cl_2).

Table S1. UV-Vis data and photochromic ring-opening/closing times for compounds **1-4** in toluene. The initial spectrum was recovered after bleaching at 750 nm.

	UV-Vis data, λ_{max} / nm (ϵ / $\text{L} \cdot \text{mol}^{-1} \text{cm}^{-1}$)	closing/opening time (min)
1o	348 (59620)	$\approx 1 / 120$
1c	320 (44300), 444 (15374), 684 (36275) (sh), 716 (40336)	
2o	340 (26109), 462 (28358)	$\approx 1 / 350$
2c	318 (15775), 450 (28478), 676 (22282) (sh), 710 (24090)	
3o	346 (17822)	$\approx 1 / 210$
3c	316 (9859), 434 (8282), 688 (16064) (sh), 722 (18238)	
4o	312 (46496), 346 (51536)	$\approx 1 / 90$
4c	310 (47474), 450 (10067), 690 (28934) (sh), 722 (32726)	

$[\text{c}] \approx 4 \times 10^{-5} \text{ mol} \cdot \text{L}^{-1}$.

3. Isomerization: ^{31}P and ^1H NMR studies

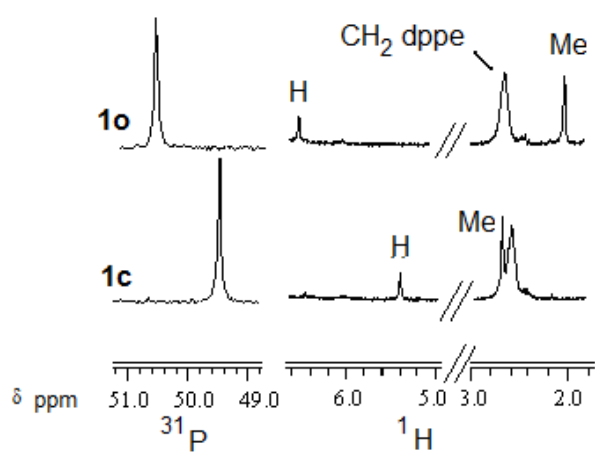


Figure S8. ^{31}P and selected ^1H NMR signals in C_6D_6 of **3o** and of **3c** after excitation at 350 nm. Initial spectra were recovered after bleaching at 750 nm.

4. Electrochemistry

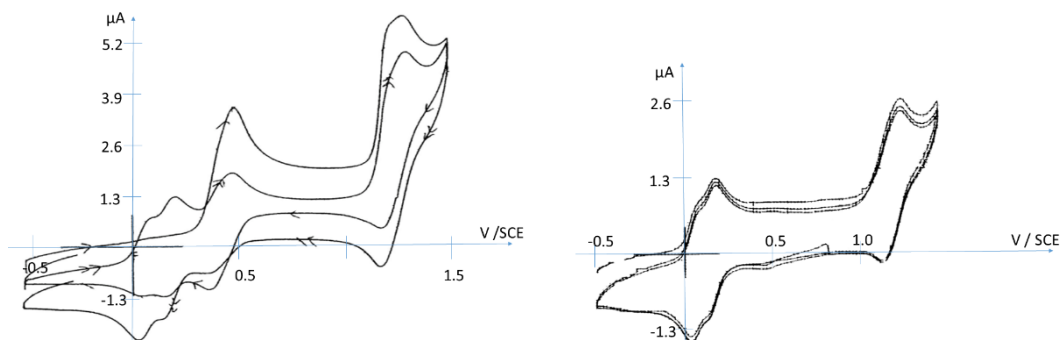


Fig. S9. Cyclic voltammetry of **1o** in CH_2Cl_2 ($0.2 \text{ mol.L}^{-1} \text{ Bu}_4\text{NPF}_6$) at 0.1 V.s^{-1} during the macroelectrolysis (Pt electrode). Left: initial CV (single arrow) and after the consumption of 1 e^- per mol (double arrow). Right: after the consumption of 2 e^- per mol (total macroelectrolysis) and the corresponding further two-electron reduction.

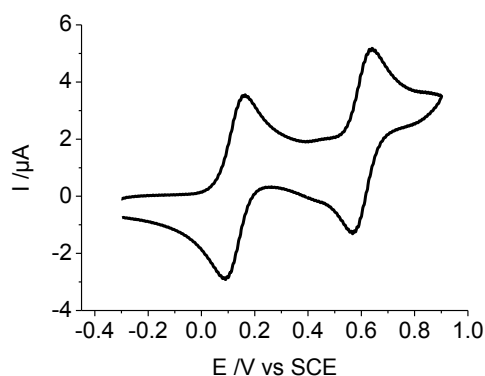


Fig. S10: CV of **6** ($[c] = 2.10^{-3} \text{ mol L}^{-1}$) in CH_2Cl_2 ($0.2 \text{ mol.L}^{-1} \text{ Bu}_4\text{NPF}_6$, $v = 0.2 \text{ V.s}^{-1}$) at a Pt electrode.

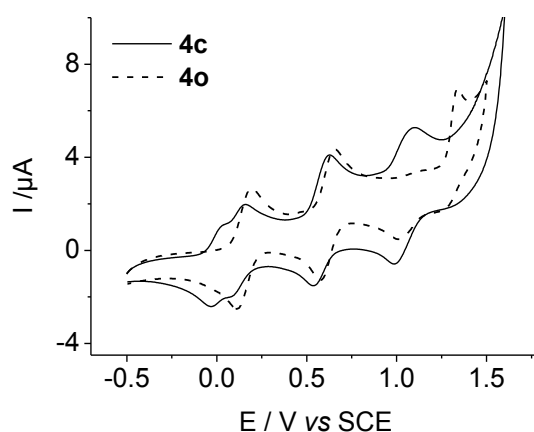


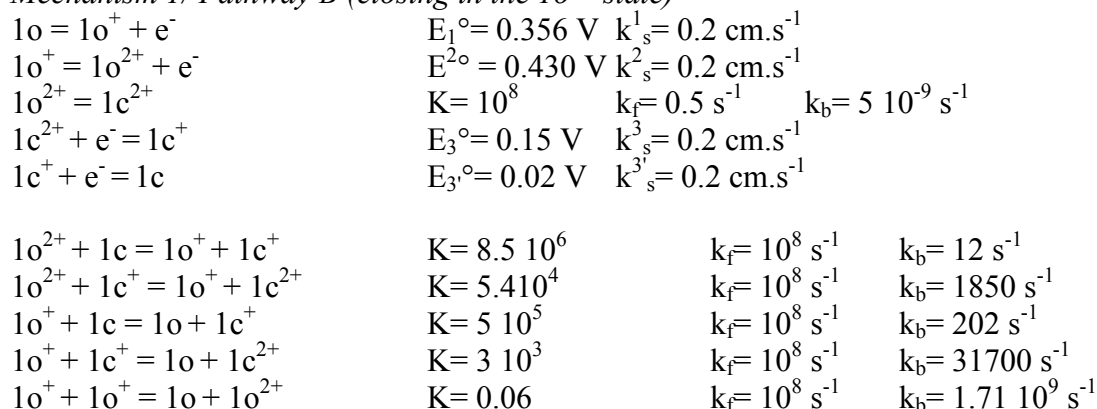
Fig. S11: CV of **4o** and **4c** after UV irradiation at $\lambda_{\text{max}} = 350 \text{ nm}$ ($[c] = 7.10^{-4} \text{ mol L}^{-1}$) in CH_2Cl_2 ($0.2 \text{ mol.L}^{-1} \text{ Bu}_4\text{NPF}_6$, $v = 0.2 \text{ V.s}^{-1}$) at a Pt electrode.

Study of the mechanism: Numerical simulations.

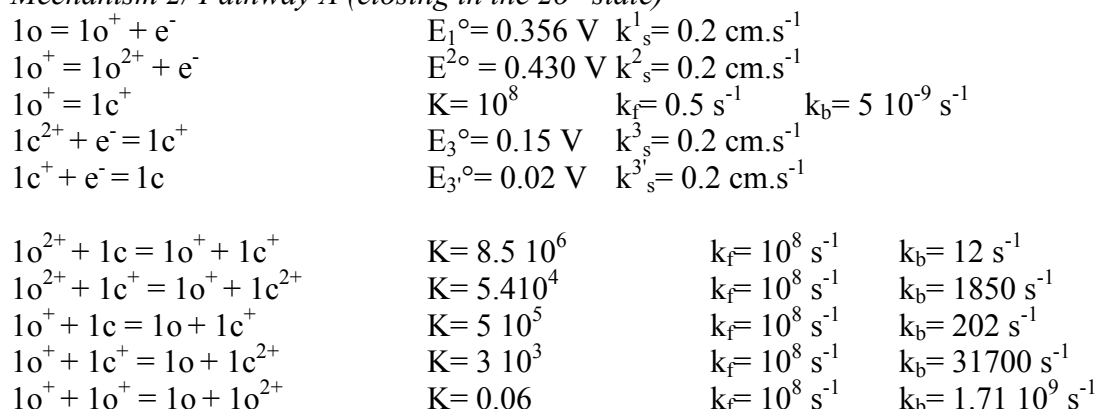
Two distinct mechanisms were tested for **1o**, **2o** and **3o**

A) Compound 1o

Mechanism 1/ Pathway B (closing in the 1o²⁺ state)

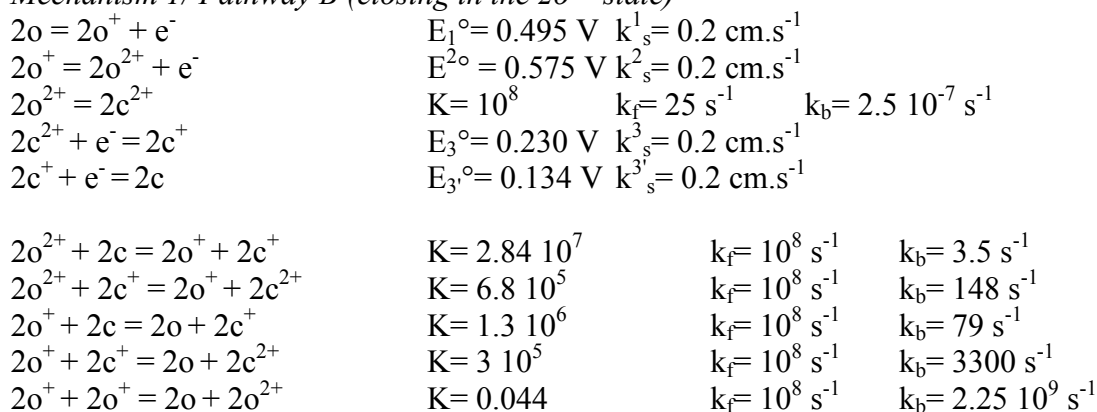


Mechanism 2/ Pathway A (closing in the 2o⁺ state)



B) Compound 2o

Mechanism 1/ Pathway B (closing in the 2o²⁺ state)



Mechanism 2/ Pathway A (closing in the 2o⁺ state)

$2o = 2o^+ + e^-$	$E_1^\circ = 0.495 \text{ V}$	$k_s^1 = 0.2 \text{ cm.s}^{-1}$	
$2o^+ = 2o^{2+} + e^-$	$E_2^\circ = 0.575 \text{ V}$	$k_s^2 = 0.2 \text{ cm.s}^{-1}$	
$2o^+ = 2c^+$	$K = 10^8$	$k_f = 25 \text{ s}^{-1}$	$k_b = 2.5 \cdot 10^{-7} \text{ s}^{-1}$
$2c^{2+} + e^- = 2c^+$	$E_3^\circ = 0.230 \text{ V}$	$k_s^3 = 0.2 \text{ cm.s}^{-1}$	
$2c^+ + e^- = 2c$	$E_{3'}^\circ = 0.134 \text{ V}$	$k_s^{3'} = 0.2 \text{ cm.s}^{-1}$	
$2o^{2+} + 2c = 2o^+ + 2c^+$	$K = 2.84 \cdot 10^7$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 3.5 \text{ s}^{-1}$
$2o^{2+} + 2c^+ = 2o^+ + 2c^{2+}$	$K = 6.8 \cdot 10^5$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 148 \text{ s}^{-1}$
$2o^+ + 2c = 2o + 2c^+$	$K = 1.3 \cdot 10^6$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 79 \text{ s}^{-1}$
$2o^+ + 2c^+ = 2o + 2c^{2+}$	$K = 3 \cdot 10^5$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 3300 \text{ s}^{-1}$
$2o^+ + 2o^+ = 2o + 2o^{2+}$	$K = 0.044$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 2.25 \cdot 10^9 \text{ s}^{-1}$

C) Compound 3o

Mechanism 1/ Pathway B (closing in the 3o²⁺ state)

$3o = 3o^+ + e^-$	$E_1^\circ = 0.405 \text{ V}$	$k_s^1 = 0.2 \text{ cm.s}^{-1}$	
$3o^+ = 3o^{2+} + e^-$	$E_2^\circ = 0.490 \text{ V}$	$k_s^2 = 0.2 \text{ cm.s}^{-1}$	
$3o^{2+} = 3c^{2+}$	$K = 10^8$	$k_f = 15 \text{ s}^{-1}$	$k_b = 1.5 \cdot 10^{-7} \text{ s}^{-1}$
$3c^{2+} + e^- = 3c^+$	$E_3^\circ = 0.130 \text{ V}$	$k_s^3 = 0.2 \text{ cm.s}^{-1}$	
$3c^+ + e^- = 3c$	$E_{3'}^\circ = 0.009 \text{ V}$	$k_s^{3'} = 0.2 \text{ cm.s}^{-1}$	
$3o^{2+} + 3c = 3o^+ + 3c^+$	$K = 1.35 \cdot 10^8$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 0.74 \text{ s}^{-1}$
$3o^{2+} + 3c^+ = 3o^+ + 3c^{2+}$	$K = 1.21 \cdot 10^6$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 83 \text{ s}^{-1}$
$3o^+ + 3c = 3o + 3c^+$	$K = 4.9 \cdot 10^6$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 20 \text{ s}^{-1}$
$3o^+ + 3c^+ = 3o + 3c^{2+}$	$K = 4.4 \cdot 10^5$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 2250 \text{ s}^{-1}$
$3o^+ + 3o^+ = 3o + 3o^{2+}$	$K = 0.037$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 2.7 \cdot 10^9 \text{ s}^{-1}$

Mechanism 2/ Pathway A (closing in the 1o⁺ state)

$3o = 3o^+ + e^-$	$E_1^\circ = 0.405 \text{ V}$	$k_s^1 = 0.2 \text{ cm.s}^{-1}$	
$3o^+ = 3o^{2+} + e^-$	$E_2^\circ = 0.490 \text{ V}$	$k_s^2 = 0.2 \text{ cm.s}^{-1}$	
$3o^+ = 3c^+$	$K = 10^8$	$k_f = 1.5 \text{ s}^{-1}$	$k_b = 1.5 \cdot 10^{-8} \text{ s}^{-1}$
$3c^{2+} + e^- = 3c^+$	$E_3^\circ = 0.130 \text{ V}$	$k_s^3 = 0.2 \text{ cm.s}^{-1}$	
$3c^+ + e^- = 3c$	$E_{3'}^\circ = 0.009 \text{ V}$	$k_s^{3'} = 0.2 \text{ cm.s}^{-1}$	
$3o^{2+} + 3c = 3o^+ + 3c^+$	$K = 1.35 \cdot 10^8$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 0.74 \text{ s}^{-1}$
$3o^{2+} + 3c^+ = 3o^+ + 3c^{2+}$	$K = 1.21 \cdot 10^6$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 83 \text{ s}^{-1}$
$3o^+ + 3c = 3o + 3c^+$	$K = 4.9 \cdot 10^6$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 20 \text{ s}^{-1}$
$3o^+ + 3c^+ = 3o + 3c^{2+}$	$K = 4.4 \cdot 10^5$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 2250 \text{ s}^{-1}$
$3o^+ + 3o^+ = 3o + 3o^{2+}$	$K = 0.037$	$k_f = 10^8 \text{ s}^{-1}$	$k_b = 2.7 \cdot 10^9 \text{ s}^{-1}$

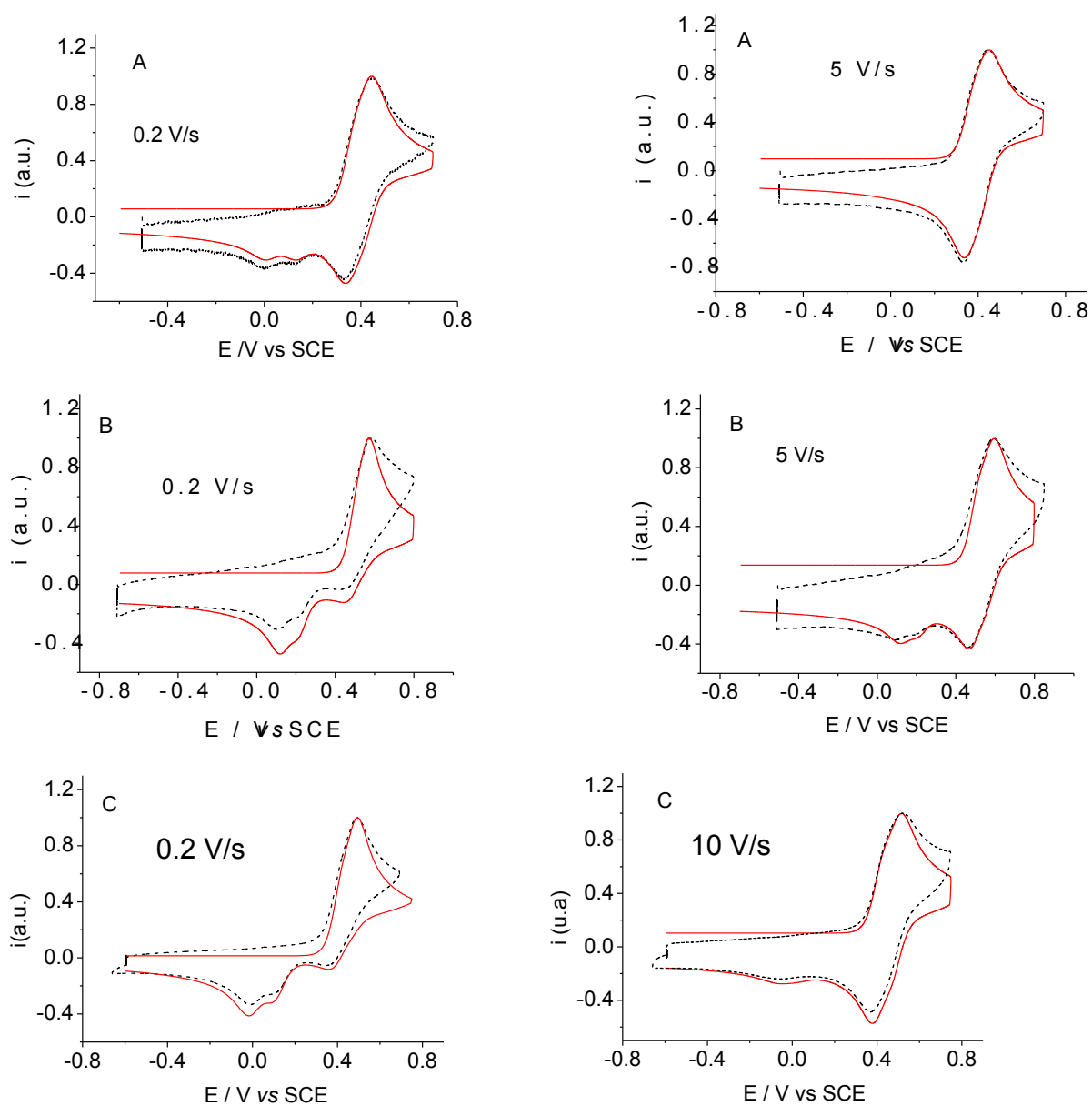


Figure S12. Cyclic voltammetry of **1o** (A), **2o** (B) and **3o** (C) in CH_2Cl_2 (0.2 mol.L^{-1} Bu_4NPF_6) on a Pt disk electrode at different scan rates. Black dashed line : experimental data. Red solid line: simulation according pathway B (mechanism 1).

5. Spectroelectrochemical studies.

A) Detailed spectroelectrochemical experiment for **1o** (0.2 mol.L⁻¹ Bu₄NPF₆ in CH₂Cl₂).

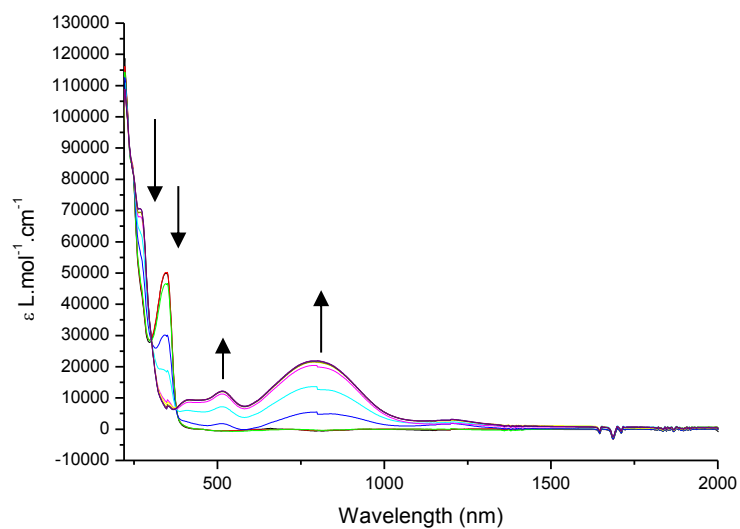


Fig. S13 UV-Vis-NIR absorption spectra obtained for oxidation of **1o** to **1c²⁺**.

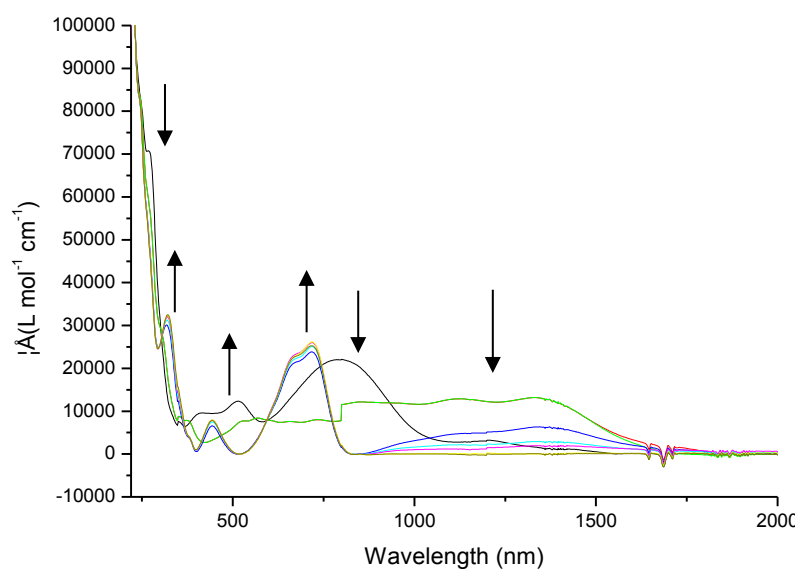


Fig. S14 UV-Vis-NIR absorption spectra obtained for reduction of **1c²⁺** to **1c** (via **1c⁺**).

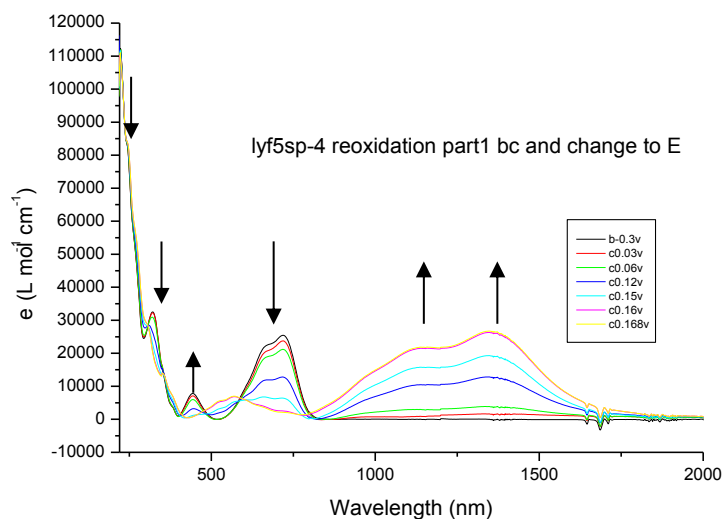


Fig. S15 UV-Vis-NIR absorption spectra obtained for oxidation of **1c** to **1c⁺**.

