

Supporting Information
for
Simple activation by acid of latent Ru-NHC-based
metathesis initiators bearing 8-quinolinolate co-
ligands

Julia Wappel¹, Roland C. Fischer², Luigi Cavallo³, Christian Slugovc¹
and Albert Poater^{3,4,*}

Address: ¹Institute for Chemistry and Technology of Materials, Graz University of Technology, NAWI Graz, Stremayrgasse 9, 8010 Graz, Austria, ²Institute of Inorganic Chemistry, Graz University of Technology, Stremayrgasse 9, 8010 Graz, Austria, ³KAUST Catalysis Center, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia and ⁴Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, Campus de Montilivi, E-17071 Girona, Spain.

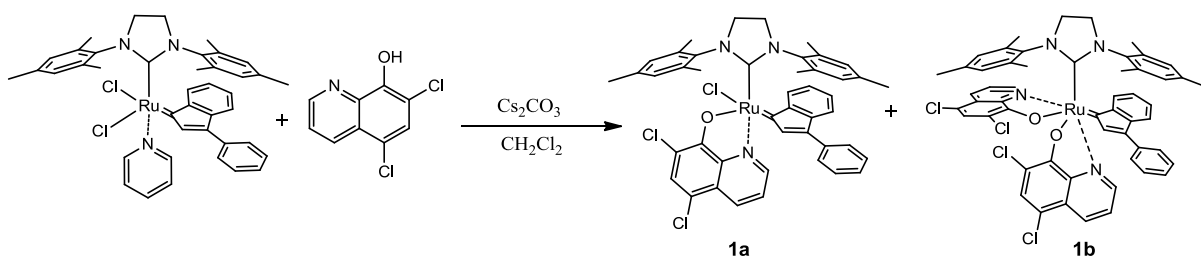
Email: Albert Poater - albert.poater@udg.edu

*Corresponding author

**Experimental data, energies, Cartesian coordinates, and 3D view for all DFT
optimized species discussed in this work**

1. Complex synthesis and characterization

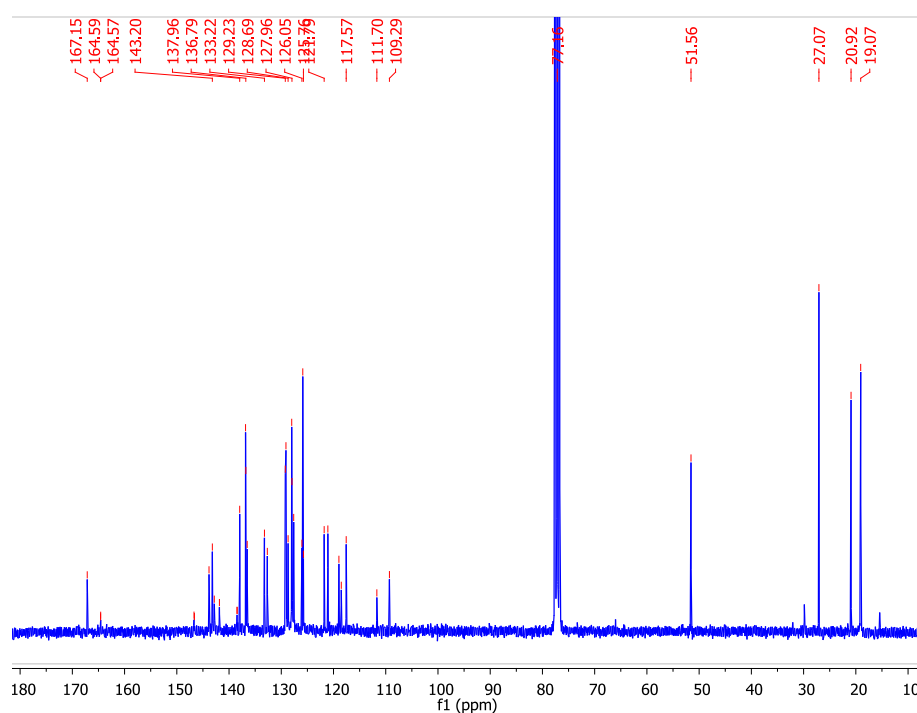
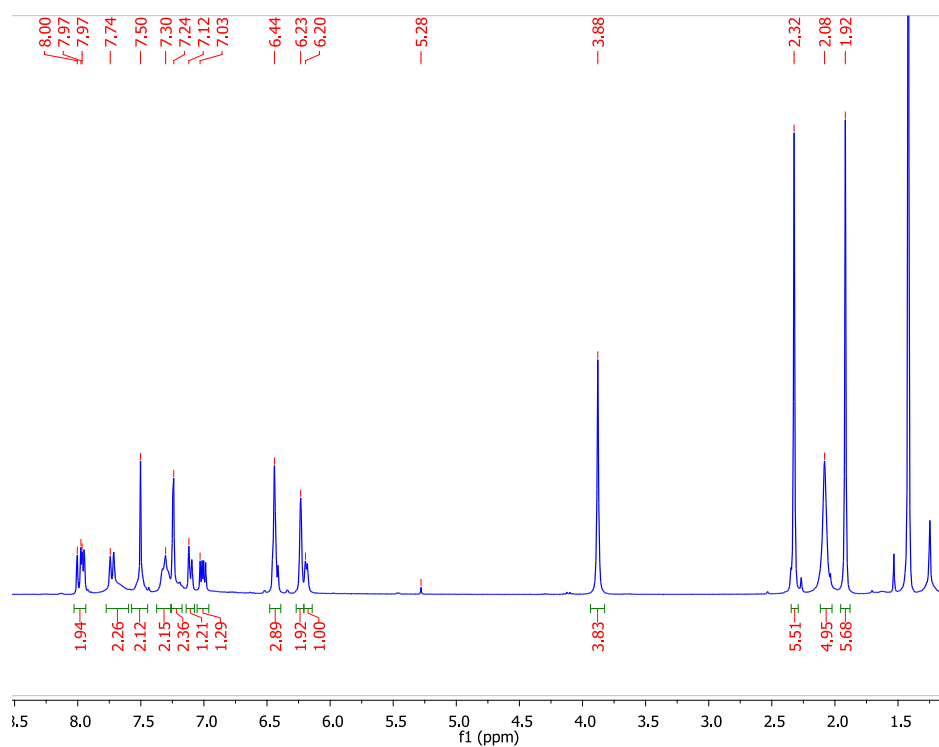
Synthesis way A