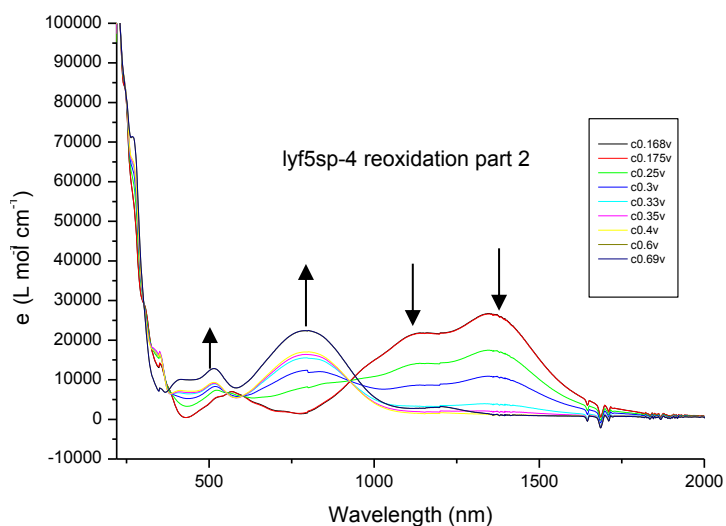


Fig. S16 UV-Vis-NIR absorption spectra obtained for oxidation of **1c⁺** to **1c²⁺**.

B) Detailed spectroelectrochemical experiment for **6 (0.2 mol.L⁻¹ Bu₄NPF₆ in CH₂Cl₂).**

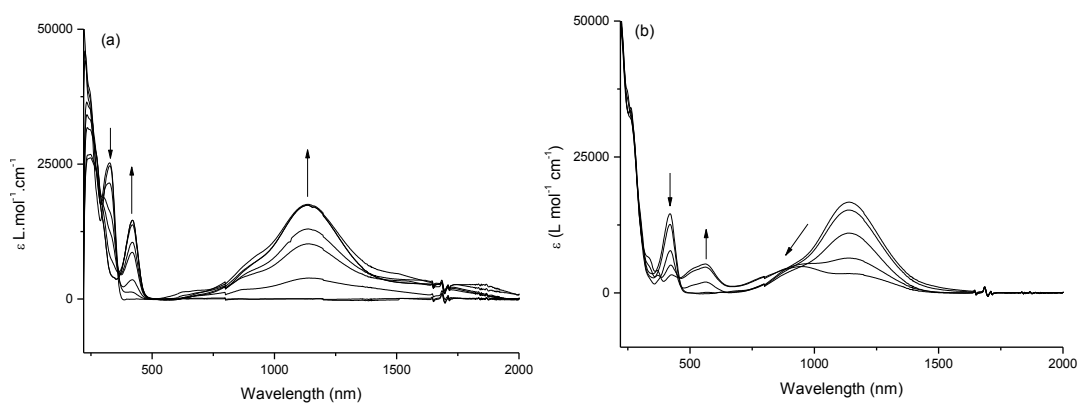


Fig. S17 UV-Vis-NIR absorption spectra obtained for oxidation of **6** to **6⁺** (left), and of **6⁺** to **6²⁺** (right).

6. EPR Spectroscopy.

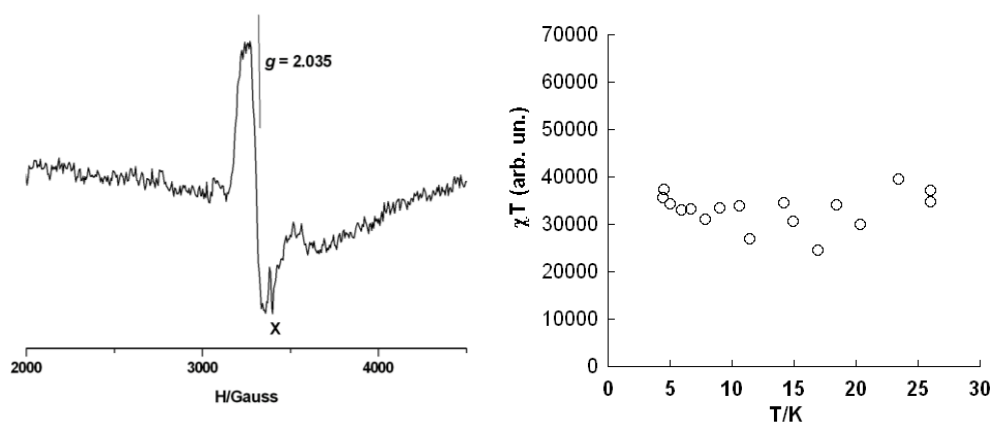


Figure S18 : (a) X-band EPR spectrum of 40^{2+} in a frozen solution at 4K in CH_2Cl_2 (peak caused by cavity impurity is marked by X), and (b) temperature dependence of the integrated EPR absorption.

7. Theoretical calculations.

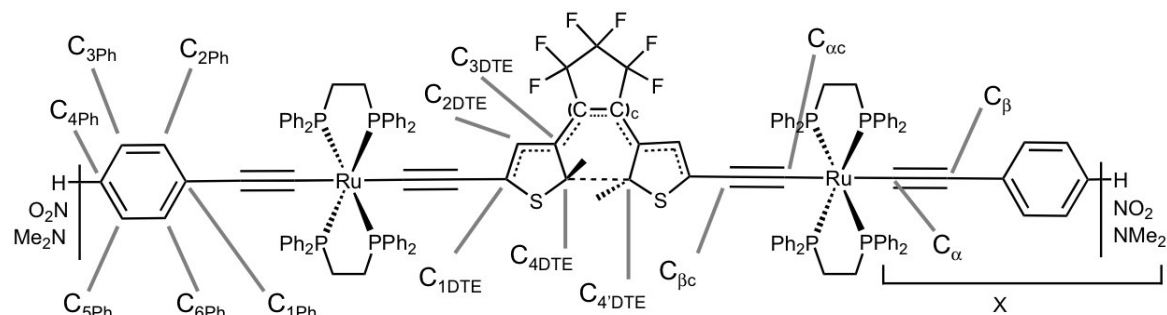


Table S2. Main distances of the optimized (DFT) geometries **1-3o/c**^{0/2+} and **4o/c**^{0/+2+/4+}. Distances in Å; Angles in °. In the cases for which the distances of each branch of the molecule diverge of less than 0.002 Å, the mean value is given.

compd	Ru-C _{αc}	C _{αc} -C _{βc}	C _{βc} -C _{1DTE}	C _{1DTE} -C _{2DTE}	C _{2DTE} -C _{3DTE}	C _{3DTE} -C _c	(C=C) _c	Ru-C _α	C _α C _β	Ru-Cl	C _{βc} -C _{1Ph}	C _{1Ph} -C _{2Ph}	C _{2Ph} -C _{3Ph}	C _{3Ph} -C _{4Ph}	C _{4Ph} -C _{5Ph}	C _{5Ph} -C _{6Ph}	C _{6Ph} -C _{1Ph}	C _{4Ph} -N
6	2.087	1.237						2.094	1.236		1.427	1.413	1.391	1.415	1.415	1.392	1.413	1.402
1o	2.097	1.239	1.404	1.382	1.433	1.462	1.375	2.107	1.237		1.428	1.416	1.394	1.400	1.400	1.395	1.415	
1o ²⁺ HS	2.056	1.248	1.391	1.391	1.421	1.465	1.368	2.064	1.247		1.415	1.420	1.390	1.402	1.402	1.390	1.420	
2o	2.100	1.239	1.405	1.382	1.433	1.464	1.375	2.090	1.240		1.416	1.420	1.387	1.401	1.401	1.387	1.421	1.460
2o ²⁺ HS	2.046	1.251	1.388	1.394	1.418	1.468	1.368	2.070	1.245		1.417	1.419	1.388	1.397	1.397	1.387	1.419	1.485
3o	2.030	1.238	1.405	1.386	1.423	1.481	1.354			2.564								
3o ²⁺ HS	1.958	1.257	1.380	1.399	1.413	1.469	1.365			2.498								
4o	2.093	1.238	1.403	1.382	1.433	1.465	1.373	2.110	1.237		1.427	1.412	1.391	1.415	1.415	1.391	1.412	1.401
4o ⁺	2.080	1.240	1.401	1.386	1.428	1.463	1.366	2.081	1.242		1.416	1.419	1.385	1.422	1.422	1.385	1.419	1.377
4o ²⁺ HS	2.078	1.243	1.398	1.385	1.426	1.465	1.369	2.056	1.249		1.404	1.424	1.379	1.427	1.427	1.378	1.424	1.368
4o ⁴⁺ HS	2.033	1.257	1.382	1.400	1.413	1.468	1.368	2.069	1.250		1.402	1.428	1.374	1.433	1.433	1.374	1.429	1.359
	2.060	1.250	1.389	1.395	1.417	1.471		2.021	1.260		1.386	1.437	1.368	1.440	1.439	1.368	1.436	1.349
1c	2.083	1.243	1.395	1.388	1.408	1.381	1.442	2.107	1.237		1.428	1.415	1.395	1.399	1.400	1.395	1.415	
1c ²⁺ LS	2.012	1.262	1.365	1.430	1.368	1.423	1.383	2.094	1.240		1.423	1.416	1.392	1.401	1.401	1.392	1.416	
2c	2.083	1.242	1.395	1.387	1.409	1.380	1.442	2.094	1.239		1.417	1.420	1.387	1.400	1.400	1.387	1.420	1.462
2c ²⁺ LS	1.994	1.255	1.351	1.441	1.353	1.438	1.360	2.104	1.222		1.427	1.407	1.385	1.389	1.389	1.385	1.407	1.476
3c	2.013	1.242	1.394	1.388	1.410	1.381	1.444			2.557								
3c ²⁺ LS	1.934	1.266	1.357	1.441	1.362	1.434	1.374			2.515								
4c	2.078	1.243	1.394	1.388	1.409	1.382	1.444	2.110	1.237		1.427	1.412	1.391	1.416	1.416	1.391	1.413	1.399
4c ⁺	2.049	1.249	1.380	1.404	1.392	1.398	1.419	2.100	1.239		1.421	1.416	1.386	1.420	1.420	1.387	1.415	1.382
4c ²⁺ HS	2.054	1.249	1.381	1.407	1.390	1.400	1.413	2.082	1.247		1.395	1.422	1.380	1.426	1.426	1.380	1.422	1.370
4c ⁴⁺ HS	2.020	1.262	1.366	1.436	1.364	1.430	1.374	2.079	1.249		1.401	1.430	1.373	1.434	1.434	1.373	1.430	1.358

Table S3. Calculated relative energies of **1-3o/c-6**^{0/2+} and **4o/c**^{0/+2+/4+} in their different spin states using BP86 and B3LYP functionals.

cpd	funct.→ charge→	BP86				B3LYP			
		0	+	2+ (spin state)	4+ (spin state)	0	+	2+ (spin state)	4+ (spin state)
1o		0.000		12.691 (HS) 12.688 (BS)		0.000		12.714 (HS) 12.713 (BS)	
1c		0.230		12.622 (LS)		0.167		12.778 (LS)	
2o		0.000		13.464 (HS) 13.461 (BS)		0.000		13.481 (HS) 13.480 (BS)	
2c		0.220		13.333 (LS)		0.128		12.918 (LS)	
3o		0.000		13.060 (HS) 13.057 (BS)		0.000		13.031 (HS) 13.029 (BS)	
3c		0.243		12.791 (LS)		0.240		13.002 (LS)	
4o		0.000	4.957	11.604 (LS) 11.492 (HS) 11.491 (BS)	30.782 (LS) n. a. ^a n. a. ^a	0.000	5.196	12.081 (LS) 11.564 (HS) 11.564 (BS)	31.068 (LS) 30.754 (HS) ^b 30.762 (BS) ^b
4c		0.240	4.684	11.479 (LS) 11.444 (HS) 11.368 (BS)	30.777 (LS) 30.684 (HS) 30.709 (BS)	0.462	4.824	11.825 (LS) 11.582 (HS) 11.577 (BS)	31.086 (LS) 30.412 (HS) 30.412 (BS)
6		0.000	5.333	13.807 (LS) 13.901 (HS) 13.853 (BS)			5.385	13.987 (LS) 13.803 (HS) 13.773 (BS)	

^a SCF convergence was not reached. ^b Optimization performed at the B3LYP level.

Table S4. Mulliken atomic spin densities of **1-3o/c-6²⁺** and **4o/c^{2+/4+}** in their different spin states using BP86 and B3LYP functionals.

cpd	Ru	C _{αc}	C _{βc}	C _{1DTE}	C _{2DTE}	C _{3DTE}	C _{4DTE}	S	C _c	C _α	C _β	Cl	C _{1Ph}	C _{2Ph}	C _{3Ph}	C _{4Ph}	C _{5Ph}	C _{6Ph}	N	X ₁	X ₂
6⁺ _{BP86}	0.19	0.04	0.10							0.13	0.10		0.06	0.03	0.03	0.05	0.03	0.02	0.13	-0.01	
6⁺ _{B3LYP}	0.21	0.02	0.10							0.16	0.11		0.06	0.03	0.02	0.06	0.03	0.03	0.14	-0.01	
6²⁺ _{HS/BP86}																					
6²⁺ _{HS/B3LYP}	0.29	0.19	0.22							0.25	0.03		0.19	-0.03	0.11	0.04	0.11	-0.03	0.28	-0.02	
6²⁺ _{BS/BP86}																					
6²⁺ _{BS/B3LYP}	0.22	0.19	0.20							-0.28	0.06		-0.20	0.04	-0.11	-0.03	-0.11	0.04	-0.27	0.02	
1o²⁺ _{HS/BP86}	0.27	0.05	0.13	0.00	0.09	-0.01	0.10	0.00	0.00	0.07	0.15		0.00	0.06	-0.03	0.10	-0.03	0.06			
1o²⁺ _{HS/B3LYP}	0.34	0.02	0.14	-0.02	0.09	-0.02	0.10	0.00	0.00	0.06	0.16		-0.01	0.07	-0.04	0.10	-0.04	0.07			
1o²⁺ _{BS/BP86}	0.27	0.05	0.13	0.00	0.08	0.00	0.09	0.00	0.00	0.07	0.15		0.00	0.06	-0.03	0.10	-0.03	0.06			
1o²⁺ _{BS/B3LYP}	-0.27	-0.05	-0.13	0.00	-0.08	0.01	-0.09	0.00	0.00	-0.07	-0.15		0.00	-0.06	0.03	-0.10	0.03	-0.06			
1o²⁺ _{BS/B3LYP}	0.34	0.02	0.15	-0.02	0.09	-0.02	0.10	0.00	0.00	0.06	0.16		-0.01	0.07	-0.04	0.10	-0.04	0.07			
2o²⁺ _{HS/BP86}	-0.34	-0.02	-0.14	0.02	-0.09	0.02	-0.10	0.00	0.00	-0.06	-0.16		0.01	-0.07	0.04	-0.10	0.04	-0.07			
2o²⁺ _{HS/B3LYP}	0.28	0.07	0.15	0.01	0.10	-0.01	0.12	0.00	0.01	0.03	0.14		-0.01	0.05	-0.02	0.06	-0.02	0.05	0.00	0.01	0.01
2o²⁺ _{BS/BP86}	0.36	0.05	0.18	-0.01	0.12	-0.03	0.13	0.00	0.00	0.00	0.14		-0.03	0.05	-0.03	0.06	-0.03	0.05	0.00	0.01	0.01
2o²⁺ _{BS/B3LYP}	-0.28	-0.06	-0.15	0.01	-0.12	-0.03	-0.13	0.00	0.00	-0.01	-0.14		0.03	-0.06	0.03	-0.05	0.03	-0.05	0.00	-0.01	-0.01
2o²⁺ _{BS/B3LYP}	0.36	0.05	0.18	-0.01	0.12	-0.03	0.13	0.00	0.00	0.00	0.14		-0.03	0.05	-0.03	0.06	-0.03	0.05	0.00	0.01	0.01
3o²⁺ _{HS/BP86}	-0.37	-0.04	-0.17	0.02	-0.12	0.03	-0.13	0.00	0.00	-0.01	-0.14		0.03	-0.06	0.03	-0.05	0.03	-0.05	0.00	-0.01	-0.01
3o²⁺ _{HS/B3LYP}	0.34	0.08	0.22	0.01	0.15	-0.02	0.16	0.00	0.00			0.07									
3o²⁺ _{HS/B3LYP}	0.40	0.05	0.24	-0.03	0.16	-0.04	0.17	0.00	0.00			0.05									
3o²⁺ _{BS/BP86}	0.21	0.07	0.21	0.00	0.14	0.02	0.16	0.00	0.00			0.07									
3o²⁺ _{BS/B3LYP}	-0.21	-0.08	-0.21	0.00	-0.14	-0.02	-0.16	0.00	0.00			-0.07									
3o²⁺ _{BS/B3LYP}	0.40	0.05	0.24	-0.04	0.16	-0.04	0.17	0.00	0.01			0.05									
4o⁺ _{BP86}	-0.40	-0.05	-0.24	0.03	-0.16	0.04	-0.18	0.00	-0.01			-0.05									
4o⁺ _{B3LYP}	0.08	0.01	0.04	0.00	0.02	0.00	0.03	0.00	0.00	0.07	0.05		0.03	0.01	0.02	0.02	0.02	0.01	0.07	-0.01	-0.01
4o²⁺ _{HS/BP86}	0.08	0.01	0.03	0.00	0.02	0.00	0.03	0.00	0.00	0.09	0.04		0.04	0.01	0.02	0.03	0.02	0.01	0.08	0.00	0.00
4o²⁺ _{HS/B3LYP}	0.18	0.02	0.07	0.00	0.05	0.00	0.05	0.00	0.00	0.10	0.10		0.07	0.02	0.03	0.06	0.05	0.03	0.14	-0.01	-0.01
4o²⁺ _{BS/BP86}	0.20	0.00	0.06	-0.01	0.04	-0.01	0.04	0.00	0.00	0.17	0.10		0.08	0.03	0.04	0.06	0.04	0.04	0.15	-0.01	-0.01
4o²⁺ _{BS/B3LYP}	0.18	0.02	0.07	0.00	0.05	0.00	0.05	0.00	0.00	0.14	0.10		0.07	0.02	0.04	0.05	0.04	0.02	0.14	-0.01	-0.01
4o²⁺ _{BS/B3LYP}	-0.18	-0.02	-0.07	0.01	-0.05	0.00	-0.05	0.00	0.00	-0.14	-0.10		-0.07	-0.02	-0.04	-0.05	-0.04	-0.02	-0.14	0.01	0.01
4o⁴⁺ _{HS/B3LYP^a}	0.19	0.00	0.06	-0.01	0.04	-0.01	0.04	0.00	0.00	0.17	0.10		0.08	0.03	0.03	0.06	0.03	0.03	0.15	-0.01	-0.01
4o⁴⁺ _{HS/B3LYP^a}	-0.20	0.00	-0.06	0.01	-0.04	0.01	-0.04	0.00	0.00	-0.17	-0.10		-0.08	-0.03	-0.03	-0.06	-0.03	-0.03	-0.15	0.01	0.01
4o⁴⁺ _{BS/B3LYP}	0.34	0.13	0.20	0.01	0.15	-0.03	0.20	-0.01	0.00	0.24	0.03		0.21	-0.02	0.13	0.02	0.12	-0.05	0.31	-0.02	-0.02
4o⁴⁺ _{BS/B3LYP}	0.29	0.09	0.15	0.01	0.11	-0.02	0.14	-0.01	0.00	-0.25	0.12		-0.20	0.06	-0.11	0.00	-0.11	0.06	-0.25	-0.02	-0.02
4o⁴⁺ _{BS/B3LYP}	-0.28	-0.14	-0.19	-0.01	-0.15	0.03	-0.20	0.01	0.00	0.29	-0.10		0.22	-0.05	0.13	0.02	0.13	-0.05	0.31	-0.02	-0.02
4c⁺ _{BP86}	-0.25	0.09	0.15	0.01	0.11	-0.02	0.14	-0.01	0.00	-0.25	0.11		-0.20	0.06	-0.11	0.00	-0.11	0.06	-0.25	0.02	0.02
4c⁺ _{B3LYP}	0.05	0.04	0.02	0.02	0.07	0.02	0.00	0.04	0.08	0.03	0.02		0.02	0.00	0.01	0.01	0.01	0.00	0.04	0.00	0.00
4c⁺ _{B3LYP}	0.05	0.07	0.02	0.03	0.08	0.02	0.00	0.04	0.10	0.02	0.02		0.01	0.00	0.00	0.01	0.00	0.00	0.02	0.00	0.00

$4\mathbf{c}^{2+}$ HS/BP86	0.08	0.05	0.02	0.04	0.07	0.04	0.00	0.06	0.10	0.13	0.04	0.08	0.00	0.05	0.03	0.05	0.00	0.14	-0.01	-0.01
$4\mathbf{c}^{2+}$ HS/B3LYP	0.08	0.07	0.02	0.05	0.07	0.03	0.00	0.04	0.10	0.15	0.03	0.09	0.00	0.05	0.04	0.05	0.00	0.14	-0.01	-0.01
$4\mathbf{c}^{2+}$ BS/BP86	0.05	-0.03	0.03	-0.03	0.03	-0.04	0.00	-0.02	0.04	0.10	0.03	0.06	0.00	0.04	0.02	0.03	0.02	0.11	-0.01	-0.01
$4\mathbf{c}^{2+}$ BS/B3LYP	-0.05	0.03	-0.03	0.03	-0.03	0.04	0.00	0.02	-0.03	-0.10	-0.03	-0.06	0.00	-0.04	-0.02	-0.04	-0.02	-0.11	0.01	0.01
$4\mathbf{c}^{2+}$ BS/B3LYP	0.11	-0.07	0.06	-0.10	0.09	-0.11	0.01	-0.03	0.11	0.14	0.04	0.08	0.01	0.04	0.04	0.04	0.04	0.13	-0.01	-0.01
$4\mathbf{c}^{2+}$ BS/B3LYP	-0.11	0.07	-0.07	0.11	-0.09	0.12	-0.01	0.03	-0.11	-0.14	-0.04	-0.08	-0.01	-0.04	-0.04	-0.04	-0.04	-0.13	0.01	0.01
$4\mathbf{c}^{4+}$ HS/BP86	0.05	0.01	0.01	0.02	0.01	0.01	0.00	0.02	0.01	0.22	0.01	0.18	-0.02	0.11	0.02	0.11	-0.02	0.26	-0.02	-0.02
$4\mathbf{c}^{4+}$ HS/B3LYP	0.01	0.00	0.00	0.01	0.01	0.01	0.00	0.01	0.00	0.27	-0.04	0.22	-0.05	0.13	0.02	0.13	-0.05	0.30	-0.02	-0.02
$4\mathbf{c}^{4+}$ BS/BP86	0.02	0.01	0.00	0.02	-0.01	0.02	0.00	0.01	-0.02	0.23	-0.01	0.18	-0.02	0.11	0.02	0.11	-0.02	0.27	-0.02	-0.02
$4\mathbf{c}^{4+}$ BS/BP86	-0.05	0.00	0.00	-0.01	0.01	-0.01	0.00	-0.01	0.01	-0.21	0.01	-0.17	0.02	-0.10	-0.03	-0.10	0.02	-0.25	0.02	0.02
$4\mathbf{c}^{4+}$ BS/B3LYP	0.01	0.00	0.00	0.00	-0.01	0.01	0.00	0.00	-0.01	0.27	-0.04	0.22	-0.05	0.12	0.02	0.12	-0.05	0.30	-0.02	-0.02
$4\mathbf{c}^{4+}$ BS/B3LYP	0.00	0.00	0.00	-0.01	0.01	-0.01	0.00	-0.01	0.01	-0.27	0.05	-0.22	0.05	-0.13	-0.02	-0.13	0.05	-0.31	0.02	0.02

Table S5. Cartesian coordinates of $1\text{-}3\mathbf{o}/\mathbf{c}\text{-}6^{0/2+}$ and $4\mathbf{o}/\mathbf{c}^{0/+2+/4+}$ in their different spin states using BP86

[illegible]