In a Schlenk flask **M31** (Py)(H₂IMes)(Cl₂)Ru(3-phenyl-1*H*-inden-1-ylidene) (142 mg, 0.189 mmol, 1 equiv) was dissolved in degassed CH₂Cl₂ (≈18 mL). 5,7-Dichloro-8-hydroxyquinoline (810 mg, 3.785 mmol, 20 equiv) and Cs₂CO₃ (1.24 g, 3.815 mmol, 20 equiv) were added. The reaction mixture was stirred in a Schlenk flask under argon atmosphere overnight. The insoluble residue was filtered over celite. According to a TLC (CH/EE 5:1) two derivatives were formed. The two catalysts were separated via column chromatography (CH/EE 10:1) and fully characterized by NMR. Yield = 90% (117 mg **1** and 33 mg **2**).

1a: ¹H-NMR (δ, 20°C, CDCl₃, 300 MHz): 8.0 (d, *j* = 8.1 Hz, 1H, CH^{hq 3}), 7.97 (d, *j* = 4.8 Hz, 1H, CH^{hq 1}), 7.74 (d, *j* = 8.1 Hz, CH), 7.30 (t, 2H, CH), 7.05 (s, 2H, CH), 7.23 (d, 2H, CH), 7.12 (d, *j* = 7.14 Hz, 1H, CH), 7.03 (q, 1H, CH^{hq 2}), 6.44 (s, 3H, CH), 6.23 (s, 2H, CH), 6.20 (d, 1H, CH), 3.87 (s, 4H, CH₂), 2, 32, 2.08, 1.92 (s, 18H, CH₃^{mes 7,7',8,8',9,9'}).

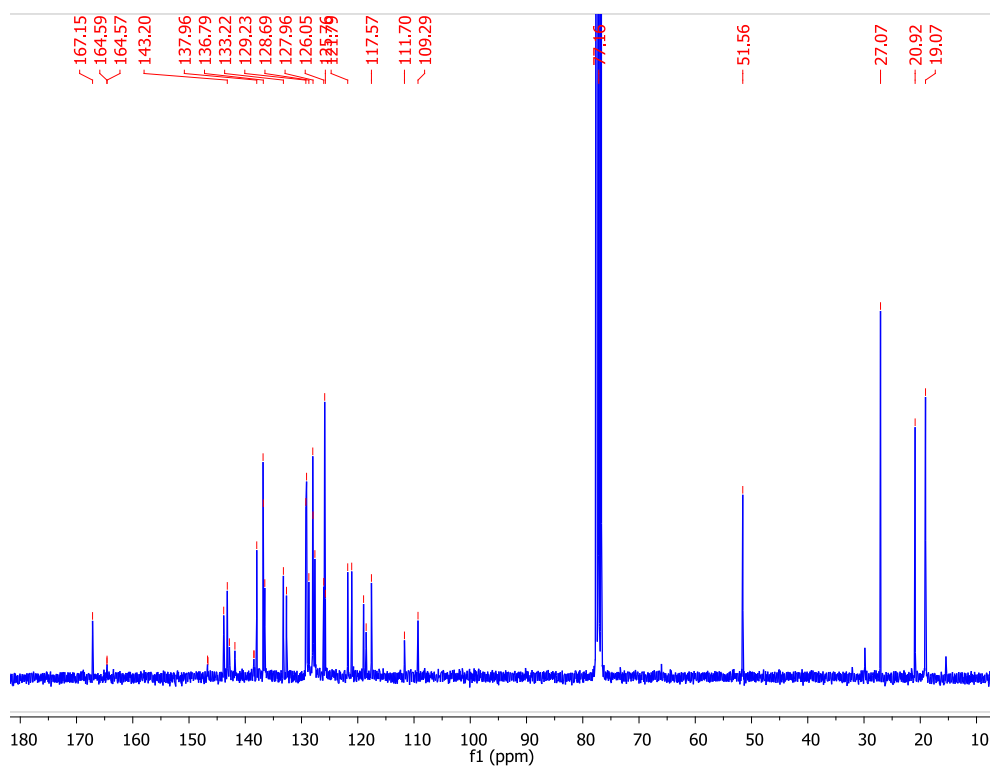
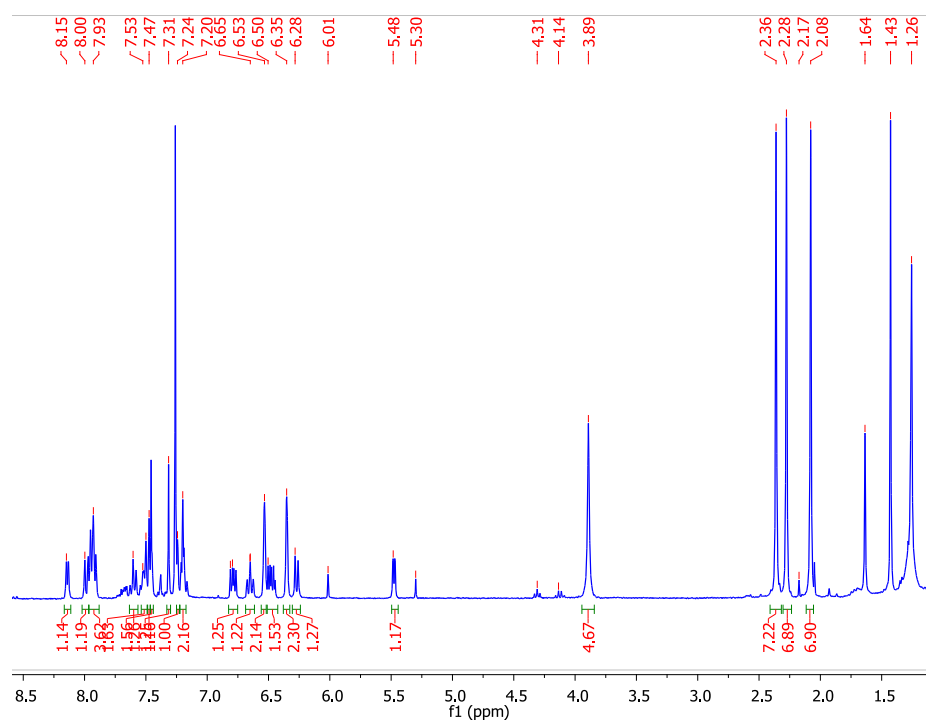
¹³C-NMR (δ, 20°C, CDCl₃, 300 MHz): Ru=C and Ru-C not observed, 167.2 (C_q), 164.6 (CH), 146.7 (CH), 143.8 (C_q), 143.2 (CH), 142.8 (CH), 141.8 (C_q), 138.0 (C_q), 136.9 (C_q), 136.8 (C_q), 136.5 (C_q), 133.2 (CH), 132.7 (CH), 129.1 (CH), 129.1 (CH), 128.7 (CH), 128.0 (CH), 127.9 (CH), 127.6 (CH), 126.0 (C_q), 125.9 (CH), 125.7 (C_q), 121.8 (CH), 121.0 (CH), 118.9 (C_q), 118.5 (C_q), 117.6 (CH), 111.7 (C_q), 109.3 (C_q), 51.6 (2C, CH₂-N), 20.9, 18.1 (12C, CH₃).



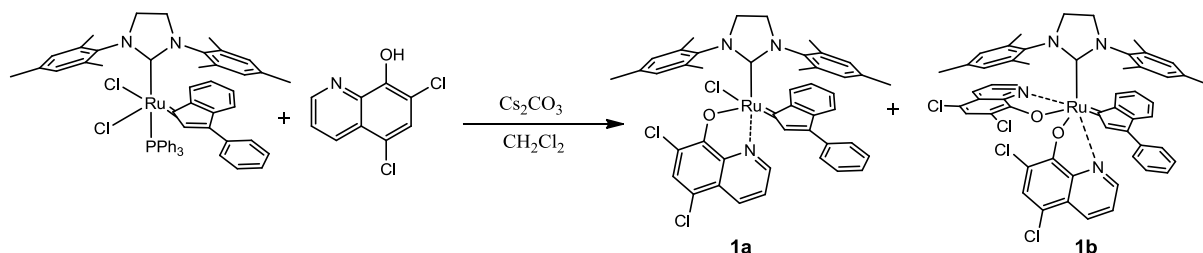
1b: ¹H-NMR (δ, 20°C, CDCl₃, 300 MHz): 8.15 (d j= 4.8 hZ, 1H, CH^{hq} 1), 7.99 (dd j= 8.4, 1H, CH^{hq} 3), 7.9 (3H, CH^{hq} 3), 7.60 (1H, CH), 7.52 (1H, CH), 7.47 (1H, CH), 7.31 (s, 1H, CH), 7.24 (s, 1H, CH), 7.2 (t, 2H, CH^{ind} 2 or 3), 6.81 (q, 1H, CH^{hq} 2), 6.65 (t, 1H, CH^{ind} 2 or 3), 6.53 (s, 2H, CH^{mes}), 6.50 (q, 1H, CH^{hq} 2), 6.35 (s, 2H, CH^{mes}), 6.28 (d j=7.2 Hz, CH^{ind} 1 or 4), 5.48 (dd j=4.8 Hz, 1H, CH^{hq} 1), 3.89 (s, 4H, CH₂^{mes}), 2.36, 2.28, 2.08 (s, 18H, CH₃^{mes}).