58.C	11.376112	0.987519	-5.149429	2.C	4.820561	19.268063	3.584862	59.P	2.509460	0.052938	1.012008
59.P	11.365134	0.983266	-3.276598	3.C	5.633472	19.357275	4.739859	60.P	5.183368	14.014626	2.788301
60.P	-4.346103	5.958129	-0.081121	4.C	6.042388	20.593938	5.238367	61.C	6.670859	14.293452	1.679564
61.C	-5.057755	5.054481	1.393488	5.C	5.654883	21.779386	4.603566	62.C	6.233557	14.255299	0.207617
62.C	-4.944986	3.537105	1.184349	6.C	4.852913	21.710942	3.458241	63.P	4.683146	15.287733	-0.019766
63.P	-5.516961	3.081123	-0.538331	7.C	4.394541	18.004736	3.074592	64.H	-1.263530	1.025595	2.842918
64.H	6.319332	1.837346	-4.666721	8.C	4.011896	16.917943	2.624818	65.H	-0.876610	-1.094578	2.911119
65.H	1.674796	-0.031376	-4.466765	9.Ru	3.299042	15.082889	1.873623	66.H	1.282811	1.508341	3.438739
66.H	1.616223	0.405510	-2.748896	10.P	1.947811	14.978873	3.801568	67.H	0.943914	0.088301	4.459527
67.H	2.021905	-1.257889	-3.225192	11.C	0.477112	16.123041	3.597011	68.H	3.314969	0.050196	3.362661
68.H	9.940907	-1.847124	1.882550	12.C	-0.022468	16.068567	2.145603	69.H	2.315767	-1.370249	2.959394
69.H	11.579422	0.112263	0.502717	13.P	1.433537	16.195928	0.967860	70.H	3.520721	-0.880725	0.637993
70.H	9.430985	0.283760	0.331970	14.H	5.974230	22.746035	4.995501	71.H	3.311392	1.233601	0.975371
71.H	11.314675	-2.516678	0.972015	15.C	2.532107	13.280161	1.169482	72.H	-2.786568	-0.990364	-0.418393
72.H	8.324899	-2.715760	0.186946	16.C	2.010686	12.225917	0.766147	73.H	-2.629663	1.101313	-0.906781
73.H	9.385447	-4.070706	0.632453	17.C	1.381312	11.054673	0.344639	74.H	-1.565590	-1.612907	-2.702952
74.H	8.685205	-3.881073	-2.184541	18.C	0.199730	10.954713	-0.376368	75.H	-2.610602	-0.257153	-3.203858
75.H	10.738600	-4.303919	-1.661339	19.C	-0.242191	9.643970	-0.636443	76.H	-0.243395	-0.223150	-4.308978
76.H	9.577755	-1.832192	-5.552449	20.C	0.825904	8.575673	-0.339089	77.H	-0.627717	1.255238	-3.394131
77.H	11.416199	-2.911872	-5.172725	21.S	2.054200	9.453057	0.776598	78.H	1.930557	0.909423	-2.769116
78.H	11.562030	-0.485854	-6.762706	22.C	0.145942	7.343022	0.306610	79.H	1.624600	-1.223511	-2.695280
79.H	12.799588	-0.635447	-5.493685	23.C	-0.967282	6.831892	-0.627422	80.H	-1.857380	4.890021	-1.158413
80.H	12.067536	1.755057	-5.522380	24.C	-1.758615	7.790780	-1.227937	81.H	0.285030	7.951285	2.406396
81.H	10.358684	1.270578	-5.460315	25.C	-1.442882	9.195389	-1.151692	82.H	-1.221919	8.458729	1.595895
82.H	12.697186	1.367025	-2.952003	26.C	-3.001613	7.593177	-2.019882	83.H	-0.991535	6.746916	2.055803
83.H	10.711716	2.215589	-2.990433	27.C	-3.709086	8.990611	-1.963260	84.H	-0.360045	11.841531	-0.665209
84.H	15.880415	-1.032060	-3.172306	28.C	-2.538531	10.011439	-1.740991	85.H	1.966991	9.170584	-2.086569
85.H	3.564254	4.169774	-1.259795	29.S	1.277526	5.861381	0.527324	86.H	2.374687	7.534856	-1.485758
86.H	4.109678	3.923864	-2.936312	30.C	0.028954	4.749465	-0.113551	87.H	0.855700	7.802772	-2.383328
87.H	3.915728	2.532019	-1.856096	31.C	-1.041884	5.426798	-0.679335	88.H	5.227313	16.556324	-0.354814
88.H	-0.426871	2.948973	-4.824326	32.C	1.557432	8.245262	-1.660777	89.H	4.285918	14.889594	-1.330619
89.H	-6.954622	3.498861	-4.317084	33.C	-0.484213	7.647511	1.685807	90.H	1.497292	17.602067	0.733682
90.H	-5.099997	2.398969	-4.434947	34.C	0.199081	3.366651	-0.041538	91.H	0.817949	15.815848	-0.261589
91.H	-5.639632	4.422834	-6.452805	35.C	0.304755	2.129563	0.012652	92.H	1.317954	13.754876	4.179862
92.H	-3.993613	4.419127	-5.783112	36.Ru	0.355336	0.047967	0.070789	93.H	2.421974	15.370246	5.087058
93.H	-6.197192	6.517715	-5.207123	37.C	0.355054	-2.058123	0.111452	94.H	5.200399	12.595931	2.947711
94.H	-4.659539	6.809044	-6.053026	38.C	0.327187	-3.294862	0.120490	95.H	5.729433	14.361350	4.059479
95.H	-4.823102	7.910049	-3.369158	39.C	0.288467	-4.721671	0.131861	96.H	-0.755126	16.860368	1.937443
96.H	-3.024983	6.833096	-3.920622	40.C	-0.941621	-5.420168	0.085089	97.H	-0.498629	15.098609	1.933905
97.H	-5.045210	1.743974	-0.661883	41.C	-0.978453	-6.814213	0.094033	98.H	-0.316590	15.860222	4.309784
98.H	-6.901319	2.808361	-0.353819	42.C	0.207096	-7.556213	0.151709	99.H	0.847437	17.129708	3.845203
99.H	-5.524040	2.981283	1.933985	43.C	1.432980	-6.882711	0.199623	100.H	5.959692	13.231392	-0.090772
100.H	-6.112638	5.362374	1.457322	44.C	1.476347	-5.488782	0.189195	101.H	7.030363	14.605532	-0.462898
101.H	-4.554184	5.374397	2.315631	45.F	-2.201525	10.583255	-2.966089	102.H	7.453608	13.551766	1.890274
102.H	-3.896533	3.208783	1.255043	46.F	-2.963889	11.074662	-0.959616	103.H	7.058166	15.289586	1.944314
103.H	-4.776101	7.293571	0.156466	47.F	-4.454884	9.263623	-3.069907	104.H	-1.868313	-4.846100	0.043095
104.H	-2.974325	6.107123	0.274577	48.F	-4.547109	9.019607	-0.878006	105.H	-1.941354	-7.326903	0.057030
105.H	-9.108421	7.298280	0.219725	49.F	-2.761207	7.275367	-3.359191	106.H	2.364733	-7.449471	0.244876
106.H	14.508263	-4.189433	-0.558701	50.F	-3.842005	6.599305	-1.559425	107.H	2.434367	-4.968179	0.224867
107.H	16.853115	-4.963426	-0.268048	51.H	0.174642	-8.646568	0.158961	108.H	5.935068	18.435879	5.240085
108.H	18.223113	-1.810750	-2.878817	52.P	1.030868	-0.031095	-2.185842	109.H	6.668720	20.633687	6.131402
109.H	-9.629829	6.359163	-3.966450	53.C	-0.461076	0.170398	-3.306626	110.H	4.544362	22.628044	2.953186
110.H	-11.878477	7.417375	-3.921339	54.C	-1.681674	-0.518337	-2.678496	111.H	3.817820	20.428373	2.060581
111.H	-11.358611	8.354634	0.259149	55.P	-1.801322	-0.060995	-0.863939				
				56.P	-0.326111	0.083756	2.325224				
				57.C	1.152430	0.415056	3.431496				
				58.C	2.396772	-0.277085	2.855790				
1c								1c ²⁺ LS			
1.C	4.442271	20.477272	2.953773					1.C	3.481173	20.734943	1.785902

2.C	4.065986	19.797280	2.672288	59.P	2.465541	-0.668742	0.831169	3.C	5.287346	20.094888	3.811021
3.C	4.916135	20.276176	3.698304	60.P	5.243125	14.704629	3.029513	4.C	5.626694	21.432391	3.971191
4.C	5.165581	21.639319	3.830662	61.C	6.609267	15.296518	1.898871	5.C	5.088943	22.404557	3.114465
5.C	4.584536	22.553253	2.942528	62.C	6.267856	14.966253	0.437970	6.C	4.203822	22.030260	2.092278
6.C	3.744192	22.095018	1.919926	63.P	4.492873	15.425639	0.059602	7.C	4.043126	18.338368	2.607046
7.C	3.805307	18.406177	2.526330	64.H	-0.968875	0.732809	2.980414	8.C	3.728928	17.145134	2.429450
8.C	3.572332	17.198350	2.373117	65.H	-1.209172	-1.367707	2.507363	9.Ru	3.177669	15.182447	2.057173
9.Ru	3.145855	15.177309	2.023719	66.H	1.563260	0.309253	3.628003	10.P	1.918533	15.250628	4.082644
10.P	1.891867	15.381418	4.048112	67.H	0.850781	-1.212108	4.206354	11.C	0.366696	16.256312	3.804123
11.C	0.401661	16.457599	3.721180	68.H	3.174436	-1.505320	3.050419	12.C	-0.210809	15.962457	2.411059
12.C	-0.219590	16.097516	2.363136	69.H	1.874616	-2.477228	2.313938	13.P	1.148772	15.995607	1.120970
13.P	1.110845	15.938893	1.050761	70.H	3.271450	-1.636722	0.169938	14.H	5.359335	23.452969	3.243136
14.H	4.785871	23.619735	3.046769	71.H	3.472942	0.309022	1.080590	15.C	2.608174	13.250724	1.636760
15.C	2.719216	13.248501	1.647049	72.H	-2.942089	-0.417813	-0.434673	16.C	2.228776	12.100649	1.325216
16.C	2.431886	12.053692	1.359347	73.H	-2.407386	1.582395	-1.028476	17.C	1.686814	10.909623	0.881211
17.C	1.933970	10.858770	0.927502	74.H	-1.871448	-1.360255	-2.721159	18.C	0.519607	10.794426	0.097785
18.C	0.723547	10.713738	0.179469	75.H	-2.714278	0.115331	-3.260074	19.C	0.161577	9.501048	-0.246058
19.C	0.396032	9.431861	-0.169391	76.H	-0.404844	-0.271814	-4.418241	20.C	1.218849	8.441430	0.096109
20.C	1.465033	8.378613	0.138407	77.H	-0.546144	1.296646	-3.598518	21.S	2.389740	9.327050	1.262000
21.S	2.683031	9.281145	1.237740	78.H	1.946654	0.698987	-2.957943	22.C	0.494254	7.205789	0.702434
22.C	0.757166	7.153127	0.804922	79.H	1.423485	-1.397904	-2.831524	23.C	-0.542116	6.709185	-0.315009
23.C	-0.321191	6.649086	-0.157330	80.H	-1.131898	4.774435	-0.898203	24.C	-1.321324	7.682232	-0.957708
24.C	-1.142563	7.627834	-0.783390	81.H	0.886544	7.796477	2.889212	25.C	-1.012891	9.052059	-0.869806
25.C	-0.815718	8.971969	-0.760722	82.H	-0.586541	8.348590	2.050658	26.C	-2.528186	7.465352	-1.821586
26.C	-2.399335	7.385541	-1.572196	83.H	-0.436338	6.644788	2.558916	27.C	-3.222921	8.874900	-1.853255
27.C	-3.059667	8.809200	-1.674438	84.H	0.106397	11.580910	-0.042516	28.C	-2.052862	9.884705	-1.560991
28.C	-1.857952	9.802185	-1.459088	85.H	2.623660	8.896333	-1.636176	29.S	1.586835	5.710865	1.002672
29.S	1.849930	5.655398	1.076988	86.H	3.027277	7.301327	-0.944521	30.C	0.444527	4.623362	0.192115
30.C	0.696143	4.559684	0.292326	87.H	1.519578	7.514761	-1.871320	31.C	-0.589127	5.331959	-0.455710
31.C	-0.369314	5.291467	-0.320273	88.H	4.594435	16.740141	-0.470787	32.C	2.020537	8.100636	-1.182972
32.C	2.208397	7.997821	-1.162472	89.H	4.258639	14.711723	-1.150872	33.C	-0.219922	7.522840	2.037876
33.C	0.114367	7.508479	2.165436	90.H	1.120538	17.228953	0.451535	34.C	0.576172	3.248122	0.197052
34.C	0.807488	3.199489	0.263964	91.H	0.411117	15.237781	0.025165	35.C	0.534621	1.999518	0.132964
35.C	0.684035	1.949337	0.140919	92.H	1.324865	14.235891	4.680852	36.Ru	0.332057	-0.040722	-0.001150
36.Ru	0.354662	-0.026626	-0.045982	93.H	2.476831	15.995566	5.187882	37.C	0.056381	-2.089716	-0.155238
37.C	-0.081200	-2.065865	-0.241831	94.H	5.622828	13.358475	3.306982	38.C	-0.149961	-3.314104	-0.264847
38.C	-0.400982	-3.256870	-0.367248	95.H	5.613398	15.290383	4.271742	39.C	-0.392969	-4.700792	-0.393499
39.C	-0.781684	-4.620129	-0.512548	96.H	-0.966632	16.840781	2.053892	40.C	-1.721854	-5.198357	-0.476125
40.C	-2.148576	-4.979186	-0.607466	97.H	-0.722196	15.118933	2.410380	41.C	-1.957953	-6.560902	-0.605848
41.C	-2.522409	-6.312683	-0.745517	98.H	-0.326163	16.355961	4.537504	42.C	-0.883031	-7.460952	-0.657049
42.C	-1.546946	-7.316140	-0.802725	99.H	0.777624	17.491811	3.719134	43.C	0.435211	-6.988052	-0.576337
43.C	-0.190959	-6.976727	-0.714905	100.H	6.349165	13.884332	0.250587	44.C	0.682962	-5.627447	-0.445594
44.C	0.191948	-5.646635	-0.565955	101.H	6.943587	15.478863	-0.259824	45.F	-1.589207	10.409484	-2.749142
45.F	-1.409344	10.262875	-2.674786	102.H	7.569929	14.855126	2.196475	46.F	-2.497616	10.952604	-0.815094
46.F	-2.252431	10.905941	-0.741080	103.H	6.668205	16.385297	2.048342	47.F	-3.856741	9.125947	-3.020446
47.F	-3.699433	9.008225	-2.846942	104.H	-2.906282	-4.196451	-0.561791	48.F	-4.129923	8.938842	-0.835388
48.F	-3.948218	8.956788	-0.651585	105.H	-3.578874	-6.574457	-0.810074	49.F	-2.184521	7.097758	-3.109976
49.F	-2.121197	6.912293	-2.838617	106.H	0.569799	-7.756215	-0.761967	50.F	-3.384385	6.498656	-1.358124
50.F	-3.248967	6.481223	-0.992375	107.H	1.246776	-5.379989	-0.496790	51.H	-1.072587	-8.529757	-0.759582
51.H	-1.842983	-8.359450	-0.915247	108.H	5.368351	19.562433	4.387357	52.P	0.939251	-0.012209	-2.313039
52.P	0.961449	-0.139323	-2.361092	109.H	5.817581	21.994821	4.628854	53.C	-0.560738	0.391758	-3.359598
53.C	-0.531903	0.207396	-3.438199	110.H	3.293136	22.804369	1.225465	54.C	-1.830996	-0.191341	-2.722209
54.C	-1.820049	-0.261365	-2.745470	111.H	2.827739	20.375181	0.990684	55.P	-1.862212	0.182806	-0.888965
55.P	-1.820646	0.283137	-0.957937	1c ²⁺ HS				56.P	-0.285690	-0.162547	2.301904
56.P	-0.320983	-0.292677	2.233406		1.C	3.855632	20.696276	57.C	1.251701	-0.207298	3.368292
57.C	1.166170	-0.666219	3.307057		2.C	4.392209	19.696882	58.C	2.370369	-0.982438	2.655709
58.C	2.219501	-1.450740	2.510647					59.P	2.505097	-0.426652	0.873416

60.P	5.237115	14.476315	3.001461	4.C	-10.483241	7.962140	0.396732	61.P	6.360295	-7.352712	-5.057160
61.C	6.620503	14.790834	1.779579	5.C	-11.275698	8.439038	-0.654942	62.O	12.837810	-13.801195	-1.420785
62.C	6.146852	14.483978	0.350535	6.C	-10.965548	8.138134	-1.987290	63.P	-6.286992	2.291068	-1.880378
63.P	4.465668	15.248736	0.047102	7.C	-7.880173	6.072683	-1.516448	64.C	-6.446568	1.949752	-0.042243
64.H	-1.058649	0.848690	2.938820	8.C	-6.872953	5.398711	-1.779525	65.C	-5.174326	2.408949	0.685484
65.H	-1.015577	-1.303474	2.737782	9.Ru	-5.136444	4.319561	-2.214601	66.P	-4.675315	4.114642	0.081950
66.H	1.542312	0.842668	3.527124	10.P	-3.980651	6.350046	-2.550012	67.O	-13.127847	9.676574	-1.316375
67.H	1.018176	-0.644560	4.348355	11.C	-4.334855	7.009956	-4.269499	68.H	-0.926526	2.207566	-5.421892
68.H	3.334460	-0.859372	3.167231	12.C	-4.464890	5.843663	-5.260260	69.H	3.556497	1.421998	-3.271477
69.H	2.138549	-2.058009	2.620815	13.P	-5.552135	4.504201	-4.525251	70.H	2.876381	-0.029251	-2.519542
70.H	3.371162	-1.414489	0.325911	14.N	-12.442765	9.264548	-0.357898	71.H	2.955088	1.493138	-1.599355
71.H	3.435828	0.649701	0.951113	15.O	-12.693252	9.515370	0.838944	72.H	-6.654927	0.885612	0.134973
72.H	-2.936901	-0.636134	-0.442622	16.C	-3.353497	3.306556	-2.665879	73.H	-7.629896	2.074727	-2.308178
73.H	-2.526464	1.443483	-0.839865	17.C	-2.262071	2.800074	-2.960073	74.H	-5.727703	1.068667	-2.359438
74.H	-1.840938	-1.288759	-2.806570	18.C	-0.986268	2.295148	-3.264045	75.H	-7.319125	2.530536	0.294925
75.H	-2.738212	0.195019	-3.206066	19.C	-0.394334	2.050805	-4.488809	76.H	-4.328629	1.745951	0.445517
76.H	-0.416377	0.020261	-4.383038	20.C	0.954868	1.574196	-4.417465	77.H	-5.307925	2.410845	1.776028
77.H	-0.613786	1.490447	-3.405634	21.C	1.416793	1.455341	-3.104890	78.H	-3.360901	4.214489	0.625986
78.H	1.913953	0.881108	-2.840139	22.S	0.178306	1.927536	-1.982204	79.H	-5.340074	4.962838	1.018222
79.H	1.417108	-1.221808	-2.889461	23.C	1.793081	1.344651	-5.599273	80.H	-2.555533	6.352041	-2.515007
80.H	-1.340246	4.811234	-1.044678	24.C	2.700060	0.344684	-5.858139	81.H	-4.210835	7.516305	-1.762649
81.H	0.508644	7.812056	2.805090	25.C	3.540518	0.696845	-7.063317	82.H	-3.552217	7.717273	-4.575925
82.H	-0.933107	8.349047	1.901740	26.C	2.728814	1.794711	-7.808554	83.H	-5.283690	7.562727	-4.189700
83.H	-0.770543	6.639383	2.384995	27.C	1.827299	2.392780	-6.688009	84.H	-4.863475	6.175280	-6.228921
84.H	-0.062917	11.672930	-0.168537	28.C	2.950308	-0.923314	-5.174852	85.H	-3.485527	5.371950	-5.434596
85.H	2.454418	9.015602	-1.605810	29.C	1.953885	-1.768428	-4.681694	86.H	-6.846427	4.886623	-4.990676
86.H	2.829386	7.395952	-0.954197	30.S	2.655749	-3.227622	-4.056705	87.H	-5.320956	3.437908	-5.443206
87.H	1.360956	7.645704	-1.936530	31.C	4.309032	-2.727391	-4.456838	88.H	-9.603068	7.115789	-3.298291
88.H	4.784858	16.524082	-0.497167	32.C	4.265378	-1.480594	-5.048927	89.H	-0.037491	-2.584589	-4.647135
89.H	4.054793	14.597138	-1.149902	33.C	5.390243	-3.586071	-4.195123	90.H	0.140408	-1.102740	-5.615855
90.H	1.111933	17.342945	0.662300	34.C	6.271880	-4.428868	-3.978400	91.H	0.112219	-0.999016	-3.850104
91.H	0.503714	15.378165	0.010922	35.Ru	7.670715	-5.964624	-3.671741	92.H	5.166132	-0.972573	-5.383774
92.H	1.416860	14.039967	4.641036	36.C	9.003601	-7.544412	-3.364474	93.H	9.980387	-5.878241	-6.044593
93.H	2.446839	15.832941	5.267769	37.C	9.762487	-8.503497	-3.160278	94.H	8.905426	-4.014607	-6.097335
94.H	5.423460	13.103620	3.336060	38.C	10.623190	-9.604981	-2.932092	95.H	8.236010	-6.013738	-8.063903
95.H	5.761853	15.057166	4.190103	39.C	10.273316	-10.628833	-2.011422	96.H	6.840457	-5.248176	-7.261445
96.H	-1.002531	16.675777	2.145399	40.C	11.108588	-11.712015	-1.785226	97.H	7.856518	-8.135684	-6.792763
97.H	-0.643871	14.950892	2.373835	41.C	12.321977	-11.797615	-2.479482	98.H	6.296205	-7.676551	-7.517501
98.H	-0.366206	16.051093	4.596049	42.C	12.702692	-10.808224	-3.395198	99.H	6.183149	-8.748440	-4.824015
99.H	0.672295	17.310578	3.887394	43.C	11.862204	-9.727479	-3.615538	100.H	4.996901	-7.008503	-5.293422
100.H	6.019041	13.400295	0.204092	44.N	13.204009	-12.937567	-2.244589	101.H	9.124847	-3.145961	-2.589028
101.H	6.865233	14.843146	-0.398629	45.O	14.277136	-12.988047	-2.879827	102.H	10.296357	-4.848334	-1.985355
102.H	7.506131	14.198108	2.045378	46.C	0.464891	-1.610084	-4.696328	103.H	8.892986	-4.070081	0.141302
103.H	6.879818	15.855590	1.883935	47.F	4.776256	1.221410	-6.690957	104.H	8.421415	-6.522264	-0.003941
104.H	-2.551926	-4.493266	-0.433556	48.F	3.813290	-0.359601	-7.891239	105.H	6.975122	-5.753923	0.696805
105.H	-2.981411	-6.931067	-0.667773	49.F	1.949493	1.206002	-8.767252	106.H	7.353788	-3.695020	-0.674913
106.H	1.268274	-7.689863	-0.616602	50.F	3.512366	2.724736	-8.417821	107.H	6.470105	-7.882250	-1.197857
107.H	1.704372	-5.252263	-0.384145	51.F	0.583365	2.711375	-7.201444	108.H	5.311749	-6.073844	-1.356052
108.H	5.700591	19.333699	4.472604	52.F	2.364514	3.583164	-6.241406	109.H	9.324864	-10.552146	-1.480147
109.H	6.313238	21.726938	4.764936	53.C	2.769249	1.065034	-2.592748	110.H	-8.746148	6.809188	0.919727
110.H	3.788023	22.787791	1.427739	54.P	6.633024	-6.534784	-1.636745	111.H	-10.754458	8.216761	1.418920
111.H	3.169588	20.397017	1.132178	55.C	7.603748	-5.812098	-0.202443	112.H	-11.604891	8.524643	-2.777908
				56.C	8.163894	-4.436383	-0.594483	113.H	12.147451	-8.950184	-4.324172
				57.P	8.941041	-4.530149	-2.299760	114.H	13.652834	-10.908186	-3.915495
				58.P	8.689256	-5.369158	-5.708256	115.H	10.845539	-12.499987	-1.082674
				59.C	7.645747	-5.988694	-7.137583				
				60.C	7.065682	-7.369609	-6.795822				
2o	1.C	-9.854083	7.357442	-2.265791				2o ⁺	HS		
	2.C	-9.022931	6.858238	-1.227610							
	3.C	-9.373169	7.182293	0.110324							