¹³C-NMR (δ, 20°C, CDCl₃, 300 MHz): Ru=C not observed, 204.3 (1C, C_q, Ru-C), 166.3 (C_q), 161.2 (C_q), 150.0 (CH), 145.8 (C_q), 145.1 (C_q), 143.1 (CH), 142.0 (C_q), 141.7 (CH), 140.4 (C_q),

137.9 (C_q), 137.5 (C_q), 137.3 (C_q), 136.8 (C_q), 136.4 (C_q), 136.3 (C_q), 136.4 (C_q), 136.3 (C_q), 136.2 (C_q), 133.3 (CH), 133.2 (CH), 130.0 (CH), 129.7 (CH), 129.6 (CH), 129.4 (CH), 129.3 (CH), 129.1 (CH), 128.5 (CH), 128.2 (CH), 128.1 (CH), 126.6 (CH), 126.0 (CH), 125.9 (C_q), 125.8 (CH), 125.4 (C_q), 120.9 (CH), 120.7 (CH), 120.1 (C_q), 118.5 (CH), 118.2 (C_q), 112.2 (C_q), 108.2 (C_q), 53.3 (2C, CH₂-N), 20.9, 20.3, 19.5 (18C, CH₃).

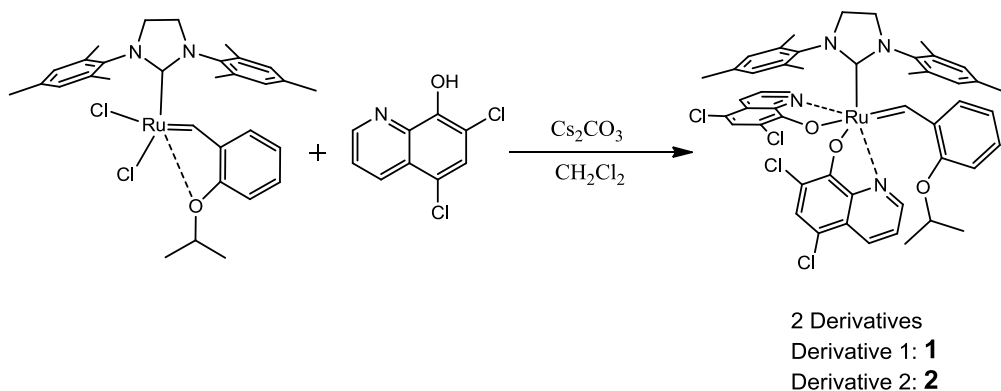


Synthesis way B



In a Schlenk flask $(\text{PPh}_3)(\text{H}_2\text{IMes})(\text{Cl}_2)\text{Ru}(3\text{-phenyl-1}H\text{-inden-1-ylidene})$ (26 mg, 0,0278 mmol, 1 equiv) was dissolved in degassed CH_2Cl_2 (≈ 3 mL). 5,7-Dichloro-8-hydroxyquinoline (88 mg, 0,411 mmol, 15 equiv) and Cs_2CO_3 (150 mg, 0,461 mmol, 16 equiv) were added. The reaction mixture was stirred in a Schlenk flask under argon atmosphere overnight. The insoluble residue was filtered over celite. According to a TLC (CH/EE 5:1) two derivatives were formed. The two catalysts were separated via column chromatography (CH/EE 20:1) and fully characterized by NMR. Yield = 73% (10,3 mg **1a** and 8,4 mg **1b**).

Di-(5,7-dichloro-8-quinolinolate)(isopropylbenzylidene)(1,3-bis(2,4,6-trimethylphenyl)-4,5-dihydroimidazol-2-ylidene)ruthenium, **2a** and **2b**

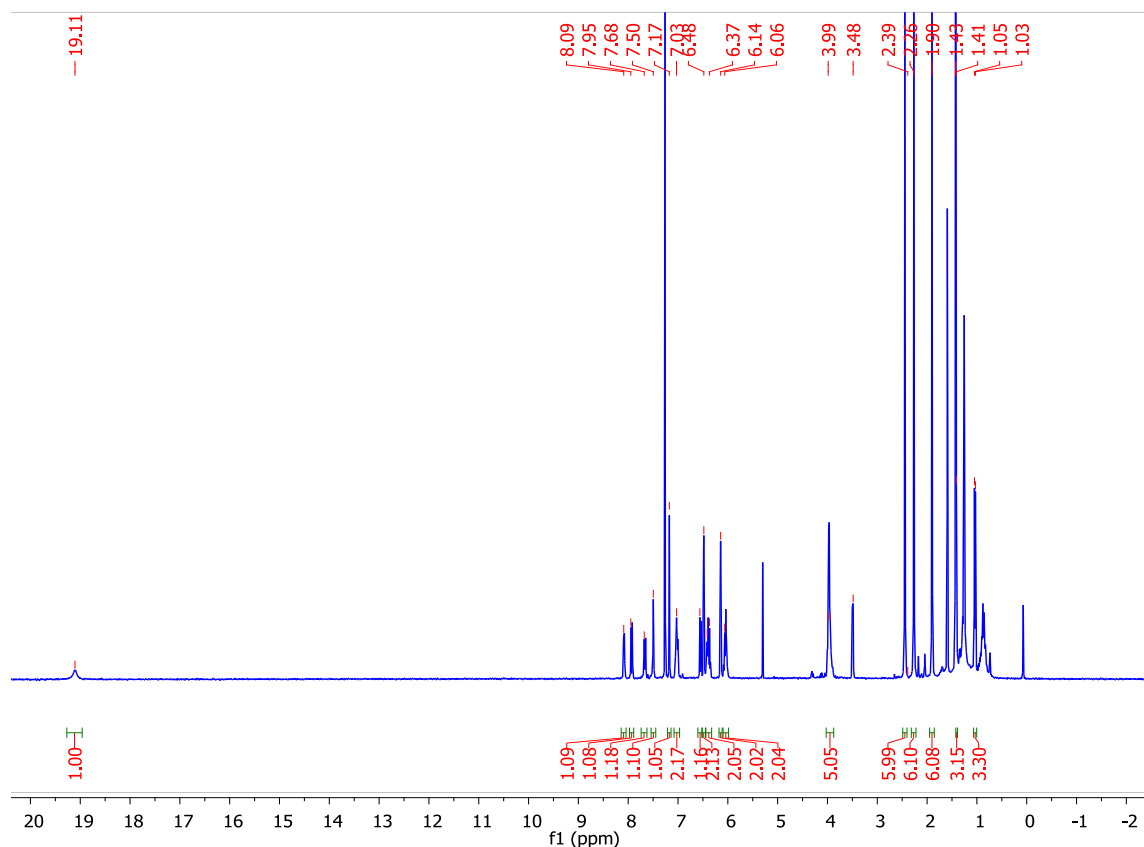


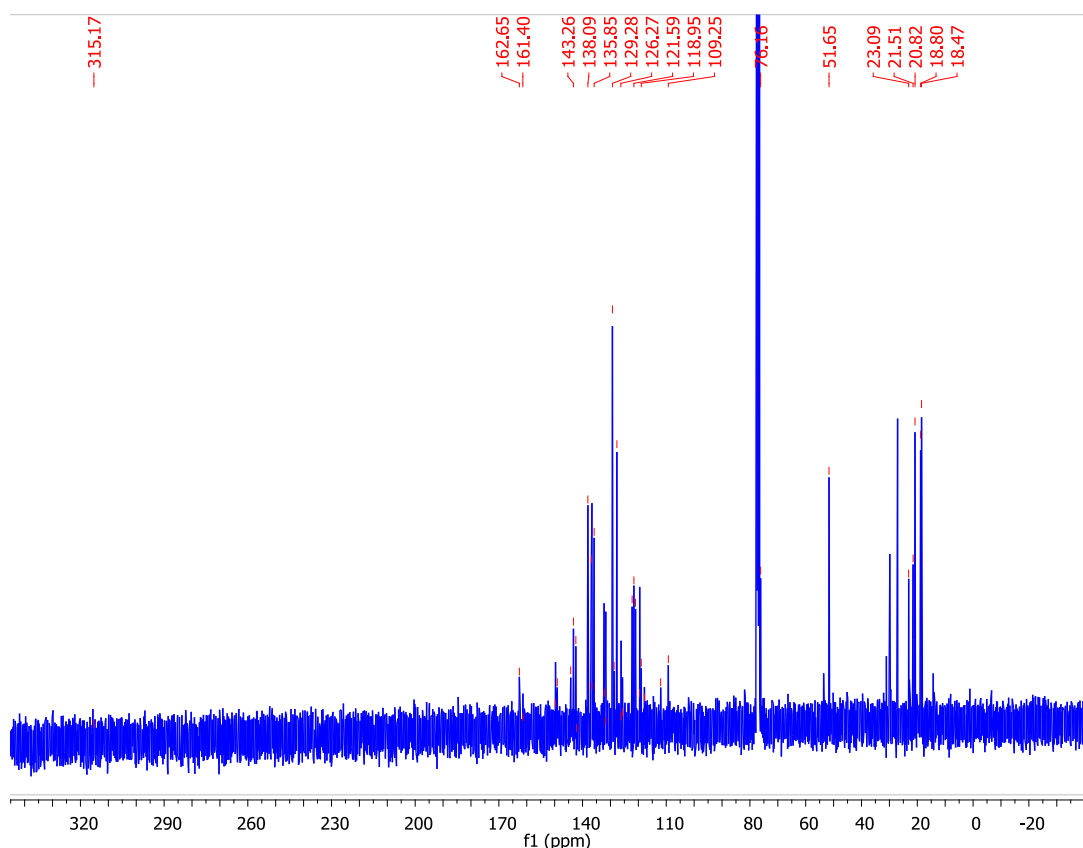
In a Schlenk flask, $(\text{H}_2\text{IMes})\text{Cl}_2\text{Ru}(\text{CH-}o\text{-OiPrC}_6\text{H}_4)$ (106 mg, 0.169 mmol, 1 equiv) was dissolved in degassed CH_2Cl_2 (≈ 18 mL). 5,7-Dichloro-8-hydroxyquinoline (707 mg, 3.303 mmol, 19 equiv) and Cs_2CO_3 (150 mg, 0,461 mmol, 16 equiv) were added. The reaction mixture was stirred under a nitrogen atmosphere overnight. The insoluble residue was filtered over celite. According to a TLC (CH/EE 5:1) two derivatives were formed. The products were separated via column chromatography (CH/EE 5:1) and fully characterized by NMR and crystal structure analysis. Yield = 83% (46.5 mg **2a** and 91 mg **2b**).