1.C	-9.974440	7.148509	-2.593850	58.P	9.279882	-4.508897	-4.118915	115.H	11.371283	-12.719255	-2.367877	
2.C	-8.987601	7.117729	-1.574958	59.C	9.346124	-4.243739	-5.971403	2c				
3.C	-9.210148	7.864771	-0.389560	60.C	9.037543	-5.555580	-6.708139					
4.C	-10.367865	8.612941	-0.228836	61.P	7.539527	-6.376119	-5.951884		1.C	4.824587	20.364152	2.764570
5.C	-11.316697	8.614189	-1.253881	62.O	13.528016	-13.646601	-2.800830		2.C	5.065186	19.140188	3.442841
6.C	-11.136104	7.890895	-2.435016	63.P	-5.774811	3.163422	-0.370148		3.C	5.921345	19.168926	4.575024
7.C	-7.803244	6.357406	-1.739243	64.C	-5.563610	4.036808	1.268154		4.C	6.506612	20.350388	5.005715
8.C	-6.764334	5.688861	-1.885754	65.C	-4.249748	4.832313	1.273799		5.C	6.246145	21.536700	4.309151
9.Ru	-5.025299	4.594151	-2.137612	66.P	-4.071868	5.803504	-0.317048		6.C	5.406209	21.549499	3.188950
10.P	-4.440333	6.135673	-3.875015	67.O	-13.379774	9.384654	-2.009165		7.C	4.471625	17.931073	3.001155
11.C	-5.458012	5.772082	-5.398877	68.H	-1.090811	1.932586	-5.033642		8.C	3.955146	16.877887	2.601294
12.C	-5.613129	4.254615	-5.577729	69.H	3.517023	1.433925	-3.132095	9.Ru	3.081117	15.107276	1.901890	
13.P	-6.074122	3.451291	-3.949930	70.H	2.898376	0.119516	-2.114417	10.P	1.720807	15.075575	3.831318	
14.N	-12.557153	9.410446	-1.082571	71.H	3.060019	1.756389	-1.442134	11.C	0.291515	16.269439	3.614993	
15.O	-12.682264	10.044183	-0.024928	72.H	-5.601706	3.311721	2.092260	12.C	-0.193651	16.241916	2.157792	
16.C	-3.289148	3.546847	-2.410893	73.H	-7.122878	2.715809	-0.304290	13.P	1.276274	16.321268	0.995000	
17.C	-2.210582	2.954454	-2.638738	74.H	-5.118685	1.917478	-0.155696	14.N	6.862481	22.783896	4.758739	
18.C	-0.981890	2.369214	-2.910925	75.H	-6.430605	4.707885	1.365339	15.C	2.222519	13.346492	1.203132	
19.C	-0.488221	1.907982	-4.131236	76.H	-3.382580	4.155518	1.317897	16.C	1.702132	12.302183	0.777724	
20.C	0.842398	1.421877	-4.083055	77.H	-4.190946	5.508715	2.137080	17.C	1.107600	11.126814	0.319410	
21.C	1.403101	1.515412	-2.794767	78.H	-2.697754	6.173385	-0.281612	18.C	-0.062521	11.008448	-0.415656	
22.S	0.270949	2.183585	-1.670211	79.H	-4.646091	7.063432	0.011350	19.C	-0.450118	9.689765	-0.723417	
23.C	1.587839	1.003769	-5.279441	80.H	-3.105702	6.145024	-4.371578	20.C	0.654645	8.654015	-0.443815	
24.C	2.434557	-0.051749	-5.479754	81.H	-4.628341	7.535136	-3.709376	21.S	1.836746	9.541473	0.711155	
25.C	3.164559	0.098692	-6.802389	82.H	-4.998264	6.238449	-6.280567	22.C	0.014037	7.381717	0.159750	
26.C	2.324551	1.133434	-7.608626	83.H	-6.434554	6.251033	-5.231047	23.C	-1.066452	6.855251	-0.803511	
27.C	1.575405	1.921113	-6.490369	84.H	-6.362351	4.012932	-6.343533	24.C	-1.885913	7.799144	-1.388770	
28.C	2.732698	-1.232503	-4.664313	85.H	-4.659517	3.798494	-5.885157	25.C	-1.625770	9.211841	-1.267682	
29.C	1.782990	-1.997367	-3.959987	86.H	-7.496669	3.440905	-3.990729	26.C	-3.112888	7.577701	-2.201069	
30.S	2.514005	-3.394881	-3.252002	87.H	-5.840034	2.075033	-4.229478	27.C	-3.874610	8.944785	-2.110704	
31.C	4.114479	-2.999360	-3.908495	88.H	-9.812666	6.576417	-3.506387	28.C	-2.745300	10.002286	-1.849860	
32.C	4.028081	-1.812406	-4.632525	89.H	-0.204396	-2.744229	-3.610868	29.S	1.198341	5.938971	0.356653	
33.C	5.198535	-3.848813	-3.734175	90.H	-0.104173	-1.405802	-4.780891	30.C	-0.004250	4.800323	-0.318971	
34.C	6.133309	-4.674316	-3.632472	91.H	0.058298	-1.079520	-3.046036	31.C	-1.090861	5.449216	-0.887075	
35.Ru	7.594438	-6.105585	-3.573462	92.H	4.893359	-1.385007	-5.131837	32.C	1.411829	8.388163	-1.765845	
36.C	9.035136	-7.591830	-3.546389	93.H	10.627496	-4.833078	-3.795523	33.C	-0.645225	7.625410	1.537643	
37.C	9.895746	-8.490796	-3.534218	94.H	9.257385	-3.170909	-3.633011	34.C	0.205005	3.422295	-0.253270	
38.C	10.880809	-9.508941	-3.499969	95.H	10.325592	-3.839604	-6.260195	35.C	0.334746	2.188675	-0.188814	
39.C	10.604492	-10.755205	-2.879760	96.H	8.586846	-3.479745	-6.199037	36.Ru	0.399091	0.110842	-0.065194	
40.C	11.563485	-11.756992	-2.837538	97.H	9.863967	-6.273884	-6.596951	37.C	0.389619	-1.978276	0.069610	
41.C	12.812393	-11.518294	-3.415976	98.H	8.875205	-5.388433	-7.781391	38.C	0.340125	-3.213794	0.152378	
42.C	13.124535	-10.305594	-4.035596	99.H	7.564496	-7.668376	-6.543961	39.C	0.263945	-4.625416	0.253510	
43.C	12.160964	-9.306982	-4.077854	100.H	6.457019	-5.811974	-6.685163	40.C	-0.989585	-5.292261	0.230607	
44.N	13.839301	-12.589969	-3.369064	101.H	7.640617	-4.703479	-0.495760	41.C	-1.073821	-6.672680	0.332177	
45.O	14.933526	-12.353517	-3.900700	102.H	8.943934	-6.428809	-0.571849	42.C	0.102136	-7.421916	0.459731	
46.C	0.305373	-1.801014	-3.840812	103.H	6.691260	-7.212749	0.647941	43.C	1.357052	-6.801359	0.485343	
47.F	4.443290	0.599229	-6.605915	104.H	6.983677	-8.933907	-1.137114	44.C	1.433033	-5.420184	0.382829	
48.F	3.305443	-1.072372	-7.489910	105.H	5.233701	-8.747340	-0.878602	45.F	-2.414301	10.612948	-3.056168	
49.F	1.417691	0.464704	-8.378705	106.H	5.518970	-6.322223	-0.348423	46.F	-3.215285	11.028095	-1.047101	
50.F	3.075754	1.926181	-8.405914	107.H	6.034308	-9.071256	-3.646546	47.F	-4.620393	9.219664	-3.214657	
51.F	0.307789	2.259446	-6.908481	108.H	4.613545	-7.511157	-3.178402	48.F	-4.718653	8.910429	-1.031666	
52.F	2.227252	3.100641	-6.224743	109.H	9.623827	-10.920250	-2.436006	49.F	-2.843891	7.310706	-3.544087	
53.C	2.791589	1.192032	-2.343056	110.H	-8.456200	7.849693	0.396272	50.F	-3.917201	6.539307	-1.778144	
54.P	6.002448	-7.790803	-3.027826	111.H	-10.556999	9.195737	0.670047	51.N	0.017832	-8.877259	0.568486	
55.C	6.141789	-8.229365	-1.215045	112.H	-11.906671	7.926163	-3.202070	52.P	1.078468	-0.011940	-2.323756	
56.C	6.411580	-6.965564	-0.384955	113.H	12.383982	-8.353058	-4.554053	53.C	-0.406171	0.226998	-3.444226	
57.P	7.757191	-5.942100	-1.186799	114.H	14.112712	-10.170557	-4.470300	54.C	-1.642031	-0.441388	-2.823547	

55.P	-1.760256	0.000769	-1.004703	112.H	4.170265	20.359524	1.893156	52.P	0.625591	0.091110	-2.269523
56.P	-0.286276	0.284492	2.186919	113.O	7.607561	22.740433	5.758442	53.C	-0.952704	-0.088595	-3.238146
57.C	1.182049	0.743980	3.257146	114.O	-1.114393	-9.400602	0.541700	54.C	-2.022052	-0.808459	-2.411500
58.C	2.442536	0.030930	2.745211	115.O	6.610806	23.824241	4.117875	55.P	-2.091844	-0.103553	-0.696173
59.P	2.555370	0.194187	0.879030	2c ²⁺ LS				56.P	-0.338531	0.043149	2.384233
60.P	4.882339	13.884564	2.804171		1.C	4.807476	20.175965	57.C	1.242220	0.165293	3.357865
61.C	6.356450	13.977629	1.647209		2.C	5.127658	18.919134	58.C	2.426570	-0.366792	2.545864
62.C	5.876516	13.963784	0.187977		3.C	6.065873	18.856960	59.P	2.377731	0.308795	0.817465
63.P	4.446520	15.157557	-0.022594		4.C	6.660854	20.007958	60.P	5.079152	13.879474	2.455234
64.H	-1.252040	1.236962	2.623635		5.C	6.323149	21.230647	61.C	6.490279	14.429268	1.381368
65.H	-0.804722	-0.859640	2.862893		6.C	5.403062	21.330329	62.C	6.048591	14.502026	-0.083369
66.H	1.287653	1.836206	3.167018		7.C	4.518863	17.731739	63.P	4.406079	15.361990	-0.243486
67.H	0.979328	0.504565	4.309975		8.C	3.991512	16.718199	64.H	-1.186602	0.923445	3.087345
68.H	3.351848	0.423722	3.220299		9.Ru	3.101406	14.961271	65.H	-0.890851	-1.186355	2.785212
69.H	2.388053	-1.049395	2.950729	10.P	2.001425	14.993965	3.827268	66.H	1.376933	1.224513	3.587145
70.H	3.571937	-0.763222	0.588940	11.C	0.767181	16.377799	3.821254	67.H	1.140492	-0.364916	4.304816
71.H	3.346877	1.372216	0.733516	12.C	0.042249	16.435534	2.473093	68.H	3.374989	-0.121844	3.023934
72.H	-2.747840	-0.928915	-0.565187	13.P	1.249909	16.301823	1.060922	69.H	2.368421	-1.451302	2.444598
73.H	-2.580777	1.167628	-1.034197	14.N	6.960663	22.459624	4.877147	70.H	3.369561	-0.447166	0.164003
74.H	-1.550991	-1.537930	-2.861378	15.C	2.266861	13.279136	1.040861	71.H	3.071171	1.533592	0.934079
75.H	-2.563896	-0.156040	-3.348502	16.C	1.745889	12.213247	0.632555	72.H	-2.932670	-1.010779	-0.024015
76.H	-0.195113	-0.164079	-4.448867	17.C	1.174902	11.058985	0.224316	73.H	-2.989973	0.977753	-0.829728
77.H	-0.550153	1.315641	-3.523959	18.C	-0.079155	10.936982	-0.475320	74.H	-1.771497	-1.863273	-2.291280
78.H	2.006204	0.901396	-2.904173	19.C	-0.454655	9.669495	-0.762176	75.H	-2.999603	-0.745180	-2.889324
79.H	1.642048	-1.220934	-2.828993	20.C	0.568330	8.584311	-0.439305	76.H	-0.759185	-0.609579	-4.175770
80.H	-1.882327	4.893764	-1.384720	21.S	1.886716	9.476095	0.519145	77.H	-1.275066	0.924882	-3.486333
81.H	0.101931	7.938444	2.277159	22.C	-0.174044	7.461932	0.365569	78.H	1.301075	1.098074	-2.989505
82.H	-1.412220	8.410190	1.458769	23.C	-1.297621	6.932869	-0.517804	79.H	1.389988	-1.025082	-2.654150
83.H	-1.123023	6.697055	1.876988	24.C	-2.107757	7.918466	-1.178510	80.H	-2.152297	5.062852	-1.171088
84.H	-0.651729	11.883025	-0.682313	25.C	-1.716657	9.216778	-1.284320	81.H	0.037777	8.277717	2.377112
85.H	1.792041	9.339399	-2.160573	26.C	-3.423884	7.674907	-1.872682	82.H	-1.422246	8.817915	1.539103
86.H	2.252687	7.703076	-1.602250	27.C	-3.996549	9.114974	-2.107525	83.H	-1.329843	7.176447	2.181784
87.H	0.734437	7.942243	-2.509243	28.C	-2.735197	10.044183	-2.030085	84.H	-0.673095	11.813625	-0.689917
88.H	5.116178	16.364791	-0.381647	29.S	0.856859	5.958796	0.730866	85.H	1.635696	8.889619	-2.305760
89.H	3.974195	14.793733	-1.317172	30.C	-0.309812	4.857813	0.005136	86.H	1.992871	7.343553	-1.528765
90.H	1.405106	17.726071	0.779413	31.C	-1.380412	5.587192	-0.625426	87.H	0.458615	7.576217	-2.375332
91.H	0.659102	15.984774	-0.245512	32.C	1.204983	8.061587	-1.746545	88.H	4.746763	16.701970	-0.499645
92.H	1.051132	13.874271	4.209777	33.C	-0.758492	7.969145	1.703166	89.H	3.992821	14.971936	-1.533906
93.H	2.202333	15.454189	5.118203	34.C	-0.169606	3.514579	0.021458	90.H	1.515725	17.644484	0.730971
94.H	4.751358	12.478180	3.003658	35.C	-0.050311	2.265704	0.035990	91.H	0.402503	15.966658	-0.015269
95.H	5.496704	14.208118	4.049796	36.Ru	0.128006	0.279925	0.056369	92.H	1.237310	13.885477	4.252931
96.H	-0.894201	17.061632	1.947719	37.C	0.320768	-1.815542	0.075497	93.H	2.744185	15.225814	4.998697
97.H	-0.703175	15.291540	1.935324	38.C	0.435068	-3.031872	0.095109	94.H	5.173276	12.471035	2.408728
98.H	-0.518643	16.028685	4.316762	39.C	0.571372	-4.451966	0.118767	95.H	5.578921	14.095583	3.753605
99.H	0.688229	17.262825	3.875701	40.C	-0.563686	-5.282408	0.155780	96.H	-0.546090	17.348279	2.380686
100.H	5.481858	12.972367	-0.083337	41.C	-0.434252	-6.661041	0.175756	97.H	-0.643781	15.592172	2.368649
101.H	6.688915	14.211891	-0.508706	42.C	0.838354	-7.216685	0.151213	98.H	0.062570	16.260256	4.644681
102.H	7.056910	13.156229	1.851029	43.C	1.981247	-6.428596	0.110639	99.H	1.340257	17.289614	3.993877
103.H	6.863205	14.926827	1.880715	44.C	1.844354	-5.050756	0.095450	100.H	5.907198	13.499954	-0.493888
104.H	-1.897159	-4.696887	0.133778	45.F	-2.292388	10.343471	-3.282553	101.H	6.795588	15.005176	-0.697305
105.H	-2.030971	-7.189539	0.316719	46.F	-3.020916	11.219129	-1.408659	102.H	7.344299	13.762970	1.502851
106.H	2.248605	-7.416675	0.584798	47.F	-4.651384	9.228568	-3.268823	103.H	6.776391	15.416121	1.747537
107.H	2.403610	-4.924975	0.399888	48.F	-4.830194	9.422446	-1.087270	104.H	-1.549202	-4.836785	0.172002
108.O	1.082452	-9.517520	0.683097	49.F	-3.233090	7.043430	-3.069219	105.H	-1.297625	-7.309882	0.205156
109.H	6.115012	18.238737	5.108848	50.F	-4.272103	6.909504	-1.143113	106.H	2.952724	-6.900926	0.091868
110.H	7.163823	20.379761	5.872117	51.N	0.980519	-8.686102	0.169818	107.H	2.726188	-4.425348	0.058031
111.H	5.227429	22.490516	2.673202					108.O	2.119791	-9.143752	0.162570

109.H	6.322054	17.897438	4.869510	49.Cl	4.507041	-4.054651	-9.742632	17.C	-3.233673	3.582673	-2.502009
110.H	7.381925	19.974819	5.733181	50.C	-1.143072	-0.198597	-0.709972	18.Ru	-4.910058	4.537967	-2.168384
111.H	5.169043	22.301166	2.915808	51.C	-1.664568	-1.387160	-1.198330	19.P	-3.895277	6.137330	-0.697281
112.H	4.091834	20.237933	2.039647	52.S	-3.148637	-1.079976	-2.055293	20.C	-3.967438	5.543673	1.076877
113.O	7.771747	22.336125	5.790445	53.C	-3.078704	0.659762	-1.755303	21.C	-5.215395	4.675542	1.299731
114.O	-0.049675	-9.353087	0.199289	54.C	-1.940744	0.939694	-1.014863	22.P	-5.386660	3.440445	-0.088382
115.O	6.641951	23.522835	4.352746	55.C	-1.112486	-2.780934	-1.095612	23.C	2.865968	1.281157	-2.484810
				56.H	-1.115063	-3.141070	-0.056358	24.F	4.447371	0.477166	-6.728984
				57.H	-0.076222	-2.821450	-1.462670	25.F	3.246693	-1.178214	-7.559120
				58.H	-1.702820	-3.485630	-1.694296	26.F	1.399154	0.400185	-8.468850
				59.H	-1.688481	1.951777	-0.706979	27.F	3.105532	1.803639	-8.552255
				60.C	-4.042767	1.562969	-2.233453	28.F	0.369334	2.272776	-7.029776
				61.C	-4.810016	2.454277	-2.619203	29.F	2.327001	3.055285	-6.384338
				62.Ru	-6.012334	4.029388	-3.058512	30.C	0.250764	-1.758600	-3.930349
				63.P	-5.587239	4.719802	-0.855427	31.C	5.115612	-3.845984	-3.673709
				64.C	-6.658672	3.741956	0.332802	32.C	6.059844	-4.665308	-3.542819
				65.C	-8.045572	3.527961	-0.292980	33.Ru	7.488537	-6.002154	-3.470607
				66.P	-7.851589	2.944426	-2.067627	34.P	7.984322	-5.841730	-5.811400
				67.H	-5.860791	6.065521	-0.459948	35.C	9.671135	-5.075645	-6.027415
				68.H	-4.304125	4.582622	-0.248422	36.C	9.841329	-3.902258	-5.050375
				69.H	-6.722060	4.250962	1.304755	37.P	9.266520	-4.393819	-3.337515
				70.H	-6.143012	2.779767	0.479491	38.Cl	-7.048562	5.762583	-1.756999
				71.H	-8.598608	4.479029	-0.348835	39.P	-4.785620	5.851626	-4.174079
				72.H	-8.648203	2.813193	0.284456	40.C	-6.138316	5.309423	-5.338616
				73.H	-9.184741	3.097120	-2.550945	41.C	-6.238280	3.776334	-5.345889
				74.H	-7.851503	1.525742	-1.905010	42.P	-6.208039	3.111087	-3.595355
				75.P	-4.226285	5.210688	-4.040071	43.Cl	9.252819	-7.770960	-3.488882
				76.C	-4.138651	4.867671	-5.886293	44.P	5.981576	-7.859379	-3.600392
				77.C	-5.549746	4.598436	-6.431839	45.C	6.007209	-8.782338	-1.979262
				78.P	-6.445556	3.407331	-5.295106	46.C	6.011672	-7.785927	-0.809712
				79.H	-2.857692	5.037552	-3.670657	47.P	7.265072	-6.429350	-1.116022
				80.H	-4.269731	6.636452	-4.009867	48.H	-1.053854	1.944285	-5.137700
				81.H	-3.654705	5.706313	-6.405996	49.H	3.577288	1.506012	-3.291505
				82.H	-6.154739	5.518499	-6.416067	50.H	2.975965	0.213857	-2.234154
				83.H	-5.522747	4.211344	-7.460064	51.H	3.149085	1.864035	-1.600444
				84.H	-3.497570	3.979847	-6.004618	52.H	-5.179877	4.155610	2.266832
				85.H	-7.758303	3.439983	-5.850689	53.H	-6.675478	2.885893	0.140149
				86.H	-6.038222	2.140969	-5.820289	54.H	-4.585374	2.343889	0.345066
				87.Cl	-7.507274	6.043769	-3.589707	55.H	-6.130784	5.285908	1.267798
								56.H	-3.047527	4.962842	1.246953
								57.H	-3.949346	6.404885	1.758440
								58.H	-2.541415	6.561495	-0.820141
								59.H	-4.539272	7.403997	-0.651257
								60.H	-3.612769	5.809224	-4.982804
								61.H	-4.970027	7.259445	-4.108129
								62.H	-5.952548	5.707900	-6.345384
								63.H	-7.063306	5.763045	-4.951479
								64.H	-7.147956	3.434897	-5.858169
								65.H	-5.375178	3.328415	-5.862503
								66.H	-7.584552	3.009440	-3.254334
								67.H	-5.913912	1.733069	-3.804661
								68.H	-0.277935	-2.686314	-3.681836
								69.H	-0.133847	-1.385046	-4.889598
								70.H	0.001245	-1.010699	-3.161124
								71.H	4.863446	-1.428539	-5.143626
								72.H	10.454155	-4.866437	-2.714084
								73.H	9.145438	-3.133276	-2.685828
3o											
1.C	0.133568	-0.089908	0.033189								
2.C	0.176753	-0.239897	1.532466								
3.C	1.688466	-0.080109	1.937019								
4.C	2.424502	0.215991	0.577006								
5.C	1.350783	0.204317	-0.481783								
6.F	-0.586639	0.725838	2.155512								
7.F	-0.312312	-1.452617	1.962314								
8.F	2.161825	-1.219412	2.515893								
9.F	1.858038	0.941720	2.822766								
10.F	3.392263	-0.736060	0.334970								
11.F	3.081077	1.424539	0.642356								
12.C	1.671065	0.474641	-1.902271								
13.C	2.128326	-0.537789	-2.797031								
14.C	2.322925	-0.100039	-4.097250								
15.S	1.952034	1.628578	-4.183123								
16.C	1.529141	1.718973	-2.495440								
17.H	2.300145	-1.570951	-2.503058								
18.C	1.058634	3.011643	-1.896669								
19.H	1.063734	2.953277	-0.800675								
20.H	0.033904	3.253615	-2.217977								
21.H	1.707080	3.850647	-2.186238								
22.H	0.026556	-5.033364	-8.300322								
23.C	2.722111	-0.821000	-5.234401								
24.C	3.062722	-1.470442	-6.231146								
25.Ru	3.691933	-2.591956	-7.801625								
26.P	2.193287	-4.340520	-7.299996								
27.C	0.875238	-4.417885	-8.630097								
28.C	0.435125	-2.994401	-9.005337								
29.P	1.943220	-1.892204	-9.223001								
30.H	2.601512	-5.705860	-7.248221								
31.H	1.410298	-4.317717	-6.104831								
32.H	1.358207	-4.914280	-9.486148								
33.H	-0.159187	-2.543757	-8.195052								
34.H	-0.176021	-2.986547	-9.918653								
35.H	1.330350	-0.602573	-9.191009								
36.H	2.168292	-1.977883	-10.629024								
37.P	5.463101	-3.341907	-6.450874								
38.C	6.831643	-2.058383	-6.421625								
39.C	6.943357	-1.393717	-7.802521								
40.P	5.232720	-0.924413	-8.414246								
41.H	5.095863	0.405171	-7.911106								
42.H	5.513837	-0.599270	-9.774758								
43.H	7.600920	-0.513501	-7.780061								
44.H	7.340474	-2.103365	-8.545397								
45.H	7.781559	-2.514823	-6.110336								
46.H	6.537275	-1.322241	-5.657133								
47.H	6.170403	-4.523153	-6.829261								
48.H	5.321249	-3.617629	-5.058260								
				3o ²⁺ HS							
				1.C	3.983698	-1.830755	-4.648215				
				2.C	2.700071	-1.241896	-4.720977				
				3.C	1.726725	-1.979651	-4.013398				
				4.S	2.423406	-3.362817	-3.249820				
				5.C	4.043971	-3.002216	-3.886170				
				6.C	2.430172	-0.077696	-5.571512				
				7.C	1.618959	1.005475	-5.391481				
				8.C	1.627803	1.898098	-6.621530				
				9.C	2.337607	1.057547	-7.728472				
				10.C	3.152274	0.014605	-6.904418				
				11.C	0.889559	1.463326	-4.199192				
				12.C	-0.438322	1.942843	-4.243228				
				13.C	-0.919305	2.432347	-3.022691				
				14.S	0.356344	2.284353	-1.794161				
				15.C	1.469764	1.592679	-2.919039				
				16.C	-2.143818	3.005187	-2.744331				