2a: $^1\text{H-NMR}$ (δ , 20°C, CDCl_3 , 300 MHz): 19.10 (s, 1H, $\text{Ru}=\text{CH}$), 8.09 (d $J=4,04$, 1H, CH^{hq}), 7.95 (d $J=8,56$; $j=1,43$, 1H, CH^{hq}), 7.68 (d $J=8,43$ $j=1,30$, 1H, CH^{ph}), 7.49 (s, 1H, CH^{hq}), 7.17 (s, 1H, CH^{hq}), 7.05 (m, 2H, CH^{hq}), 6.56 (d $J=8,04$, 1H, CH^{hq}), 6.48 (s, 2H, CH^{mes}), 6.43 6,39 (? , 2H,

CH^{ph}), 6.14 (s, 2H, CH^{mes}), 6.06 (2H, $CH^{hq + ph}$), 3.97 (5H, $CH_2 + CH^{isoprop}$), 2.45 (s, 6H), 2.27 (s, 6H), 1.90 (s, 6H, $CH_3^{1, 1', 2, 2', 3, 3'}$), 1.43 (d, 3H, $CH_3^{isoprop}$), 1.05 (d, 3H, $CH_3^{isoprop}$).

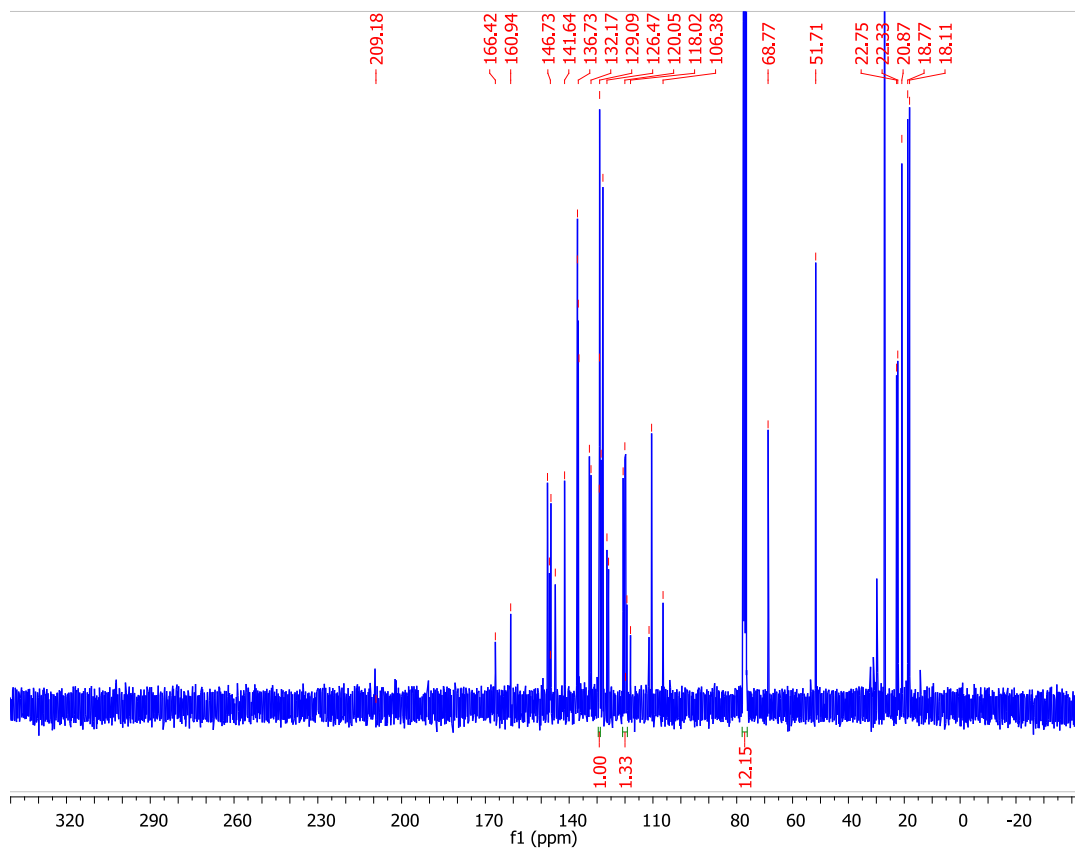
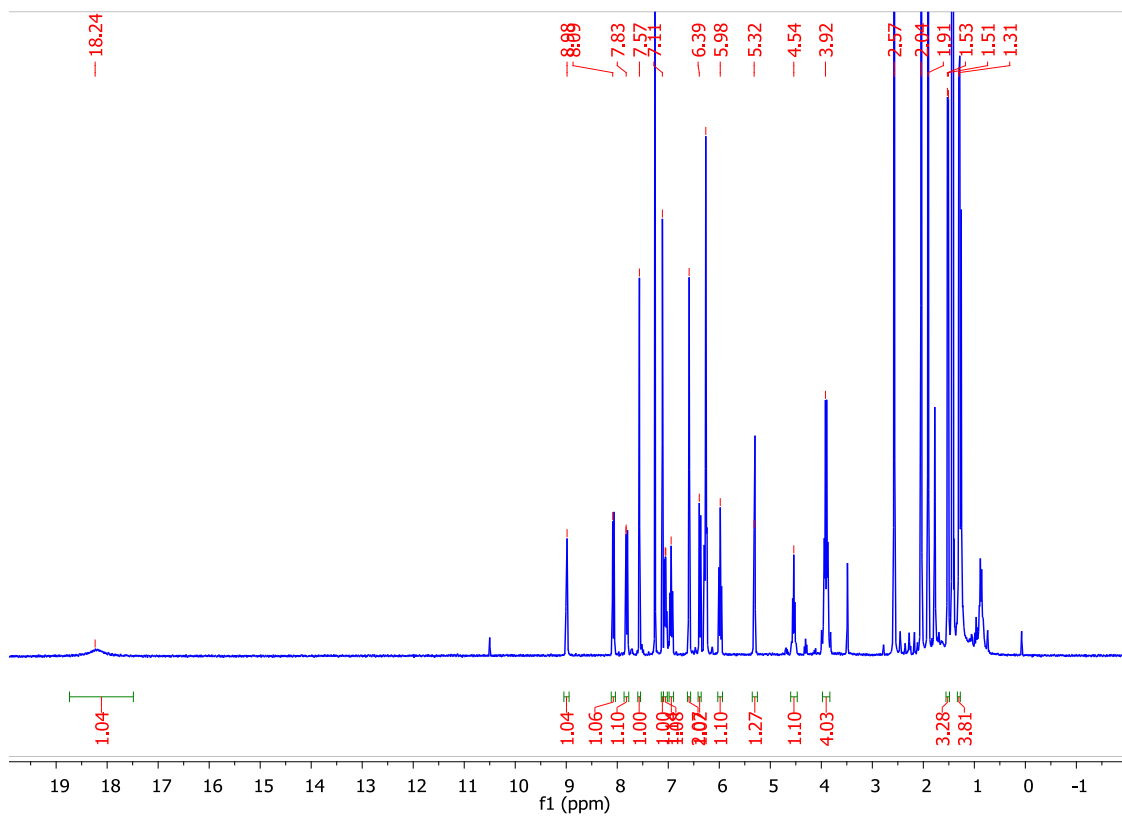
^{13}C -NMR (δ , 20°C, $CDCl_3$, 75 MHz): 315.5 (1C, Ru=CH), Ru-C was not observed, 162.6, 161.3, 149.7, 149.4, 149.0, 144.2, 143.2, 142.4, 142.3, 138.1 (C_q), 136.9 (C_q), 136.6 (C_q), 135.8 (C_q), 132.3 (CH), 131.7 (CH), 129.3 (CH), 129.2 (CH), 128.7, 127.7 (CH), 126.2, 125.8, 125.7, 122.2 (CH), 121.6 (CH), 121.0 (CH), 119.5 (CH), 118.9, 112.0, 109.2, 76.2 (1C, $CH^{isoprop}$), 51.6 (2C, CH_2-N), 23.1 (1C, $CH_3^{isoprop}$), 21.5 (1C, $CH_3^{isoprop}$), 20.8, 18.8, 18.5 (2C, $CH_3^{mes 7, 7', 8, 8', 9, 9'}$).





2b: $^1\text{H-NMR}$ (δ , 20°C, CDCl_3 , 300 MHz): 18.24 (bs, 1H, Ru=CH), 9.00 (d $j=4.67$ Hz, 1H, $\text{CH}^{\text{hq}1}$), 8.09 (d $J=8.56$ Hz, 1H, $\text{CH}^{\text{hq}3}$), 7.83 (d $J=8.30$ Hz, 1H, $\text{CH}^{\text{hq}3}$), 7.57 (s, 1H, $\text{CH}^{\text{hq}4 \text{ or } 4}$), 7.12 (s, 1H, $\text{CH}^{\text{hq}4 \text{ or } 4}$), 7.06 (q, 1H, $\text{CH}^{\text{hq}2}$), 6.94 (t, 1H; $\text{CH}^{\text{ph}3 \text{ or } 4}$), 6.59 (s, 2H, $\text{CH}^{\text{mes}3+3' \text{ or } 5+5'}$), 6.39 (d, 1H, $\text{CH}^{\text{ph}2 \text{ or } 5}$), 6.26 (s, 2H, $\text{CH}^{\text{mes}3+3' \text{ or } 5+5'}$), (d, 1H, $\text{CH}^{\text{ph}2 \text{ or } 5}$), (t, 1H, $\text{CH}^{\text{hq}2}$), 5.98 (t, 1H, $\text{CH}^{\text{ph}3 \text{ or } 4}$), 5.32 (d $j=4.54$ Hz, 1H, $\text{CH}^{\text{hq}1}$), 4.54 (m, 1H, $\text{CH}^{\text{isoprop}}$), 3.92 (q, 4H, CH_2^{mes}), 2.57 (s, 6H), 2.04 (s, 6H), 1.91 (s, 6H, $\text{CH}_3^{\text{mes}7,7',8,8',9,9'}$), 1.53 (d, 3H, $\text{CH}_3^{\text{isoprop}}$), 1.31 (d, 3H, $\text{CH}_3^{\text{isoprop}}$).