74.H	10.884441	-3.560446	-5.009436	42.F	-3.817854	7.650793	1.660653	10.H	3.726469	-1.200142	2.135458
75.H	9.219520	-3.044967	-5.352173	43.F	-2.650506	6.864043	3.359017	11.H	2.313323	-2.207119	1.724412
76.H	10.392459	-5.878047	-5.810185	44.C	1.724100	7.649699	1.588511	12.H	3.095324	-1.279824	-0.688573
77.H	9.810801	-4.757901	-7.069704	45.H	2.708256	7.899198	1.173251	13.H	3.448621	0.667006	0.199073
78.H	8.067315	-7.023948	-6.595533	46.H	1.396717	8.474636	2.238630	14.Cl	-0.170757	-2.319289	-0.152708
79.H	7.151988	-5.054499	-6.659565	47.H	1.806784	6.735529	2.190863	15.P	-2.227821	0.233151	-0.394004
80.H	6.879829	-5.440383	-0.166449	48.F	-4.084994	9.635019	3.361979	16.H	-3.068079	-0.542285	0.450441
81.H	8.441993	-6.916496	-0.484051	49.F	-2.130916	9.241539	4.308555	17.H	-2.944504	1.465919	-0.353717
82.H	6.229009	-8.285306	0.144240	50.F	-3.009801	10.903109	1.346455	18.C	-2.624827	-0.434603	-2.092715
83.H	6.931497	-9.379698	-1.992076	51.F	-1.441879	11.275205	2.847460	19.H	-2.539349	-1.528075	-2.005639
84.H	5.152202	-9.469674	-1.921785	52.S	2.014104	9.438012	-1.102627	20.H	-3.660739	-0.188505	-2.363052
85.H	5.034347	-7.287895	-0.712412	53.C	1.472897	11.082115	-0.642481	21.C	-1.628607	0.112971	-3.127697
86.H	6.209548	-8.888169	-4.554009	54.C	0.345932	11.063148	0.166843	22.H	-1.715117	-0.418351	-4.085272
87.H	4.592568	-7.633795	-3.828758	55.H	-0.069808	11.981131	0.576989	23.H	-1.811224	1.181555	-3.321631
3c	1.Ru	0.427570	0.269993	-0.277493	56.C	2.205351	12.182946	-1.084574	24.H	0.822379	0.880375
	2.P	0.456006	-0.101225	2.051044	57.C	-0.502346	8.414369	-1.602928	25.P	0.130822	-0.008379
	3.C	2.189220	0.160991	2.722437	58.H	-0.665571	9.356135	-2.143073	26.H	0.591497	-1.252970
	4.C	3.224297	-0.305050	1.686822	59.H	-0.074892	7.673303	-2.289479	27.C	0.388183	2.092926
5.P	2.768592	0.357822	-0.007245	60.H	-1.471744	8.041144	-1.240544	28.C	0.547551	3.348046	-0.018570
6.H	-0.313119	0.651289	2.988098	61.C	2.926054	13.099282	-1.512331	29.C	0.595175	4.697202	0.116416
7.H	0.145819	-1.411243	2.522789	62.Ru	4.126403	14.554406	-2.212228	30.S	1.848607	5.724271	-0.605212
8.H	2.282176	1.242669	2.907493	63.P	4.008616	13.711202	-4.413141	31.C	-0.356122	5.494742	0.847821
9.H	2.311536	-0.360125	3.682113	64.P	2.276563	15.838109	-2.908524	32.H	-1.225223	5.029392	1.308893
10.H	4.242163	0.005017	1.961128	65.P	4.315592	15.487870	-0.057079	33.C	-0.100765	6.832847	0.866585
11.H	3.209596	-1.401697	1.588351	66.P	6.049425	13.357186	-1.554998	34.C	-0.952867	7.874471	1.360746
12.H	3.659907	-0.382827	-0.837725	67.C	2.892433	14.813628	-5.439527	35.C	1.222563	7.265610	0.239279
13.H	3.452504	1.610895	-0.032199	68.C	1.688706	15.261158	-4.595624	36.C	0.918605	8.463722	-0.727137
14.Cl	0.642679	-2.253201	-0.630145	69.C	6.755008	14.119454	0.006593	37.C	0.276293	9.578388	0.098841
15.P	-1.901062	0.037832	-0.565399	70.C	5.610110	14.557628	0.933283	38.C	-0.762576	9.189378	1.009534
16.H	-2.635328	-1.038350	0.013486	71.H	2.477760	17.233803	-3.126306	39.C	-2.164578	7.708051	2.242048
17.H	-2.784454	1.103851	-0.215841	72.H	1.040078	15.911411	-2.200084	40.C	-2.471592	9.169533	2.738486
18.C	-2.281279	-0.206687	-2.385284	73.H	4.769989	16.836250	0.051362	41.C	-1.786053	10.087918	1.658353
19.H	-2.081866	-1.270543	-2.587841	74.H	3.244344	15.549655	0.883132	42.F	-3.237203	7.223828	1.526336
20.H	-3.342935	-0.008029	-2.587371	75.H	5.950087	11.979314	-1.194186	43.F	-1.961394	6.853928	3.288680
21.C	-1.363604	0.688811	-3.232129	76.H	7.213624	13.278810	-2.373797	44.C	2.237514	7.638156	1.344059
22.H	-1.420756	0.434693	-4.299682	77.H	3.460463	12.416687	-4.663778	45.H	3.211425	7.878196	0.900131
23.H	-1.639982	1.748845	-3.118652	78.H	5.156557	13.621280	-5.253116	46.H	1.886951	8.513405	1.910543
24.H	1.014917	1.644095	-3.297691	79.H	5.974541	15.176006	1.765363	47.H	2.363617	6.799554	2.040490
25.P	0.404952	0.547283	-2.618992	80.H	5.095028	13.681915	1.358541	48.F	-3.791759	9.411761	2.866779
26.H	0.917539	-0.513986	-3.422830	81.H	7.434833	13.415133	0.505752	49.F	-1.858663	9.363454	3.938614
27.C	0.265574	2.256918	0.000412	82.H	7.340841	14.990083	-0.327206	50.F	-2.718698	10.517936	0.748035
28.C	0.163559	3.480707	0.183817	83.H	1.007783	14.416065	-4.407956	51.F	-1.238542	11.205849	2.232859
29.C	0.094623	4.862681	0.356177	84.H	1.115713	16.055406	-5.093960	52.S	2.428709	9.263700	-1.473400
30.S	1.255755	5.915777	-0.509614	85.H	2.576663	14.296507	-6.356218	53.C	1.950000	10.888616	-0.946488
31.C	-0.806603	5.585055	1.125063	86.H	3.512347	15.678377	-5.723167	54.C	0.787945	10.826109	-0.097019
32.H	-1.607305	5.089754	1.669845	87.Cl	5.701755	16.341850	-3.140761	55.H	0.398972	11.727773	0.371092
33.C	-0.636244	6.984508	1.099527	3c ²⁺ LS	1.Ru	0.146520	0.174729	56.C	2.608045	12.021678	-1.297869
34.C	-1.433601	7.995832	1.597412					57.C	-0.019197	8.063181	-1.889328
35.C	0.694515	7.418422	0.457672					58.H	-0.262980	8.942659	-2.498688
36.C	0.451062	8.672953	-0.412464					59.H	0.465672	7.314551	-2.527802
37.C	-0.163873	9.782043	0.460538	2.P	0.095888	-0.101329	2.278399	60.H	-0.955993	7.637316	-1.500700
38.C	-1.140185	9.388770	1.355365	3.C	1.824498	-0.440540	2.915974	61.C	3.140754	13.132748	-1.587490
39.C	-2.666846	7.874808	2.419542	4.C	2.664305	-1.172708	1.856630	62.Ru	3.957409	14.821911	-2.056707
40.C	-2.796614	9.275145	3.110693	5.P	2.458694	-0.359205	0.187390	63.P	4.034216	14.409031	-4.412014
41.C	-2.059806	10.259484	2.136596	6.H	-0.365894	0.893765	3.187686	64.P	1.899370	15.912430	-2.621888
				7.H	-0.662175	-1.213590	2.733720	65.P	4.063766	15.660936	0.185106
				8.H	2.261388	0.541807	3.154540	66.P	6.206896	14.154469	-1.591974
				9.H	1.769258	-1.015740	3.850260				

67.C	2.842982	15.578390	-5.251087	35.S	3.700439	-1.821123	-3.083433	92.H	-7.088228	-0.455470	-3.468893	
68.C	1.537511	15.682390	-4.445729	36.C	2.402902	-2.097089	-1.963118	93.H	-8.302264	2.238605	-4.394451	
69.C	6.809229	15.119636	-0.110164	37.C	4.887331	-3.978921	-4.336212	94.H	-7.535364	1.016797	-5.443986	
70.C	5.707479	15.202073	0.958976	38.C	5.738691	-4.284236	-5.183251	95.H	-5.987810	3.411540	-5.004564	
71.H	1.906395	17.324236	-2.455962	39.Ru	7.118686	-4.795392	-6.672036	96.H	-4.988969	1.510999	-4.837379	
72.H	0.639610	15.610968	-2.028274	40.C	9.913929	-6.016537	-10.336947	97.H	-5.250697	1.974137	1.500064	
73.H	4.025402	17.077851	0.293167	41.C	10.038903	-5.165033	-11.457133	98.H	-6.508233	3.694231	1.206224	
74.H	3.143574	15.320292	1.218351	42.C	10.767536	-5.529661	-12.584872	99.H	-4.115045	4.623813	1.853931	
75.H	6.509951	12.804714	-1.245547	43.C	11.414276	-6.786336	-12.666056	100.H	-4.603742	5.853878	-0.272620	
76.H	7.227336	14.381468	-2.554235	44.C	11.322279	-7.630015	-11.533098	101.H	-2.832885	5.642385	-0.182505	
77.H	3.668316	13.136635	-4.941805	45.C	10.590176	-7.254312	-10.411065	102.H	-3.114401	3.442852	0.974342	
78.H	5.242885	14.620361	-5.128355	46.C	1.768814	-0.936606	-1.258265	103.H	-3.959107	5.308442	-2.808141	
79.H	5.964725	15.927371	1.742885	47.C	-0.335790	-3.616590	-3.922419	104.H	-2.558681	3.822153	-2.122608	
80.H	5.556186	14.225283	1.444662	48.N	12.091967	-7.187174	-13.824409	105.H	-9.751769	5.935298	-0.434182	
81.H	7.724159	14.662919	0.291083	49.C	12.986824	-8.332116	-13.743639	106.H	9.548002	-4.191291	-11.432109	
82.H	7.059940	16.120110	-0.493232	50.P	5.941516	-6.753667	-7.224422	107.H	10.828577	-4.825062	-13.412473	
83.H	0.949381	14.754844	-4.527604	51.C	5.027867	-6.488509	-8.839182	108.H	11.824279	-8.595903	-11.524455	
84.H	0.909331	16.507851	-4.807404	52.C	4.438961	-5.070410	-8.871098	109.H	11.498640	-5.705488	-15.205552	
85.H	2.653207	15.248237	-6.281472	53.P	5.730516	-3.828917	-8.306032	110.H	12.909739	-6.665608	-15.671890	
86.H	3.360047	16.548889	-5.287520	54.P	8.538527	-5.767150	-5.072090	111.H	13.078916	-5.381680	-14.439239	
87.C1	5.063841	16.983304	-2.713217	55.C	9.579347	-4.440038	-4.246778	112.H	13.405759	-8.526706	-14.737578	
4o				56.C	9.938252	-3.351222	-5.268771	113.H	13.823793	-8.180964	-13.033962	
				57.P	8.409480	-2.879780	-6.249091	114.H	12.437676	-9.232755	-13.435898	
	1.C	-9.585753	6.640289	-1.249500	58.P	-7.443448	1.113488	-1.658635	115.H	-11.646723	11.493033	-3.616402
	2.C	-8.539861	6.385420	-2.163588	59.C	-7.786670	0.388379	-3.356111	116.H	-9.989146	10.973056	-3.950891
	3.C	-8.381894	7.318479	-3.212104	60.C	-7.533017	1.451840	-4.434985	117.H	-7.595261	7.150356	-3.948750
	4.C	-9.200447	8.436553	-3.336243	61.P	-5.904204	2.317382	-4.093582	118.H	-9.030859	9.112430	-4.172461
	5.C	-10.230678	8.699315	-2.401855	62.C	12.413725	-6.179542	-14.823929	119.H	-11.358190	10.028733	-4.600803
	6.C	-10.410695	7.754907	-1.362967	63.C	-11.003249	10.612952	-3.729212	120.H	-11.203965	7.888666	-0.629684
	7.Ru	-5.638349	2.615869	-1.778567	64.H	2.980275	-5.352084	-2.678268	121.H	-12.972427	9.121466	-1.977283
	8.P	-3.916122	4.210189	-1.900018	65.H	1.472593	-1.218193	-0.238223	122.H	-12.722150	10.888369	-1.866646
9.C	-3.791351	5.110855	-0.261175	66.H	0.860288	-0.592387	-1.778076	123.H	-12.029178	9.824957	-0.634195	
10.C	-3.984466	4.112734	0.890214	67.H	2.463182	-0.089011	-1.189424	124.C	8.438503	-5.322893	-8.230595	
11.P	-5.457683	3.002679	0.531803	68.H	4.252105	-7.254518	-8.976217	125.C	9.137610	-5.646123	-9.198164	
12.N	-11.019333	9.853961	-2.487383	69.H	6.599757	-7.989834	-7.489884	126.C	-7.691608	5.244313	-2.040617	
13.C	-12.246855	9.913623	-1.707444	70.H	4.903758	-7.260221	-6.382271	127.C	-6.956265	4.255778	-1.933172	
14.C	-4.292800	1.015165	-1.695946	71.H	5.786127	-6.612562	-9.627636	4o+				
15.C	-3.492950	0.068655	-1.716542	72.H	3.603339	-4.979645	-8.159640		1.C	-9.379450	6.866060	-0.097323
16.C	-2.576087	-0.980389	-1.885747	73.H	4.065989	-4.807409	-9.870510		2.C	-8.973509	6.457129	-1.392686
17.S	-2.152021	-1.523354	-3.521303	74.H	4.907357	-2.687125	-8.070313		3.C	-9.574255	7.126133	-2.489189
18.C	-1.030751	-2.716973	-2.946790	75.H	6.297574	-3.413748	-9.547812		4.C	-10.507321	8.133075	-2.311112
19.C	-0.979562	-2.698488	-1.552857	76.H	7.890456	-1.800123	-5.470303		5.C	-10.904593	8.541799	-1.009421
20.C	-1.866094	-1.734500	-0.970448	77.H	8.995485	-2.100459	-7.290494		6.C	-10.313459	7.869639	0.094405
21.C	-0.164151	-3.614943	-0.756001	78.H	10.375335	-2.466705	-4.785156		7.Ru	-5.786722	3.011609	-2.050647
22.C	-0.751800	-4.265010	0.471938	79.H	10.659401	-3.733500	-6.007718		8.P	-4.166794	4.695128	-2.397131
23.C	0.175778	-5.483901	0.754754	80.H	10.475857	-4.882091	-3.790624		9.C	-3.640912	5.382189	-0.739009
24.C	1.512959	-5.084869	0.059674	81.H	8.953550	-4.026097	-3.440878	10.C	-3.556612	4.248009	0.289466	
25.C	1.136781	-4.014123	-0.934899	82.H	9.536699	-6.702221	-5.482572	11.P	-5.093330	3.182996	0.193842	
26.F	-0.723861	-3.409368	1.571615	83.H	8.066456	-6.476777	-3.927673	12.N	-11.823306	9.550636	-0.825057	
27.F	-2.056042	-4.658649	0.333623	84.H	10.534906	-7.933278	-9.559222	13.C	-12.270174	9.900890	0.517224	
28.F	-0.346981	-6.596849	0.152491	85.H	-0.209555	-4.622583	-3.498156	14.C	-4.387127	1.504587	-2.357269	
29.F	0.321251	-5.755415	2.080417	86.H	0.669472	-3.243716	-4.175624	15.C	-3.572718	0.583992	-2.521679	
30.F	2.106557	-6.194275	-0.511320	87.H	-0.910657	-3.708340	-4.853216	16.C	-2.657201	-0.454239	-2.730789	
31.F	2.408735	-4.623050	1.004150	88.H	-1.963543	-1.580323	0.101475	17.S	-2.321044	-1.069784	-4.360066	
32.C	2.152825	-3.464078	-1.839513	89.H	-8.736139	1.590551	-1.284481	18.C	-1.192464	-2.254893	-3.781573	
33.C	3.026172	-4.267432	-2.641614	90.H	-7.434001	-0.071166	-0.863523	19.C	-1.071420	-2.175444	-2.393337	
34.C	3.926080	-3.549385	-3.407932	91.H	-8.811046	-0.005884	-3.406141					

20.C	-1.905509	-1.171024	-1.815217	77.H	9.033534	-2.353773	-8.112149	5.C	-10.716390	8.564518	-1.586094
21.C	-0.248905	-3.078139	-1.589218	78.H	10.005931	-2.183215	-5.382912	6.C	-10.151082	8.048708	-0.381875
22.C	-0.819403	-3.678501	-0.321857	79.H	10.480756	-3.645835	-6.278172	7.Ru	-5.871921	2.744451	-1.781422
23.C	0.113444	-4.892847	-0.004371	80.H	9.951662	-4.338193	-3.930910	8.P	-4.167302	4.357406	-1.369498
24.C	1.436659	-4.532138	-0.757942	81.H	8.381879	-3.505101	-4.009613	9.C	-4.103551	4.752503	0.458770
25.C	1.032747	-3.502766	-1.794234	82.H	9.335901	-6.491822	-5.401202	10.C	-4.366456	3.481106	1.279506
26.F	-0.771144	-2.768831	0.727283	83.H	7.628612	-6.065273	-4.139229	11.P	-5.840028	2.557277	0.581865
27.F	-2.126846	-4.067443	-0.443340	84.H	10.165975	-8.727832	-9.457533	12.N	-11.564430	9.638426	-1.567497
28.F	-0.428483	-6.025651	-0.550244	85.H	-0.407900	-4.192612	-4.242152	13.C	-11.920938	10.280977	-0.303021
29.F	0.294136	-5.097781	1.324259	86.H	0.420352	-2.874233	-5.081328	14.C	-4.448907	1.250728	-1.940871
30.F	2.013660	-5.659382	-1.299955	87.H	-1.198704	-3.384076	-5.613739	15.C	-3.591317	0.358347	-2.070207
31.F	2.358611	-4.010715	0.127467	88.H	-1.953142	-0.969733	-0.747572	16.C	-2.641698	-0.643182	-2.270213
32.C	2.018766	-3.010364	-2.760038	89.H	-8.646768	1.686605	-1.056470	17.S	-2.425630	-1.383627	-3.866853
33.C	2.854008	-3.863320	-3.543713	90.H	-7.140047	0.133551	-0.997806	18.C	-1.174990	-2.442534	-3.308667
34.C	3.757878	-3.193608	-4.352546	91.H	-8.969209	0.186330	-3.249533	19.C	-0.920792	-2.229531	-1.945658
35.S	3.567686	-1.448040	-4.109235	92.H	-7.255219	-0.051093	-3.664925	20.C	-1.760128	-1.232993	-1.374202
36.C	2.290530	-1.654240	-2.951796	93.H	-8.892539	2.536132	-4.111043	21.C	0.032294	-3.011565	-1.156925
37.C	4.718609	-3.703160	-5.235041	94.H	-8.244201	1.477256	-5.386334	22.C	-0.363584	-3.517599	0.212352
38.C	5.585127	-4.157326	-5.997488	95.H	-6.867187	4.007513	-5.052935	23.C	0.660216	-4.654712	0.521892
39.Ru	7.074385	-4.918886	-7.234698	96.H	-5.676372	2.213899	-5.254175	24.C	1.876740	-4.296913	-0.390990
40.C	10.492891	-6.661477	-10.014292	97.H	-4.703997	2.052212	0.968653	25.C	1.310523	-3.386204	-1.459189
41.C	11.300273	-5.822307	-10.824743	98.H	-5.955575	3.806778	1.142896	26.F	-0.241999	-2.517287	1.168418
42.C	12.299276	-6.330357	-11.638096	99.H	-3.421619	4.635161	1.308442	27.F	-1.649999	-3.969185	0.285181
43.C	12.558020	-7.727350	-11.696261	100.H	-4.416418	6.109173	-0.456013	28.F	0.129298	-5.849464	0.127052
44.C	11.758526	-8.574029	-10.880034	101.H	-2.686414	5.917870	-0.830357	29.F	0.986207	-4.738089	1.833775
45.C	10.761820	-8.053357	-10.071969	102.H	-2.711876	3.580192	0.064510	30.F	2.456519	-5.438494	-0.898712
46.C	1.695978	-0.462503	-2.269038	103.H	-4.450110	5.885165	-3.126937	31.F	2.848693	-3.662712	0.348270
47.C	-0.563524	-3.223386	-4.733241	104.H	-2.917718	4.363423	-3.001031	32.C	2.166956	-2.928451	-2.559640
48.N	13.541655	-8.240297	-12.512794	105.H	-8.944402	6.368563	0.769276	33.C	2.954757	-3.798597	-3.362157
49.C	13.831111	-9.669320	-12.508290	106.H	11.125014	-4.746940	-10.803037	34.C	3.750495	-3.151650	-4.299534
50.P	5.905638	-6.950444	-7.485520	107.H	12.889461	-5.639391	-12.236770	35.S	3.511146	-1.401123	-4.153966
51.C	5.040824	-6.958778	-9.145446	108.H	11.923987	-9.649558	-10.880709	36.C	2.366406	-1.573775	-2.866489
52.C	4.500281	-5.558663	-9.458993	109.H	13.782382	-6.730225	-13.982578	37.C	4.653091	-3.683163	-5.220204
53.P	5.822321	-4.274467	-9.131233	110.H	15.073472	-7.946913	-13.901663	38.C	5.496404	-4.137810	-6.014645
54.P	8.273868	-5.545152	-5.298015	111.H	14.981017	-6.676580	-12.658211	39.Ru	6.955975	-4.875301	-7.284649
55.C	9.138222	-4.037403	-4.604863	112.H	14.620326	-9.875825	-13.236905	40.C	10.289439	-6.513984	-10.189953
56.C	9.649827	-3.155369	-5.749972	113.H	14.175461	-10.014016	-11.519182	41.C	11.052642	-5.636434	-11.010870
57.P	8.301400	-2.917520	-7.026885	114.H	12.944283	-10.257253	-12.791345	42.C	12.024576	-6.106881	-11.868945
58.P	-7.421236	1.341463	-1.698202	115.H	-13.126519	10.975425	-1.619820	43.C	12.304749	-7.502868	-11.963158
59.C	-8.001458	0.695097	-3.354701	116.H	-11.715745	10.636692	-2.642480	44.C	11.545683	-8.388223	-11.140883
60.C	-8.074716	1.845745	-4.365629	117.H	-9.288919	6.835381	-3.499982	45.C	10.574471	-7.905096	-10.289098
61.P	-6.504082	2.860620	-4.288939	118.H	-10.937321	8.610538	-3.189397	46.C	1.808796	-0.353443	-2.200859
62.C	14.384970	-7.347760	-13.298717	119.H	-13.059909	9.463637	-2.556583	47.C	-0.599159	-3.464486	-4.239008
63.C	-12.461473	10.182141	-1.972998	120.H	-10.593053	8.137565	1.111243	48.N	13.267738	-7.976126	-12.812431
64.H	2.794445	-4.947418	-3.524953	121.H	-12.782616	9.059616	1.011860	49.C	13.547488	-9.409013	-12.892364
65.H	1.387347	-0.722491	-1.248623	122.H	-12.970537	10.738557	0.452070	50.P	5.769266	-6.908843	-7.548791
66.H	0.803267	-0.093040	-2.795883	123.H	-11.425117	10.212030	1.149730	51.C	4.862043	-6.895142	-9.188114
67.H	2.418679	0.361175	-2.207829	124.C	8.575086	-5.680931	-8.457440	52.C	4.321128	-5.487340	-9.481042
68.H	4.242659	-7.713141	-9.158644	125.C	9.471799	-6.136024	-9.186321	53.P	5.647971	-4.204850	-9.156305
69.H	6.566877	-8.212974	-7.503946	126.C	-8.019963	5.429029	-1.582770	54.P	8.213268	-5.534182	-5.373268
70.H	4.847095	-7.277165	-6.586571	127.C	-7.187183	4.524274	-1.752241	55.C	9.092911	-4.040635	-4.665492
71.H	5.803495	-7.255878	-9.880221					56.C	9.565758	-3.118357	-5.799665
72.H	3.663599	-5.305529	-8.791305	4o ²⁺ LS				57.P	8.188071	-2.864223	-7.044478
73.H	4.143098	-5.485240	-10.495167	1.C	-9.291953	6.969936	-0.408351	58.P	-7.564297	1.116892	-2.179370
74.H	5.063845	-3.068418	-9.175956	2.C	-8.936488	6.324646	-1.626349	59.C	-7.648620	0.734098	-4.009441
75.H	6.468705	-4.169108	-10.398453	3.C	-9.510358	6.839803	-2.822708	60.C	-7.405630	2.013183	-4.824517
76.H	7.651015	-1.733157	-6.568597	4.C	-10.366069	7.921424	-2.810832	61.P	-5.925870	2.937384	-4.142129

62.C	14.031165	-7.056694	-13.654816	119.H	-12.730533	9.409479	-3.329114	47.C	-0.593932	-2.319152	-4.871379
63.C	-12.120360	10.165945	-2.812562	120.H	-10.393430	8.506296	0.574970	48.N	11.512504	-12.005619	-12.141574
64.H	2.947267	-4.880558	-3.266065	121.H	-12.410461	9.570119	0.379594	49.C	11.674192	-13.383505	-11.678404
65.H	1.675332	-0.531389	-1.125077	122.H	-12.617732	11.098947	-0.502862	50.P	4.653778	-6.259018	-9.577358
66.H	0.825200	-0.080084	-2.615070	123.H	-11.033314	10.697358	0.197678	51.C	5.304967	-5.100131	-10.896296
67.H	2.478872	0.506273	-2.324745	124.C	8.416910	-5.596562	-8.549618	52.C	6.026441	-3.911538	-10.243733
68.H	4.058548	-7.644024	-9.186655	125.C	9.297667	-6.028297	-9.320283	53.P	7.175878	-4.519217	-8.895725
69.H	6.421804	-8.173731	-7.598990	126.C	-8.048318	5.235060	-1.649902	54.P	5.141008	-8.108288	-6.563580
70.H	4.734449	-7.245562	-6.628066	127.C	-7.252968	4.274395	-1.678659	55.C	5.834769	-8.205496	-4.827114
71.H	5.603015	-7.192935	-9.945846					56.C	7.339425	-7.899084	-4.844367
72.H	3.489923	-5.239939	-8.802873	4o ²⁺ HS				57.P	7.675608	-6.386549	-5.894928
73.H	3.954220	-5.402056	-10.512802	1.C	-9.926917	7.213595	-2.508643	58.P	-4.131075	4.937582	-0.253481
74.H	4.888337	-3.000406	-9.165984	2.C	-9.023798	6.883503	-1.458420	59.C	-4.351212	3.584438	1.022070
75.H	6.270547	-4.073944	-10.431036	3.C	-9.371350	7.314580	-0.146487	60.C	-5.747839	2.959359	0.889180
76.H	7.535605	-1.698668	-6.547744	4.C	-10.534716	8.010466	0.104051	61.P	-6.127392	2.609461	-0.910467
77.H	8.892987	-2.263751	-8.126829	5.C	-11.440734	8.326924	-0.952094	62.C	12.257569	-11.561745	-13.319200
78.H	9.913591	-2.150755	-5.413402	6.C	-11.093572	7.908457	-2.271419	63.C	-12.948815	9.421461	0.650920
79.H	10.395628	-3.579644	-6.356922	7.Ru	-5.175103	4.305015	-2.286382	64.H	2.654517	-4.527340	-3.735496
80.H	9.929325	-4.358890	-4.028666	8.P	-6.185143	3.648424	-4.326885	65.H	2.454371	0.363624	-2.644435
81.H	8.355087	-3.530200	-4.027589	9.C	-5.825342	4.914050	-5.660967	66.H	1.548854	0.619163	-4.147098
82.H	9.269779	-6.477554	-5.526191	10.C	-4.412455	5.487444	-5.475177	67.H	3.302720	0.911122	-4.108488
83.H	7.596709	-6.084837	-4.214713	11.P	-4.139323	5.935733	-3.678552	68.H	4.486404	-4.768861	-11.549449
84.H	10.007740	-8.599899	-9.669803	12.N	-12.602791	9.006187	-0.708182	69.H	4.316016	-7.408299	-10.347045
85.H	-0.385735	-4.396409	-3.697744	13.C	-13.525013	9.315589	-1.800358	70.H	3.339252	-5.761925	-9.346823
86.H	0.347204	-3.119725	-4.685184	14.C	-3.604650	3.000837	-2.675232	71.H	6.003239	-5.695869	-11.504146
87.H	-1.295606	-3.693794	-5.054909	15.C	-2.778977	2.090913	-2.860051	72.H	5.306170	-3.243090	-9.747494
88.H	-1.720897	-0.940364	-0.327907	16.C	-1.954397	0.981530	-3.069842	73.H	6.583842	-3.320958	-10.983303
89.H	-8.916953	1.433239	-1.864447	17.S	-2.030226	0.058155	-4.578756	74.H	7.513760	-3.300151	-8.242140
90.H	-7.506956	-0.185851	-1.609777	18.C	-0.897449	-1.127333	-4.018199	75.H	8.397078	-4.723676	-9.601690
91.H	-8.614252	0.273147	-4.257251	19.C	-0.458568	-0.817118	-2.724432	76.H	7.610394	-5.324395	-4.949980
92.H	-6.858282	-0.008090	-4.200108	20.C	-1.066121	0.363772	-2.204736	77.H	9.088835	-6.454850	-6.052907
93.H	-8.261004	2.700328	-4.734209	21.C	0.418501	-1.659633	-1.910866	78.H	7.734077	-7.750594	-3.830226
94.H	-7.259239	1.792249	-5.890431	22.C	0.106346	-1.819975	-0.438428	79.H	7.902153	-8.722924	-5.309603
95.H	-6.045623	4.193552	-4.803033	23.C	0.892531	-3.090735	-0.000519	80.H	5.627087	-9.190443	-4.387649
96.H	-4.850626	2.400002	-4.907971	24.C	2.029258	-3.185764	-1.063026	81.H	5.290397	-7.449465	-4.240772
97.H	-5.733725	1.305813	1.252856	25.C	1.538840	-2.372391	-2.242742	82.H	5.293878	-9.446150	-7.031745
98.H	-6.923794	3.103534	1.328757	26.F	0.557895	-0.728637	0.292843	83.H	3.740011	-8.137827	-6.310104
99.H	-4.529074	3.711469	2.341042	27.F	-1.227217	-1.941685	-0.162285	84.H	8.574944	-11.025115	-8.781213
100.H	-4.891098	5.501642	0.633083	28.F	0.074364	-4.179419	-0.106262	85.H	-1.394258	-2.500204	-5.599452
101.H	-3.138360	5.209149	0.716231	29.F	1.355563	-3.022537	1.270977	86.H	-0.486609	-3.217782	-4.247912
102.H	-3.513164	2.788925	1.210376	30.F	2.288501	-4.504788	-1.370773	87.H	0.349355	-2.191680	-5.425473
103.H	-4.194901	5.658252	-1.946849	31.F	3.198239	-2.674053	-0.548858	88.H	-0.864904	0.755862	-1.211348
104.H	-2.814182	4.020303	-1.661963	32.C	2.338239	-2.346877	-3.473109	89.H	-4.597237	6.092455	0.440135
105.H	-8.872154	6.594187	0.524473	33.C	2.859471	-3.521272	-4.088066	90.H	-2.733064	5.191972	-0.161008
106.H	10.855579	-4.566036	-10.955951	34.C	3.656290	-3.283317	-5.197291	91.H	-4.179113	3.979919	2.032204
107.H	12.579585	-5.396182	-12.477448	35.S	3.766604	-1.538783	-5.470238	92.H	-3.569489	2.838889	0.810429
108.H	11.727680	-9.459993	-11.179119	36.C	2.755689	-1.171402	-4.110409	93.H	-6.524861	3.659254	1.232990
109.H	13.369915	-6.496867	-14.333228	37.C	4.344810	-4.197467	-5.999939	94.H	-5.836996	2.038115	1.480498
110.H	14.737254	-7.630663	-14.260251	38.C	5.006118	-4.982180	-6.700391	95.H	-7.527680	2.355356	-0.865958
111.H	14.601669	-6.338956	-13.046233	39.Ru	6.178738	-6.337521	-7.750147	96.H	-5.664182	1.273851	-1.077349
112.H	14.348233	-9.576085	-13.617283	40.C	8.958026	-9.335923	-10.086332	97.H	-2.735581	6.168832	-3.647028
113.H	13.874468	-9.805265	-11.919298	41.C	9.686900	-8.928130	-11.239529	98.H	-4.580331	7.289780	-3.627279
114.H	12.660240	-9.970547	-13.221898	42.C	10.520141	-9.794071	-11.915049	99.H	-4.242251	6.362355	-6.117062
115.H	-12.758687	11.022953	-2.583041	43.C	10.683492	-11.142845	-11.478532	100.H	-6.583904	5.703497	-5.545389
116.H	-11.323283	10.501442	-3.493462	44.C	9.953072	-11.560086	-10.325832	101.H	-5.952921	4.465667	-6.655473
117.H	-9.256358	6.366214	-3.770914	45.C	9.123033	-10.684292	-9.659194	102.H	-3.649047	4.732159	-5.717416
118.H	-10.773928	8.281418	-3.752876	46.C	2.504796	0.256536	-3.736757	103.H	-7.593009	3.482600	-4.465124

104.H	-5.768412	2.431685	-4.940158	32. C	2.208393	-2.034899	-4.179913	89. H	-9.005196	2.160828	-3.049318		
105.H	-9.685559	6.899377	-3.523695	33. C	2.966394	-3.059729	-4.796935	90. H	-7.482578	0.656546	-3.383284		
106.H	9.581281	-7.901249	-11.588577	34. C	3.848832	-2.614794	-5.782638	91. H	-8.452060	2.168662	-5.680430		
107.H	11.057769	-9.434171	-12.789476	35. S	3.702657	-0.856569	-5.948336	92. H	-6.687368	1.981862	-5.587211		
108.H	10.046123	-12.580258	-9.960127	36. C	2.504691	-0.758893	-4.708364	93. H	-8.289590	4.578447	-5.049762		
109.H	11.577350	-11.234349	-14.119529	37. C	4.795340	-3.345368	-6.488954	94. H	-7.129454	4.312713	-6.366922		
110.H	12.856421	-12.394308	-13.696877	38. C	5.705288	-3.996042	-7.047608	95. H	-6.216825	6.074754	-4.225844		
111.H	12.936491	-10.732316	-13.070787	39. Ru	7.278856	-5.068812	-7.829914	96. H	-4.850627	4.566023	-4.965527		
112.H	12.373237	-13.902064	-12.339383	40. C	10.868829	-7.520291	-9.529320	97. H	-5.927012	0.742648	-0.105671		
113.H	12.078146	-13.414138	-10.655441	41. C	11.920061	-6.892995	-10.280414	98. H	-7.211864	2.246482	0.779564		
114.H	10.716016	-13.923809	-11.696592	42. C	12.988275	-7.606516	-10.751707	99. H	-4.850119	2.389855	2.050588		
115.H	-13.908545	9.943890	0.630474	43. C	13.098345	-9.019523	-10.501359	100. H	-5.296076	4.759105	1.404726		
116.H	-13.042034	8.553122	1.320244	44. C	12.046867	-9.654784	-9.751383	101. H	-3.534151	4.543823	1.384105		
117.H	-8.695716	7.082064	0.676245	45. C	10.979445	-8.932423	-9.292008	102. H	-3.774977	2.167050	0.654288		
118.H	-10.757085	8.315941	1.124086	46. C	1.992295	0.579847	-4.285738	103. H	-4.618853	6.174227	-0.776359		
119.H	-12.191829	10.105439	1.062433	47. C	-0.770197	-2.209737	-5.669749	104. H	-3.134541	4.677276	-1.269662		
120.H	-11.753299	8.132437	-3.106764	48. N	14.154398	-9.726263	-10.954519	105. H	-8.743981	6.280071	1.524869		
121.H	-13.043421	9.949463	-2.559691	49. C	14.359161	-11.137019	-10.591466	106. H	11.861360	-5.821523	-10.465543		
122.H	-14.385473	9.856049	-1.397965	50. P	7.278430	-6.434963	-5.853410	107. H	13.773327	-7.087746	-11.296445		
123.H	-13.889240	8.397582	-2.285474	51. C	6.371280	-8.036544	-6.179117	108. H	12.081104	-10.725620	-9.566367		
124.C	7.374786	-7.660298	-8.773967	52. C	5.182685	-7.795224	-7.121358	109. H	14.700787	-8.473782	-12.579108		
125.C	8.120862	-8.445788	-9.395136	53. P	5.708289	-6.737052	-8.568579	110. H	15.686169	-9.935340	-12.365747		
126.C	-7.853845	6.147434	-1.703257	54. P	8.764541	-3.349774	-7.036252	111. H	15.906328	-8.562243	-11.251573		
127.C	-6.810800	5.492640	-1.911070	55. C	8.696164	-1.875402	-8.180627	112. H	15.415298	-11.382518	-10.735336		
4o ⁴⁺ LS				56. C	8.558420	-2.340190	-9.637945	113. H	14.102776	-11.309647	-9.541604		
	1. C	-9.596373	6.516375	0.889577	57. P	7.244778	-3.662732	-9.777883	114. H	13.755140	-11.793817	-11.235264	
	2. C	-9.593085	6.050030	-0.468938	58. P	-7.618969	2.071258	-3.358240	115. H	-14.369191	9.641330	0.693297	
	3. C	-10.722781	6.392432	-1.287076	59. C	-7.548000	2.525473	-5.168586	116. H	-13.504584	9.126640	-0.769714	
	4. C	-11.763868	7.132965	-0.797076	60. C	-7.369842	4.042445	-5.329792	117. H	-10.746958	6.040474	-2.317422	
	5. C	-11.764065	7.591485	0.567362	61. C	-6.033040	4.665244	-4.181459	118. H	-12.610573	7.349240	-1.443916	
	6. C	-10.634822	7.251625	1.392556	62. C	15.168076	-9.129499	-11.838018	119. H	-14.634670	7.999660	0.052991	
	7. Ru	-6.089267	3.440499	-2.111227	63. C	-13.886337	8.792879	0.200081	120. H	-10.587060	7.602411	2.420604	
	8. P	-4.500040	4.760801	-0.880004	64. H	2.898265	-4.108204	-4.525530	121. H	-12.560590	7.839540	3.113920	
	9. C	-4.471745	4.223104	0.910111	65. H	1.884101	0.617785	-3.192511	122. H	-13.920922	8.909375	2.716843	
	10. C	-4.666238	2.703203	1.014079	66. H	1.001950	0.784578	-4.722874	123. H	-12.262268	9.560441	2.697281	
	11. P	-6.079764	2.155549	-0.077864	67. H	2.668953	1.384889	-4.595221	124. C	8.823137	-6.129856	-8.589982	
	12. N	-12.790345	8.316692	1.057966	68. H	6.049256	-8.485669	-5.229899	125. C	9.794027	-6.790464	-9.045925	
	13. C	-12.878743	8.674697	2.482198	69. H	8.487567	-6.882753	-5.253266	126. C	-8.543422	5.294930	-0.968101	
	14. C	-4.562742	2.232509	-2.779364	70. H	6.630555	-5.916209	-4.698336	127. C	-7.598400	4.596541	-1.422379	
	15. C	-3.649390	1.458633	-3.139768	71. H	7.104101	-8.717248	-6.638520	4o ⁴⁺ HS				
	16. C	-2.664151	0.548932	-3.500541	72. H	4.382506	-7.238642	-6.610025		1.C	-9.551610	7.372768	0.011056
	17. S	-2.615533	-0.202014	-5.106186	73. H	4.755979	-8.740430	-7.483288		2.C	-9.611866	5.992774	-0.350933
	18. C	-1.270536	-1.201074	-4.687668	74. H	4.466278	-6.370397	-9.154544		3.C	-10.841264	5.300764	-0.125245
	19. C	-0.851530	-0.964846	-3.360494	75. H	6.141691	-7.688692	-9.533480		4.C	-11.930587	5.935491	0.420042
	20. C	-1.645113	0.014209	-2.713248	76. H	6.057120	-2.922368	-10.030952		5.C	-11.864318	7.318613	0.789115
	21. C	0.154550	-1.743354	-2.630745	77. H	7.469265	-4.183002	-11.082358		6.C	-10.632785	8.015280	0.564876
	22. C	-0.145701	-2.071828	-1.176120	78. H	8.320733	-1.502857	-10.307939		7.Ru	-5.918448	3.651537	-2.124892
	23. C	0.803836	-3.254970	-0.824215	79. H	9.494122	-2.797464	-9.994314		8.P	-4.521305	5.084020	-0.789265
	24. C	1.955801	-3.095290	-1.864196	80. H	9.587379	-1.249138	-8.039056		9.C	-4.624905	4.562849	1.001032
	25. C	1.365225	-2.264565	-2.996412	81. H	7.819002	-1.287336	-7.870478		10.C	-4.675122	3.031336	1.105298
	26. F	0.148192	-0.986875	-0.364180	82. H	10.154192	-3.645605	-6.958676		11.P	-5.911619	2.335168	-0.112505
	27. F	-1.451005	-2.392616	-0.944564	83. H	8.584332	-2.762596	-5.754427		12.N	-12.937255	7.949422	1.334697
	28. F	0.148652	-4.428415	-1.051603	84. H	10.186675	-9.432494	-8.737552		13.C	-12.842736	9.331620	1.825352
	29. F	1.236551	-3.228276	0.453913	85. H	-0.528708	-3.151389	-5.156522		14.C	-4.357911	2.553443	-2.825761
	30. F	2.404925	-4.330030	-2.273745	86. H	0.148441	-1.861003	-6.167709		15.C	-3.440187	1.795666	-3.230299
	31. F	3.026339	-2.455139	-1.294398	87. H	-1.515443	-2.418545	-6.446013					
				88. H	-1.496817	0.325057	-1.682917						

16.C	-2.492586	0.890985	-3.669375	73.H	4.788226	-8.644910	-7.511686	1.C	-0.848972	11.107695	-0.400535
17.S	-2.290823	0.484411	-5.386376	74.H	4.568824	-6.275973	-9.193383	2.C	-1.308833	9.805617	-0.682865
18.C	-1.111269	-0.728522	-5.040061	75.H	6.220239	-7.629668	-9.544909	3.C	-0.172748	8.818301	-1.005579
19.C	-0.852470	-0.817540	-3.650989	76.H	6.256072	-2.866235	-10.069704	4.S	1.370319	9.657733	-0.352630
20.C	-1.633009	0.092991	-2.904473	77.H	7.638053	-4.178701	-11.099929	5.C	0.518530	11.225346	-0.195483
21.C	-0.032431	-1.843505	-2.995228	78.H	8.566105	-1.518693	-10.336204	6.C	-2.595429	9.304481	-0.741940
22.C	-0.558633	-2.405810	-1.682677	79.H	9.695826	-2.847245	-10.004493	7.C	-2.857125	7.893734	-0.905780
23.C	0.209373	-3.744550	-1.478332	80.H	9.820002	-1.291405	-8.056772	8.C	-1.851907	6.950527	-0.821546
24.C	1.501242	-3.534861	-2.327205	81.H	8.049869	-1.270584	-7.906201	9.C	-0.481020	7.458656	-0.335216
25.C	1.157556	-2.433347	-3.324511	82.H	10.298213	-3.696404	-6.955888	10.S	0.708288	6.087273	-0.795980
26.F	-0.270398	-1.543318	-0.636768	83.H	8.748676	-2.753812	-5.773648	11.C	-0.641100	4.929659	-1.026776
27.F	-1.909225	-2.598312	-1.672376	84.H	9.989045	-9.531277	-9.002658	12.C	-1.878801	5.556957	-1.035024
28.F	-0.524547	-4.759819	-2.015395	85.H	-0.518461	-2.621472	-5.836612	13.C	-3.870004	10.070188	-0.700752
29.F	0.466169	-4.018521	-0.182298	86.H	0.442447	-1.255671	-6.431852	14.C	-4.982793	8.970703	-0.586066
30.F	1.871857	-4.715754	-2.928537	87.H	-1.207082	-1.506349	-7.045181	15.C	-4.307133	7.673800	-1.148900
31.F	2.544115	-3.156112	-1.522703	88.H	-1.600946	0.170350	-1.821229	16.C	-0.353987	3.573440	-1.164702
32.C	2.173423	-2.093833	-4.332527	89.H	-8.820674	2.313345	-2.959507	17.C	-0.029964	2.374302	-1.220441
33.C	2.911370	-3.074547	-5.041129	90.H	-7.283383	0.916280	-3.574331	18.Ru	0.621139	0.405093	-1.115103
34.C	3.958783	-2.568587	-5.811331	91.H	-8.511024	2.627874	-5.608351	19.P	0.133266	-0.051764	-3.371064
35.S	4.002161	-0.804198	-5.651744	92.H	-6.745381	2.461977	-5.696689	20.C	-1.669345	-0.545580	-3.558788
36.C	2.658958	-0.788193	-4.566310	93.H	-8.310679	4.968349	-4.763249	21.C	-2.130194	-1.322076	-2.316413
37.C	4.922333	-3.269545	-6.526007	94.H	-7.275319	4.846759	-6.202339	22.P	-1.542983	-0.441152	-0.768407
38.C	5.835599	-3.918116	-7.081486	95.H	-6.162093	6.418434	-4.023566	23.C	-0.518020	7.535481	1.209702
39.Ru	7.392609	-5.033271	-7.841266	96.H	-4.872677	4.971289	-4.987002	24.C	-0.035340	8.722737	-2.542613
40.C	10.928443	-7.617069	-9.452731	97.H	-5.588372	0.950047	-0.126117	25.F	-4.632656	7.561189	-2.502680
41.C	12.115443	-7.014455	-9.992125	98.H	-7.117355	2.279121	0.639666	26.F	-4.839366	6.547193	-0.554607
42.C	13.167482	-7.771210	-10.430597	99.H	-4.928865	2.705926	2.123046	27.F	-6.133938	9.303906	-1.232413
43.C	13.121782	-9.208104	-10.359782	100.H	-5.546591	5.014198	1.399087	28.F	-5.289557	8.773199	0.735727
44.C	11.934076	-9.818471	-9.821849	101.H	-3.776785	4.977010	1.562735	29.F	-4.099191	10.822087	-1.851281
45.C	10.885535	-9.051675	-9.392753	102.H	-3.701789	2.587758	0.844964	30.F	-3.975396	10.977504	0.341837
46.C	2.226206	0.504722	-3.953648	103.H	-4.765350	6.482697	-0.727652	31.C	1.239037	12.364195	0.159698
47.C	-0.575690	-1.569420	-6.151415	104.H	-3.121634	5.110418	-1.045756	32.C	1.924250	13.333333	0.529829
48.N	14.159050	-9.958790	-10.783500	105.H	-8.628810	7.924100	-0.162858	33.Ru	3.028271	14.894973	1.343892
49.C	14.199381	-11.415713	-10.586167	106.H	12.174554	-5.928119	-10.037344	34.C	4.145768	16.395276	2.320283
50.P	7.328930	-6.384108	-5.850331	107.H	14.057307	-7.273341	-10.807914	35.P	1.137232	0.765543	1.156909
51.C	6.394437	-7.967668	-6.183287	108.H	11.850655	-10.901606	-9.779388	36.C	2.814781	1.591008	1.308188
52.C	5.227147	-7.706709	-7.146560	109.H	15.007312	-8.570703	-12.147695	37.C	3.750598	1.078375	0.203349
53.P	5.795986	-6.664208	-8.589598	110.H	15.808512	-10.152587	-12.056666	38.P	2.850816	1.091923	-1.440443
54.P	8.919189	-3.357796	-7.049104	111.H	16.042085	-8.977571	-10.737637	39.C	1.407800	-1.538587	-0.872782
55.C	8.910397	-1.889199	-8.203360	112.H	15.243353	-11.740910	-10.621628	40.P	4.685992	14.812655	-0.320742
56.C	8.772067	-2.358412	-9.658965	113.H	13.783715	-11.688662	-9.611721	41.C	4.475694	16.269557	-1.483640
57.P	7.419351	-3.639339	-9.802584	114.H	13.644719	-11.929206	-11.385641	42.C	2.980848	16.526732	-1.726281
58.P	-7.466607	2.314815	-3.392578	115.H	-15.002619	8.022944	1.676997	43.P	2.053072	16.478941	-0.093691
59.C	-7.566665	2.948505	-5.148319	116.H	-14.500312	6.770173	0.521306	44.P	1.431541	15.083963	3.066848
60.C	-7.417146	4.477006	-5.177920	117.H	-10.907971	4.245196	-0.387335	45.C	1.792366	13.827528	4.413406
61.P	-5.986214	5.010187	-4.101748	118.H	-12.842525	5.367475	0.588663	46.C	3.309551	13.630733	4.551320
62.C	15.319729	-9.369880	-11.469119	119.H	-14.217849	6.540255	2.277612	47.P	4.074180	13.421282	2.853724
63.C	-14.236741	7.274647	1.458094	120.H	-10.549151	9.070751	0.813763	48.H	0.354645	1.592109	2.016076
64.H	2.707593	-4.138779	-4.988194	121.H	-11.942684	9.463207	2.436615	49.H	1.278331	-0.360282	2.020502
65.H	1.959860	0.355708	-2.897715	122.H	-13.717404	9.545933	2.444349	50.H	2.628781	2.670324	1.193315
66.H	1.340101	0.914021	-4.464654	123.H	-12.823269	10.042614	0.985919	51.H	3.235832	1.421178	2.308738
67.H	3.019907	1.259030	-4.006839	124.C	8.912304	-6.148763	-8.569408	52.H	4.671969	1.673897	0.143171
68.H	6.047287	-8.404177	-5.237192	125.C	9.870161	-6.845227	-9.000009	53.H	4.024046	0.026815	0.380864
69.H	8.518392	-6.851563	-5.226844	126.C	-8.506751	5.332400	-0.905846	54.H	3.763631	0.360444	-2.254591
70.H	6.671390	-5.840390	-4.712788	127.C	-7.532879	4.711133	-1.383064	55.H	3.147822	2.400831	-1.928115
71.H	7.121196	-8.665743	-6.625941					56.H	-1.831263	-1.426942	0.221306
72.H	4.429577	-7.133341	-6.650128					57.H	-2.641383	0.430801	-0.494767

58.H	-1.663273	-2.318651	-2.285476	115.C	6.885190	22.090243	6.802547	43.P	1.742069	16.449435	0.314032
59.H	-3.221288	-1.450216	-2.298225	116.H	9.248236	21.383643	7.448299	44.P	1.763001	15.043354	3.543536
60.H	-1.813612	-1.127718	-4.479343	117.H	9.195876	19.669618	7.012145	45.C	2.554544	13.999336	4.886012
61.H	-2.231833	0.395710	-3.659760	118.H	9.474688	20.895404	5.743659	46.C	4.084094	14.131099	4.826430
62.H	0.251118	0.904876	-4.423885	119.H	7.493120	22.600610	7.558229	47.P	4.668382	13.963532	3.055902
63.H	0.800439	-1.134255	-4.019122	120.H	6.818740	22.740659	5.908700	48.H	0.928056	0.857628	2.499161
64.H	-2.793385	4.997299	-1.217576	121.H	5.873600	21.975281	7.216409	49.H	1.456697	-1.213791	2.176315
65.H	0.460458	7.832005	1.607302	122.H	5.131142	-8.972169	1.954344	50.H	3.428985	1.580346	2.011517
66.H	-1.268596	8.270601	1.536502	123.H	4.426501	-7.540377	2.718496	51.H	3.696006	0.053508	2.884570
67.H	-0.789416	6.550214	1.611167	124.H	3.405304	-8.586582	1.692957	52.H	5.323410	0.411681	0.874119
68.H	-1.510768	11.962997	-0.282474	125.H	6.113781	-8.902919	0.055670	53.H	4.371565	-1.093125	0.768575
69.H	0.132554	9.727550	-2.951737	126.H	4.891911	-8.481448	-1.179139	54.H	4.391301	-0.245390	-1.771943
70.H	0.805836	8.075018	-2.818689	127.H	6.287440	-7.409007	-0.876455	55.H	4.119967	1.779042	-1.089042
71.H	-0.955604	8.309796	-2.981884					56.H	-1.592629	-1.367293	0.125267
72.H	2.055300	17.856831	0.279303	4c ⁺				57.H	-2.042557	0.670234	-0.407307
73.H	0.705697	16.408577	-0.560021	1.C	-0.164284	10.899926	0.023216	58.H	-1.330511	-1.976663	-2.470212
74.H	1.355323	16.299008	3.809551	2.C	-0.540904	9.585913	-0.238540	59.H	-2.740717	-0.884978	-2.473504
75.H	0.034101	14.873173	2.872696	3.C	0.640891	8.637102	-0.492577	60.H	-1.121980	-0.522983	-4.491677
76.H	3.996866	12.007293	2.668631	4.S	2.132213	9.581419	0.129227	61.H	-1.385790	0.937264	-3.512271
77.H	5.461837	13.511416	3.165579	5.C	1.207566	11.099924	0.247334	62.H	1.202174	1.162163	-4.026727
78.H	4.760822	13.719502	-1.237490	6.C	-1.819657	9.026583	-0.311466	63.H	1.427872	-0.979002	-3.864105
79.H	6.076988	14.909254	-0.020831	7.C	-2.017141	7.623798	-0.388964	64.H	-1.817617	4.753628	-0.678248
80.H	1.335806	14.141695	5.362015	8.C	-0.960439	6.722220	-0.244428	65.H	1.258477	7.824809	2.183583
81.H	1.305027	12.893929	4.091762	9.C	0.372617	7.302994	0.252113	66.H	-0.480079	8.204226	2.053212
82.H	3.550613	12.771274	5.192025	10.S	1.621159	5.953611	-0.100065	67.H	0.048882	6.510112	2.251482
83.H	3.781692	14.529236	4.977669	11.C	0.337337	4.752784	-0.394450	68.H	-0.869938	11.721992	0.119136
84.H	2.544112	15.727839	-2.345676	12.C	-0.934271	5.345919	-0.450620	69.H	0.939526	9.433310	-2.494300
85.H	2.810630	17.484574	-2.236928	13.C	-3.124795	9.752532	-0.368585	70.H	1.686281	7.829862	-2.237045
86.H	5.016007	16.094670	-2.424278	14.C	-4.203373	8.622507	-0.213293	71.H	-0.080048	7.968114	-2.445405
87.H	4.939230	17.126930	-0.971527	15.C	-3.455046	7.314113	-0.647956	72.H	1.454102	17.770487	0.763824
88.C	1.967895	-2.618142	-0.649264	16.C	0.628564	3.413082	-0.555866	73.H	0.420179	16.072353	-0.067001
89.C	4.772683	17.211763	3.005699	17.C	0.872650	2.193967	-0.677643	74.H	1.500116	16.266944	4.223166
90.C	2.644893	-3.838148	-0.349042	18.Ru	1.222681	0.178231	-0.792527	75.H	0.437280	14.517978	3.534568
91.C	5.467689	18.136647	3.841148	19.P	0.857591	0.103493	-3.135821	76.H	4.862682	12.554109	2.936746
92.C	3.557376	-4.428076	-1.251022	20.C	-0.973618	-0.083665	-3.495945	77.H	6.034339	14.348983	3.172833
93.C	4.253465	-5.592144	-0.940969	21.C	-1.645364	-0.924259	-2.400094	78.H	4.856478	14.368713	-1.147234
94.C	4.085478	-6.237385	0.307992	22.P	-1.079248	-0.337724	-0.714649	79.H	6.019139	15.753365	0.027686
95.C	3.143044	-5.672581	1.201018	23.C	0.297875	7.473172	1.787616	80.H	2.162091	14.285995	5.871086
96.C	2.452592	-4.508801	0.879266	24.C	0.810342	8.452844	-2.018397	81.H	2.243617	12.962014	4.686537
97.H	3.719265	-3.952609	-2.219256	25.F	-3.717930	7.071560	-1.989780	82.H	4.578996	13.389039	5.467767
98.H	4.939857	-5.998382	-1.681857	26.F	-3.937616	6.220514	0.032498	83.H	4.400338	15.135197	5.148031
99.N	4.835203	-7.366720	0.654869	27.F	-5.327754	8.858732	-0.933928	84.H	2.218186	15.918337	-2.002588
100.H	2.946464	-6.142810	2.162884	28.F	-4.553481	8.513638	1.104123	85.H	2.118639	17.682347	-1.805908
101.H	1.740070	-4.097029	1.595254	29.F	-3.319215	10.405173	-1.574535	86.H	4.543194	16.808545	-2.215592
102.C	4.841917	19.298302	4.345340	30.F	-3.283400	10.717106	0.605658	87.H	4.362727	17.733783	-0.700994
103.C	5.499152	20.180180	5.196896	31.C	1.821089	12.291479	0.577838	88.C	1.797729	-3.108449	-0.846414
104.C	6.833472	19.945881	5.608847	32.C	2.354110	13.363401	0.934607	89.C	4.481513	17.884281	2.943688
105.C	7.478945	18.803737	5.076307	33.Ru	3.167926	15.107375	1.636663	90.C	2.041455	-4.507907	-0.813438
106.C	6.810918	17.929293	4.225240	34.C	4.012111	16.861107	2.426583	91.C	4.996763	19.056570	3.559513
107.H	3.810828	19.505410	4.056230	35.P	1.611598	0.051446	1.542164	92.C	3.332754	-5.042010	-1.037635
108.H	4.961793	21.059518	5.547641	36.C	3.396482	0.483602	1.919237	93.C	3.581019	-6.405452	-0.988074
109.N	7.476034	20.790443	6.520374	37.C	4.307174	0.005689	0.778529	94.C	2.540449	-7.328803	-0.700746
110.H	8.515325	18.589041	5.330874	38.P	3.561744	0.483442	-0.871977	95.C	1.239216	-6.799878	-0.489767
111.H	7.336980	17.054611	3.840684	39.C	1.583444	-1.888334	-0.856411	96.C	1.005410	-5.434164	-0.545254
112.C	4.418164	-8.153133	1.806226	40.P	4.656128	15.397806	-0.178319	97.H	4.152771	-4.358251	-1.259210
113.C	5.556755	-8.072736	-0.393355	41.C	4.052413	16.821390	-1.232913	98.H	4.592725	-6.760873	-1.173819
114.C	8.918609	20.678754	6.676587	42.C	2.522723	16.761741	-1.363470	99.N	2.784965	-8.685846	-0.625109

100.H	0.404829	-7.466002	-0.278856	28.F	-3.168358	8.272391	1.642048	85.H	0.940367	16.766130	-1.534028	
101.H	-0.003634	-5.058390	-0.373067	29.F	-1.925042	10.049383	-1.106833	86.H	3.396251	16.928005	-2.395024	
102.C	4.159423	20.154226	3.872042	30.F	-1.887074	10.445009	1.061001	87.H	3.095191	17.869755	-0.912699	
103.C	4.646596	21.294863	4.491686	31.C	3.125368	12.089177	0.958183	88.C	0.797868	-3.263233	-1.180735	
104.C	6.019929	21.411665	4.834806	32.C	3.368021	13.290823	1.225563	89.C	3.527046	18.456732	2.619888	
105.C	6.864447	20.311994	4.526843	33.Ru	3.554054	15.258611	1.716272	90.C	0.350299	-4.582184	-1.413875	
106.C	6.363166	19.176957	3.907188	34.C	3.609583	17.270396	2.259231	91.C	3.362036	19.791396	3.051505	
107.H	3.099817	20.093042	3.622307	35.P	2.155082	-0.650207	1.618559	92.C	1.235650	-5.612439	-1.827327	
108.H	3.955244	22.104939	4.715689	36.C	4.006743	-0.856428	1.805168	93.C	0.792135	-6.898958	-2.066792	
109.N	6.514759	22.550799	5.439907	37.C	4.606340	-1.444675	0.519199	94.C	-0.580137	-7.245006	-1.897960	
110.H	7.922816	20.347231	4.777829	38.P	3.918788	-0.551407	-0.974944	95.C	-1.472016	-6.216910	-1.475701	
111.H	7.037010	18.349208	3.683752	39.C	1.167715	-2.094396	-0.975346	96.C	-1.016212	-4.933372	-1.247305	
112.C	1.686699	-9.614563	-0.399735	40.P	4.448496	15.943102	-0.381195	97.H	2.290334	-5.374762	-1.964713	
113.C	4.112209	-9.206235	-0.919574	41.C	3.121249	16.853361	-1.334227	98.H	1.509327	-7.651277	-2.387821	
114.C	7.902187	22.598591	5.878720	42.C	1.766552	16.152195	-1.150987	99.N	-1.026911	-8.519573	-2.132454	
115.C	5.606690	23.616530	5.839815	43.P	1.482742	15.741346	0.656526	100.H	-2.527700	-6.434849	-1.328911	
116.H	8.108273	23.584411	6.306640	44.P	2.667749	14.834225	3.887030	101.H	-1.720135	-4.166796	-0.923132	
117.H	8.122428	21.835649	6.645656	45.C	4.049093	14.336732	5.050934	102.C	2.088169	20.268959	3.462037	
118.H	8.591891	22.446801	5.034226	46.C	5.351901	15.058117	4.673192	103.C	1.902896	21.564754	3.901904	
119.H	6.187051	24.437632	6.271541	47.P	5.627601	14.963251	2.824203	104.C	2.991920	22.482600	3.950343	
120.H	5.053596	24.013118	4.974584	48.H	1.847614	0.196539	2.721845	105.C	4.270526	22.011784	3.531985	
121.H	4.873456	23.277931	6.592457	49.H	1.642290	-1.874006	2.132678	106.C	4.443688	20.709269	3.103326	
122.H	2.084740	-10.632132	-0.341186	50.H	4.407351	0.150677	1.998604	107.H	1.238606	19.586710	3.432903	
123.H	1.169272	-9.398574	0.548216	51.H	4.231081	-1.481994	2.679604	108.H	0.908264	21.878937	4.211132	
124.H	0.942604	-9.581553	-1.214066	52.H	5.703402	-1.392445	0.524389	109.N	2.814072	23.770812	4.384321	
125.H	4.110890	-10.291250	-0.778009	53.H	4.314108	-2.499273	0.400300	110.H	5.130166	22.678220	3.549965	
126.H	4.418945	-8.994342	-1.958288	54.H	4.367724	-1.384720	-2.038354	111.H	5.433127	20.373851	2.792898	
127.H	4.868510	-8.777662	-0.243226	55.H	4.843688	0.519618	-1.148182	112.C	-2.434965	-8.857284	-1.938828	
4c ²⁺ LS				56.H	-1.472320	-0.749716	0.452578	113.C	-0.101729	-9.557204	-2.581271	
	1.C	1.207459	10.608240	57.H	-1.255538	1.377953	0.189691	114.C	3.936626	24.705262	4.409359	
	2.C	0.862019	9.297141	58.H	-1.641859	-1.044202	-2.210980	115.C	1.500108	24.225422	4.832794	
	3.C	2.053082	8.365565	59.H	-2.596146	0.434424	-1.930818	116.H	3.584133	25.676912	4.765268	
	4.S	3.539783	9.356924	60.H	-1.118624	0.522191	-4.080790	117.H	4.732535	24.357935	5.085980	
	5.C	2.590547	10.851951	61.H	-0.798011	1.843536	-2.938079	118.H	4.364067	24.841099	3.404322	
	6.C	-0.425549	8.726547	62.H	1.674195	1.294854	-3.724593	119.H	1.573644	25.267299	5.155369	
	7.C	-0.609176	7.338424	63.H	1.180457	-0.809000	-3.822643	120.H	0.757125	24.167276	4.022488	
	8.C	0.471954	6.447081	64.H	-0.403972	4.499146	-0.125801	121.H	1.139760	23.626470	5.683123	
	9.C	1.816003	7.033445	65.H	2.774077	7.572525	2.648573	122.H	-2.581936	-9.917176	-2.162408	
	10.S	3.050943	5.670041	66.H	1.037665	7.972560	2.573003	123.H	-2.748880	-8.678208	-0.899141	
	11.C	1.764723	4.477748	67.H	1.552913	6.276571	2.784174	124.H	-3.083600	-8.270829	-2.607709	
	12.C	0.486387	5.084981	68.H	0.484467	11.412106	0.617022	125.H	-0.653774	-10.489755	-2.724694	
	13.C	-1.737068	9.448338	69.H	2.293102	9.125619	-2.041825	126.H	0.368871	-9.284825	-3.538261	
	14.C	-2.812581	8.319329	70.H	3.088820	7.552191	-1.760091	127.H	0.690458	-9.736198	-1.838211	
	15.C	-2.051219	6.994916	71.H	1.316384	7.635209	-1.939227	4c ²⁺ HS				
	16.C	1.980960	3.134706	72.H	0.743488	16.866333	1.119383		1.C	-0.062641	10.883501	0.025696
	17.C	1.923556	1.898254	73.H	0.408262	14.808966	0.564889		2.C	-0.430854	9.567454	-0.225765
	18.Ru	1.621081	-0.089400	74.H	2.051616	15.920852	4.568564		3.C	0.753995	8.618796	-0.458535
	19.P	1.059140	0.288437	75.H	1.693885	13.828891	4.154234		4.S	2.237893	9.576135	0.159957
	20.C	-0.750987	0.751736	76.H	6.351424	13.743124	2.681258		5.C	1.310075	11.087902	0.256506
	21.C	-1.575818	0.032566	77.H	6.709941	15.870402	2.647103		6.C	-1.712186	9.006913	-0.301307
	22.P	-0.718832	0.164745	78.H	4.906951	17.979963	-1.327299		7.C	-1.907894	7.609112	-0.358177
	23.C	1.796123	7.226791	79.H	5.541574	16.850296	-0.454159		8.C	-0.848024	6.709451	-0.197859
	24.C	2.199543	8.154821	80.H	3.759713	14.543511	6.090080		9.C	0.480815	7.293442	0.302352
	25.F	-2.315509	6.666531	81.H	4.159867	13.246700	4.942520		10.S	1.728998	5.937015	-0.022428
	26.F	-2.499231	5.938512	82.H	6.213646	14.640053	5.210822		11.C	0.450504	4.741648	-0.328599
	27.F	-3.926216	8.512346	83.H	5.285846	16.130845	4.910798		12.C	-0.822880	5.335239	-0.401404
				84.H	1.748326	15.191573	-1.688768					

13.C	-3.020115	9.735421	-0.383378	70.H	1.819236	7.793816	-2.183239	127.H	4.668800	-8.905905	-0.190460
14.C	-4.101063	8.607440	-0.209228	71.H	0.053933	7.920728	-2.409675	4c ⁴⁺ LS			
15.C	-3.348853	7.290331	-0.617268	72.H	1.425108	17.745444	0.662636				
16.C	0.736552	3.398999	-0.483154	73.H	0.374752	15.981011	0.004536	1.C	0.959495	10.498479	1.252197
17.C	0.956376	2.174256	-0.588653	74.H	1.593281	16.182617	4.267849	2.C	0.614836	9.189627	1.036163
18.Ru	0.265347	0.146856	-0.708270	75.H	0.511399	14.484829	3.484152	3.C	1.666381	8.354263	0.299848
19.P	0.869957	0.158356	-3.056311	76.H	4.996918	12.585152	2.750700	4.S	3.204410	9.427544	0.348838
20.C	-0.972275	0.120762	-3.393472	77.H	6.120824	14.392954	3.107984	5.C	2.307408	10.835060	0.919919
21.C	-1.687893	-0.726147	-2.330517	78.H	4.845155	14.326397	-1.194239	6.C	-0.588738	8.537076	1.422528
22.P	-1.064936	-0.273078	-0.623583	79.H	5.989303	15.840162	-0.167600	7.C	-0.698850	7.158684	1.399591
23.C	0.397386	7.482420	1.835899	80.H	2.246505	14.087408	5.789187	8.C	0.400400	6.328953	1.052364
24.C	0.938161	8.414978	-1.981062	81.H	2.338232	12.847540	4.517862	9.C	1.789074	6.970510	1.022933
25.F	-3.594712	7.023758	-1.953518	82.H	4.668975	13.239896	5.329752	10.S	2.847329	5.696881	0.139927
26.F	-3.823241	6.209728	0.084386	83.H	4.477986	14.999234	5.134350	11.C	1.584194	4.465334	0.211400
27.F	-5.218669	8.828464	-0.939070	84.H	2.084776	15.720782	-2.018464	12.C	0.361587	5.001091	0.714959
28.F	-4.448494	8.523068	1.109290	85.H	1.933774	17.489963	-1.941049	13.C	-1.883507	9.185824	1.846571
29.F	-3.196679	10.355537	-1.604307	86.H	4.362142	16.664713	-2.417257	14.C	-2.750555	7.988625	2.393645
30.F	-3.175233	10.717035	0.570260	87.H	4.227981	17.696559	-0.972810	15.C	-2.103721	6.717465	1.725907
31.C	1.916976	12.287205	0.574440	88.C	1.769450	-3.137897	-0.808662	16.C	1.741605	3.160804	-0.185635
32.C	2.435195	13.370468	0.917225	89.C	4.465879	17.929112	2.914172	17.C	1.680185	1.942254	-0.484911
33.Ru	3.222999	15.142670	1.592926	90.C	1.983732	-4.530912	-0.814159	18.Ru	1.481985	-0.036720	-0.937171
34.C	4.019386	16.899806	2.376290	91.C	4.945881	19.091057	3.551856	19.P	-0.237982	0.484708	-2.539014
35.P	1.663542	0.067512	1.636017	92.C	3.282343	-5.079814	-0.997789	20.C	-1.883617	0.667132	-1.668624
36.C	3.430107	0.574228	1.995541	93.C	3.502495	-6.442273	-0.993374	21.C	-1.971902	-0.297559	-0.476454
37.C	4.359653	0.077299	0.878115	94.C	2.426043	-7.356512	-0.798569	22.P	-0.396368	-0.237088	0.529328
38.P	3.610888	0.456749	-0.796592	95.C	1.120257	-6.812858	-0.617574	23.C	2.333456	7.098282	2.465685
39.C	1.579066	-1.908409	-0.788670	96.C	0.913520	-5.448202	-0.628615	24.C	1.260224	8.216194	-1.188063
40.P	4.637645	15.413579	-0.296047	97.H	4.121214	-4.400789	-1.148451	25.F	-2.797198	6.387298	0.582835
41.C	3.922879	16.734780	-1.413015	98.H	4.514637	-6.812853	-1.140179	26.F	-2.153957	5.632062	2.554447
42.C	2.391638	16.616786	-1.457077	99.N	2.639142	-8.709916	-0.785175	27.F	-4.059627	8.119720	2.107920
43.P	1.708076	16.403782	0.275303	100.H	0.268964	-7.473284	-0.467238	28.F	-2.583691	7.904291	3.741523
44.P	1.840364	14.995950	3.520702	101.H	-0.093509	-5.056950	-0.485751	29.F	-2.516002	9.775220	0.780859
45.C	2.641119	13.871200	4.787177	102.C	4.074166	20.162951	3.888331	30.F	-1.714947	10.155358	2.801598
46.C	4.169740	14.019405	4.738451	103.C	4.528922	21.292328	4.538501	31.C	2.829743	12.099617	1.037393
47.P	4.767131	13.976155	2.963164	104.C	5.902336	21.426559	4.897391	32.C	3.112921	13.313705	1.212294
48.H	0.940720	0.869431	2.564744	105.C	6.783801	20.359894	4.553462	33.Ru	3.443140	15.297735	1.542238
49.H	1.552467	-1.186349	2.301051	106.C	6.315651	19.235565	3.903542	34.C	3.675734	17.303529	1.916830
50.H	3.426525	1.674239	2.040982	107.H	3.019291	20.081098	3.627425	35.P	3.201368	-0.602305	0.648037
51.H	3.740581	0.195812	2.978797	108.H	3.821431	22.083391	4.777531	36.C	4.882764	-0.356593	-0.127509
52.H	5.361261	0.520754	0.958617	109.N	6.358709	22.540961	5.551045	37.C	4.842411	-0.730364	-1.616898
53.H	4.466302	-1.017516	0.919921	110.H	7.840547	20.421851	4.804113	38.P	3.342418	0.027732	-2.435363
54.H	4.447719	-0.306323	-1.659780	111.H	7.008332	18.432310	3.653141	39.C	1.208678	-2.029504	-1.379706
55.H	4.141784	1.748374	-1.083242	112.C	1.525987	-9.633772	-0.573609	40.P	3.746083	15.808567	-0.779780
56.H	-1.618083	-1.319848	0.167818	113.C	3.983112	-9.250625	-0.979147	41.C	2.179485	16.584489	-1.443752
57.H	-1.957588	0.769623	-0.237568	114.C	7.767737	22.658223	5.921863	42.C	0.941253	15.906331	-0.837248
58.H	-1.455713	-1.793956	-2.462984	115.C	5.440262	23.622840	5.902382	43.P	1.134201	15.717200	1.014161
59.H	-2.778233	-0.605176	-2.384439	116.H	7.924543	23.612763	6.430525	44.P	3.176812	14.984640	3.906362
60.H	-1.163787	-0.256128	-4.407135	117.H	8.068451	21.849024	6.604471	45.C	4.784578	14.379863	4.647784
61.H	-1.311012	1.167491	-3.353010	118.H	8.416568	22.629564	5.033735	46.C	5.986398	14.998151	3.916683
62.H	1.294539	1.221261	-3.903440	119.H	5.997645	24.412102	6.413151	47.P	5.751167	14.900082	2.064760
63.H	1.353838	-0.935827	-3.827539	120.H	4.973301	24.055167	5.004795	48.H	3.321731	0.083030	1.887482
64.H	-1.704410	4.743756	-0.637562	121.H	4.646276	23.267985	6.576787	49.H	3.241376	-1.940734	1.124650
65.H	1.357510	7.833606	2.233310	122.H	1.905806	-10.658557	-0.585342	50.H	5.129206	0.707980	0.004932
66.H	-0.378555	8.220236	2.087762	123.H	1.041645	-9.455930	0.398340	51.H	5.634173	-0.944679	0.416129
67.H	0.140728	6.527754	2.312579	124.H	0.770279	-9.535719	-1.367546	52.H	5.756182	-0.412237	-2.136116
68.H	-0.771501	11.704117	0.108615	125.H	3.937593	-10.341980	-0.941629	53.H	4.745065	-1.819027	-1.744578
69.H	1.067355	9.388158	-2.471461	126.H	4.393240	-8.955546	-1.956628	54.H	3.306161	-0.641761	-3.688957

55.H	3.818284	1.294102	-2.876797	112.C	-1.161384	-9.326711	-2.142011	40.P	1.892090	15.702362	0.584803
56.H	-0.545693	-1.355875	1.393526	113.C	0.617720	-9.288605	-3.923009	41.C	0.228229	16.132916	1.321701
57.H	-0.659203	0.797034	1.472432	114.C	4.348664	24.975256	2.589916	42.C	-0.094501	15.200774	2.499369
58.H	-2.072485	-1.336461	-0.824120	115.C	2.971927	24.473258	4.643363	43.P	1.386487	15.026586	3.630105
59.H	-2.837357	-0.071799	0.160648	116.H	4.239455	25.965383	3.038017	44.P	4.938874	14.753718	4.146215
60.H	-2.702629	0.502558	-2.381415	117.H	5.419716	24.747281	2.498990	45.C	6.695350	14.705838	3.504476
61.H	-1.940369	1.713855	-1.333472	118.H	3.893011	24.989926	1.589287	46.C	6.870231	15.695340	2.342574
62.H	-0.182103	1.655403	-3.343645	119.H	3.023202	25.564095	4.665791	47.P	5.458683	15.524571	1.133534
63.H	-0.503167	-0.473607	-3.554287	120.H	1.915384	24.172397	4.615644	48.H	4.689770	0.035522	0.366930
64.H	-0.533029	4.385814	0.775333	121.H	3.438325	24.080673	5.558569	49.H	4.103871	-1.986857	-0.141154
65.H	3.364645	7.472367	2.455035	122.H	-1.119123	-10.375454	-2.441197	50.H	4.535006	0.720766	-2.213465
66.H	1.712806	7.796384	3.047030	123.H	-0.999473	-9.265511	-1.059088	51.H	5.173911	-0.928785	-2.361646
67.H	2.318367	6.121601	2.965682	124.H	-2.157744	-8.931769	-2.385151	52.H	3.387231	-0.335932	-4.162003
68.H	0.291578	11.239274	1.685718	125.H	0.143787	-10.255990	-4.098614	53.H	2.979765	-1.771148	-3.195825
69.H	1.105287	9.207260	-1.633318	126.H	0.595548	-8.713662	-4.856535	54.H	0.576856	-0.572550	-3.431321
70.H	2.042581	7.694373	-1.752667	127.H	1.661354	-9.457362	-3.622598	55.H	1.534728	1.349356	-3.192059
71.H	0.323673	7.645612	-1.275415					56.H	1.752059	-1.764938	2.701696
72.H	0.532249	16.897303	1.532748	4c ⁴⁺ HS				57.H	1.645764	0.361788	3.084245
73.H	0.107133	14.787120	1.337494	1.C	1.744283	10.589438	0.119247	58.H	-0.909538	-1.807563	2.307451
74.H	2.865931	16.136457	4.680967	2.C	1.523046	9.307878	-0.290463	59.H	-0.769263	-0.670780	3.666190
75.H	2.227255	14.081985	4.462502	3.C	2.538195	8.273434	0.198278	60.H	-2.556205	0.019163	1.899801
76.H	6.306365	13.635135	1.724107	4.S	3.544461	9.206788	1.475334	61.H	-1.318159	1.258855	2.185666
77.H	6.785459	15.742865	1.573349	5.C	2.811265	10.758540	1.065373	62.H	-1.608785	1.468192	-0.458520
78.H	4.005503	14.753515	-1.699324	6.C	0.432848	8.834373	-1.087598	63.H	-1.876901	-0.672327	-0.599960
79.H	4.749954	16.723984	-1.198146	7.C	0.113443	7.498828	-1.139800	64.H	0.166562	4.656121	-1.248772
80.H	4.809828	14.605989	5.722644	8.C	0.830038	6.528252	-0.373233	65.H	1.524736	7.683376	2.826799
81.H	4.778990	13.284295	4.537271	9.C	1.734105	7.039363	0.747769	66.H	0.208321	8.236869	1.757566
82.H	6.925649	14.505087	4.202758	10.S	2.763989	5.539622	1.203783	67.H	0.268273	6.537193	2.290839
83.H	6.083441	16.068818	4.154771	11.C	1.767294	4.446298	0.243717	68.H	1.148303	11.440282	-0.199554
84.H	0.815160	14.888735	-1.238590	12.C	0.815070	5.175370	-0.546695	69.H	3.972410	8.783593	-1.370459
85.H	0.025213	16.469516	-1.062512	13.C	-0.469757	9.654077	-1.978201	70.H	4.280647	7.213113	-0.585774
86.H	2.168205	16.529317	-2.540995	14.C	-1.627666	8.659122	-2.370408	71.H	2.944733	7.378975	-1.755685
87.H	2.221657	17.647687	-1.160818	15.C	-1.003234	7.234732	-2.119545	72.H	1.183465	16.040344	4.605064
88.C	0.986958	-3.232738	-1.642820	16.C	1.865112	3.082818	0.238302	73.H	1.043461	13.889030	4.412580
89.C	3.735553	18.528105	2.179287	17.C	1.728343	1.837895	0.085729	74.H	4.994021	15.726884	5.182235
90.C	0.722999	-4.568396	-1.940103	18.Ru	1.366021	-0.130906	-0.200663	75.H	4.872873	13.580838	4.948103
91.C	3.749399	19.886525	2.500461	19.P	-0.995669	0.268288	-0.000180	76.H	5.913571	14.526930	0.226342
92.C	1.490432	-5.281503	-2.915789	20.C	-1.484124	0.238891	1.806069	77.H	5.602831	16.668580	0.303014
93.C	1.217967	-6.588548	-3.224378	21.C	-0.633026	-0.778391	2.581680	78.H	1.562669	14.722647	-0.396454
94.C	0.154307	-7.292681	-2.564678	22.P	1.174500	-0.593852	2.140702	79.H	2.132395	16.799691	-0.286783
95.C	-0.610602	-6.585607	-1.576326	23.C	0.879536	7.396474	1.987726	80.H	7.399277	14.916976	4.320644
96.C	-0.336502	-5.275256	-1.285707	24.C	3.497139	7.887619	-0.951946	81.H	6.871960	13.672125	3.169745
97.H	2.303171	-4.764592	-3.422656	25.F	-0.514456	6.723208	-3.298536	82.H	7.826988	15.544278	1.824559
98.H	1.826146	-7.094603	-3.969263	26.F	-1.934991	6.352246	-1.650644	83.H	6.841301	16.735782	2.701244
99.N	-0.118529	-8.582942	-2.864040	27.F	-2.051065	8.827695	-3.636294	84.H	-0.330720	14.185605	2.144942
100.H	-1.423956	-7.084869	-1.056755	28.F	-2.669125	8.836111	-1.512562	85.H	-0.959955	15.561324	3.071573
101.H	-0.929964	-4.753644	-0.537170	29.F	0.192649	10.074821	-3.100301	86.H	-0.551816	16.089254	0.549631
102.C	3.102082	20.365034	3.686738	30.F	-0.965742	10.772754	-1.356833	87.H	0.308413	17.176617	1.661429
103.C	3.077194	21.699829	4.001850	31.C	3.179251	11.971324	1.575453	88.C	0.525259	-3.293801	-0.771822
104.C	3.712816	22.666089	3.149430	32.C	3.318680	13.185137	1.892451	89.C	3.296467	18.407924	3.024073
105.C	4.379437	22.189564	1.968604	33.Ru	3.415923	15.149924	2.343961	90.C	0.084854	-4.593748	-1.049150
106.C	4.393551	20.851976	1.660755	34.C	3.399631	17.189136	2.772135	91.C	3.142941	19.768806	3.320918
107.H	2.610292	19.646102	4.341884	35.P	3.703381	-0.646923	-0.396232	92.C	-0.027049	-5.063970	-2.395139
108.H	2.566321	22.022592	4.906910	36.C	4.266562	-0.345284	-2.154909	93.C	-0.489865	-6.325155	-2.679434
109.N	3.680297	23.985959	3.449392	37.C	3.144869	-0.684051	-3.148847	94.C	-0.868292	-7.221875	-1.626214
110.H	4.875103	22.892719	1.302147	38.P	1.526592	0.061177	-2.583960	95.C	-0.741944	-6.761158	-0.273903
111.H	4.904741	20.507256	0.761002	39.C	0.887559	-2.120989	-0.537290	96.C	-0.285970	-5.494400	-0.002520

97.H	0.259862	-4.400240	-3.210040	25.P	-4.367565	3.420869	-0.942723	21.H	-11.211321	7.603195	-8.354188			
98.H	-0.550557	-6.645081	-3.717266	26.C	-5.505921	2.547291	0.268749	22.H	-10.302414	7.906391	-6.857103			
99.N	-1.332610	-8.467631	-1.901355	27.C	-6.448392	1.608695	-0.497249	23.H	-5.264388	4.502112	-0.858651			
100.H	-1.026055	-7.409023	0.552244	28.P	-5.461600	0.627384	-1.754721	24.H	-3.342099	3.969532	-0.021990			
101.H	-0.206137	-5.161800	1.031607	29.H	-6.061028	3.278468	0.872328	25.P	-4.403842	3.369570	-0.754939			
102.C	3.288050	20.256803	4.656712	30.C	-10.540545	7.279483	-7.545729	26.C	-5.248575	2.335119	0.555159			
103.C	3.108484	21.584646	4.957952	31.H	-4.848233	1.975299	0.940876	27.C	-6.257224	1.383759	-0.104665			
104.C	2.766344	22.528741	3.934320	32.H	-7.181141	2.186085	-1.081272	28.P	-5.478551	0.549659	-1.593685			
105.C	2.632202	22.046410	2.590636	33.H	-6.994606	0.937256	0.179639	29.H	-5.729604	2.980904	1.302167			
106.C	2.818004	20.716814	2.301084	34.H	-6.512846	0.038412	-2.518695	30.C	-10.326642	7.311352	-7.782223			
107.H	3.544523	19.553611	5.447961	35.H	-5.097982	-0.528907	-0.996686	31.H	-4.446574	1.770988	1.054409			
108.H	3.228854	21.914744	5.987118	36.H	-1.148459	3.934845	-2.980442	32.H	-7.125841	1.941199	-0.486922			
109.N	2.574912	23.840306	4.228399	37.H	-2.672765	4.587358	-4.353047	33.H	-6.625723	0.630875	0.605009			
110.H	2.380535	22.733447	1.786030	38.H	-0.913484	3.194683	-5.773338	34.H	-6.626726	0.012841	-2.245664			
111.H	2.713234	20.369339	1.273880	39.H	-3.093958	2.122173	-6.369284	35.H	-4.969143	-0.659136	-1.037322			
112.C	-1.615060	-9.433418	-0.829661	40.H	-1.846119	0.851976	-6.466716	36.H	-1.356138	4.049111	-2.850235			
113.C	-1.576640	-8.905112	-3.283451	41.H	-0.571303	1.905449	-4.592019	37.H	-2.794780	4.570285	-4.374364			
114.C	2.222050	24.807194	3.178105	42.H	-4.371541	0.028339	-5.329722	38.H	-0.858340	3.140354	-5.554902			
115.C	2.713946	24.334432	5.606450	43.H	-2.559789	-0.572448	-4.331522	39.H	-2.966302	2.040743	-6.317436			
116.H	2.126973	25.798454	3.625510	44.H	-8.463621	2.168824	-5.575447	40.H	-1.723669	0.772161	-6.228105			
117.H	3.003604	24.843254	2.407295	45.H	-6.617259	6.003520	-4.965279	41.H	-0.631629	1.906941	-4.290519			
118.H	1.263813	24.538107	2.712488	46.H	-8.464672	7.096883	-6.128981	42.H	-4.395815	0.035199	-5.312711			
119.H	2.495392	25.403894	5.623914	47.H	-9.745362	7.426198	-8.303081	43.H	-2.687793	-0.594786	-4.144056			
120.H	2.008930	23.820680	6.273831	48.H	-10.325850	3.232695	-6.742307	44.H	-8.605148	2.226454	-5.407649			
121.H	3.738819	24.178804	5.970513	49.C	-0.446735	0.061908	0.000785	45.H	-6.467488	5.969993	-5.157902			
122.H	-1.717719	-10.427909	-1.271208	50.C	-0.675067	-1.158329	0.682563	46.H	-8.205037	7.069310	-6.482254			
123.H	-0.793739	-9.457177	-0.104336	51.C	0.307326	-1.727042	1.492665	47.H	-9.433760	7.551781	-8.379352			
124.H	-2.553558	-9.178489	-0.314491	52.C	1.549801	-1.101118	1.650381	48.H	-10.344855	3.291896	-6.756618			
125.H	-2.189235	-9.810069	-3.262457	53.C	1.795107	0.105418	0.983889	49.C	-0.432391	0.118401	-0.158803			
126.H	-2.115376	-8.132324	-3.843924	54.C	0.816023	0.679308	0.173209	50.C	-0.599179	-1.123481	0.502445			
127.H	-0.628102	-9.134267	-3.792099	55.H	-1.641212	-1.650769	0.561373	51.C	0.447524	-1.690098	1.225028			
6				56.H	0.102302	-2.668580	2.006047	52.C	1.685322	-1.039573	1.303688			
	1.C	-8.468757	3.254188	-5.686259	57.H	2.316962	-1.547895	2.284630	53.C	1.868386	0.187820	0.654642		
	2.C	-7.390905	3.995845	-5.153950	58.H	2.759340	0.604723	1.098011	54.C	0.825217	0.764033	-0.065580		
	3.C	-7.438367	5.394733	-5.346502	59.H	1.011668	1.621088	-0.342110	55.H	-1.562612	-1.630269	0.436087		
	4.C	-8.493439	6.015135	-6.008339	6 ⁺				56.H	0.301172	-2.645905	1.729574		
	5.C	-9.584586	5.268216	-6.513366		1.C	-8.523884	3.286108	-5.649544	57.H	2.503890	-1.487308	1.868343	
	6.C	-9.529863	3.863426	-6.349696		2.C	-7.393211	4.009284	-5.173920	58.H	2.831050	0.697162	0.713326	
	7.Ru	-3.838250	1.994495	-2.706073		3.C	-7.321298	5.391395	-5.510383	59.H	0.964866	1.721703	-0.568560	
	8.P	-3.356390	0.600861	-4.506176		4.C	-8.302356	6.009191	-6.257292	6 ²⁺ LS				
	9.C	-2.360321	1.544799	-5.786399		5.C	-9.427507	5.275518	-6.737488		1.C	-8.540622	3.266831	-5.512358
	10.C	-1.374496	2.482085	-5.075574		6.C	-9.503846	3.889134	-6.410280		2.C	-7.360552	3.999317	-5.151686
	11.P	-2.260835	3.390167	-3.690720		7.Ru	-3.983123	2.021575	-2.642409		3.C	-7.247813	5.346951	-5.631935
	12.N	-10.680357	5.893352	-7.123947		8.P	-3.422626	0.589924	-4.432458		4.C	-8.231096	5.921171	-6.393551
	13.C	-11.605940	5.073753	-7.892121		9.C	-2.301315	1.492329	-5.633101		5.C	-9.400510	5.174610	-6.768015
	14.C	-2.333067	1.143554	-1.536785		10.C	-1.384603	2.460382	-4.871410		6.C	-9.514036	3.819912	-6.301960
	15.C	-1.452623	0.646615	-0.824693		11.P	-2.383014	3.431745	-3.619713		7.Ru	-3.978514	2.088330	-2.594567
	16.H	-11.127333	4.566313	-8.752872		12.N	-10.400503	5.881447	-7.486698		8.P	-3.408045	0.660525	-4.427217
	17.H	-12.414189	5.710316	-8.270437		13.C	-11.527809	5.107936	-8.004525		9.C	-2.295908	1.589534	-5.609188
	18.H	-12.063852	4.304495	-7.254903		14.C	-2.434199	1.193300	-1.548337		10.C	-1.379802	2.552476	-4.839372
	19.C	-6.312724	3.370926	-4.457711		15.C	-1.499648	0.699416	-0.898784		11.P	-2.362854	3.514188	-3.571369
	20.C	-5.377973	2.854000	-3.835403		16.H	-12.165044	5.764024	-8.603227		12.N	-10.364809	5.729980	-7.535946
	21.H	-11.491908	7.618861	-7.971549		17.H	-12.134338	4.687675	-7.187822		13.C	-11.484964	4.934988	-8.059453
	22.H	-10.315614	7.926057	-6.686214		18.H	-11.181569	4.283975	-8.646218		14.C	-2.458488	1.232841	-1.541216
	23.H	-5.089798	4.625561	-1.198935		19.C	-6.390901	3.390856	-4.409666		15.C	-1.519241	0.685754	-0.924378
	24.H	-3.391355	3.955885	-0.049731		20.C	-5.487214	2.860274	-3.730593		16.H	-11.937948	5.478196	-8.893405

17.H	-12.250656	4.777421	-7.285097	13.C	-11.573344	5.084150	-7.844676
18.H	-11.131681	3.965974	-8.428702	14.C	-2.404576	1.177709	-1.567604
19.C	-6.364505	3.426675	-4.373675	15.C	-1.489972	0.674067	-0.872119
20.C	-5.454363	2.914816	-3.670989	16.H	-12.376186	5.777391	-8.109316
21.H	-11.344161	7.452269	-8.210867	17.H	-11.952496	4.386148	-7.088997
22.H	-10.065171	7.764858	-7.019701	18.H	-11.281552	4.523963	-8.745830
23.H	-5.257539	4.570583	-0.798351	19.C	-6.318603	3.367692	-4.425590
24.H	-3.345065	4.015257	0.066498	20.C	-5.398524	2.833794	-3.768935
25.P	-4.413648	3.432215	-0.666260	21.H	-11.152566	7.527459	-8.351442
26.C	-5.285843	2.384902	0.610123	22.H	-10.712026	7.859728	-6.657424
27.C	-6.287893	1.442628	-0.073407	23.H	-5.269553	4.560588	-1.140406
28.P	-5.499626	0.604717	-1.551108	24.H	-3.463650	4.048467	-0.053341
29.H	-5.779034	3.028243	1.351338	25.P	-4.461519	3.426201	-0.852348
30.C	-10.342013	7.156983	-7.887975	26.C	-5.465980	2.476368	0.404342
31.H	-4.498710	1.816104	1.127423	27.C	-6.395404	1.479766	-0.303194
32.H	-7.150681	2.004500	-0.462205	28.P	-5.458066	0.547964	-1.625881
33.H	-6.670091	0.688455	0.627613	29.H	-6.029764	3.173343	1.039029
34.H	-6.629883	0.073138	-2.233016	30.C	-10.430227	7.301056	-7.562732
35.H	-4.980251	-0.601768	-1.004431	31.H	-4.739217	1.952841	1.043641
36.H	-1.342348	4.120079	-2.788185	32.H	-7.213925	2.004402	-0.818809
37.H	-2.796405	4.658983	-4.299345	33.H	-6.844885	0.774169	0.408499
38.H	-0.862095	3.241946	-5.519823	34.H	-6.504061	-0.076323	-2.360180
39.H	-2.963008	2.140166	-6.289648	35.H	-4.956681	-0.590629	-0.935500
40.H	-1.715748	0.878892	-6.213331	36.H	-1.199100	3.951905	-2.929550
41.H	-0.615252	1.997398	-4.275558	37.H	-2.728500	4.606631	-4.316093
42.H	-4.398197	0.116362	-5.291159	38.H	-0.938335	3.211865	-5.747923
43.H	-2.677806	-0.521942	-4.129167	39.H	-3.108893	2.154574	-6.384953
44.H	-8.650922	2.244926	-5.151068	40.H	-1.870393	0.882254	-6.462862
45.H	-6.357782	5.919541	-5.373297	41.H	-0.603955	1.916701	-4.578981
46.H	-8.104628	6.944369	-6.740075	42.H	-4.452681	0.070439	-5.342331
47.H	-9.636983	7.347326	-8.711077	43.H	-2.641652	-0.572826	-4.338610
48.H	-10.393772	3.230856	-6.551143	44.H	-8.306355	2.131660	-5.762333
49.C	-0.466199	0.050800	-0.238910	45.H	-6.674516	6.013309	-4.745115
50.C	-0.661126	-1.226180	0.363131	46.H	-8.449435	7.108343	-6.016295
51.C	0.381457	-1.851698	1.030146	47.H	-9.438001	7.626633	-7.896929
52.C	1.637485	-1.228445	1.113162	48.H	-10.118340	3.203347	-7.001081
53.C	1.849225	0.030156	0.526564	49.C	-0.472262	0.105031	-0.090158
54.C	0.814328	0.668209	-0.140743	50.C	-0.764956	-0.953158	0.821429
55.H	-1.639352	-1.701243	0.288818	51.C	0.246483	-1.519479	1.580613
56.H	0.227630	-2.828085	1.489354	52.C	1.560718	-1.031449	1.478679
57.H	2.454507	-1.725473	1.637295	53.C	1.865711	0.020407	0.597604
58.H	2.827646	0.505060	0.597290	54.C	0.870989	0.575624	-0.191330
59.H	0.965818	1.646609	-0.596828	55.H	-1.788760	-1.319712	0.894543

6²⁺ HS

1.C	-8.350647	3.218886	-5.817094	56.H	0.023389	-2.341991	2.259939
2.C	-7.346475	3.985105	-5.151070	57.H	2.350222	-1.472732	2.087911
3.C	-7.428024	5.407783	-5.247665	58.H	2.886435	0.397029	0.533716
4.C	-8.425841	6.021918	-5.966565	59.H	1.095864	1.389033	-0.881024
5.C	-9.441366	5.250285	-6.616624				
6.C	-9.371832	3.824268	-6.510639				
7.Ru	-3.890166	1.993239	-2.668625				
8.P	-3.404910	0.609275	-4.547445				
9.C	-2.391632	1.572964	-5.786342				
10.C	-1.406717	2.497990	-5.057065				
11.P	-2.280029	3.414418	-3.680966				
12.N	-10.441668	5.854218	-7.313808				