$^{13}\text{C-NMR}$ (δ , 20°C, CDCl_3 , 75 MHz): Ru=C not observed, 209.5 (1C, Ru-C), 166.4 (C_q), 160.9 (C_q), 147.7 (C_q), 146.7 (C_q), 147.1 (C_q), 146.7 (C_q), 164.5 (CH), 146.5 (CH), 144.9 (C_q), 141.2 (CH), 137.1 (C_q), 137.0 (C_q), 136.7 (C_q), 136.5 (C_q), 119.3 (C_q), 125.8 (C_q), 132.7 (CH), 132.2 (CH), 129.2 (CH), 129.1 (2C, CH), 129.0 (CH), 128.6 (CH), 127.9 (CH), 126.4 (C_q), 120.7 (CH), 120.1 (CH), 119.7 (CH), 118.0 (C_q), 111.3 (C_q), 110.5 (CH), 106.4 (C_q), 68.7 (1C, $\text{CH}^{\text{isoprop}}$), 51.7 (2C, CH_2), 22.7, 22.3 (2C, $\text{CH}_3^{\text{isoprop}}$), 20.9, 18.9, 18.1 (6C, $\text{CH}_3^{\text{mes}7,7',8,8',9,9'}$).



Crystal structures

The crystals for the X-ray diffraction measurement were obtained by slow diffusion of Et₂O in a saturated solution of CH₂Cl₂.

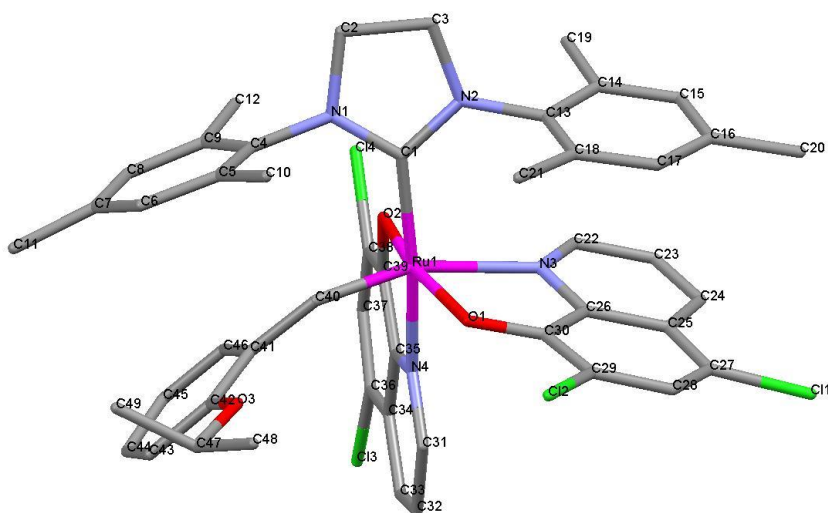


Figure 1: Crystal structure of complex 1

Empirical formula	C _{24.50} H ₂₃ Cl ₂ N ₂ O _{1.50} Ru _{0.50}	
Formula weight	490.88	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1375(5) Å	α = 72.358(3)°.
	b = 12.6359(6) Å	β = 88.303(5)°.
	c = 20.7869(12) Å	γ = 74.605(3)°.
Volume	2201.7(2) Å ³	
Z	4	
Density (calculated)	1.481 Mg/m ³	
Absorption coefficient	0.647 mm ⁻¹	
F(000)	1008	
Crystal size	0.246 x 0.112 x 0.086 mm ³	
Theta range for data collection	1.74 to 24.05°.	
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -23 ≤ l ≤ 23	
Reflections collected	87418	
Independent reflections	6894 [R(int) = 0.1038]	
Completeness to theta = 24.05°	99.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	

Data / restraints / parameters	6894 / 0 / 558
Goodness-of-fit on F^2	1.154
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0528$, $wR2 = 0.0964$
R indices (all data)	$R1 = 0.0901$, $wR2 = 0.1153$
Largest diff. peak and hole	0.802 and -0.896 e.Å ⁻³

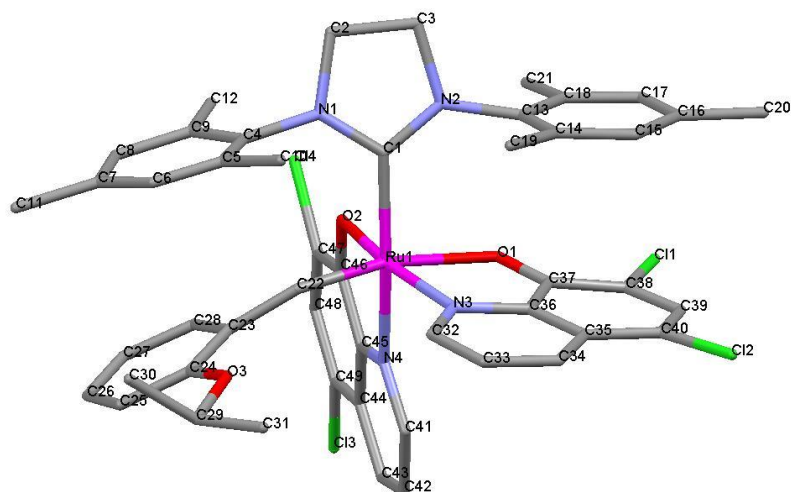
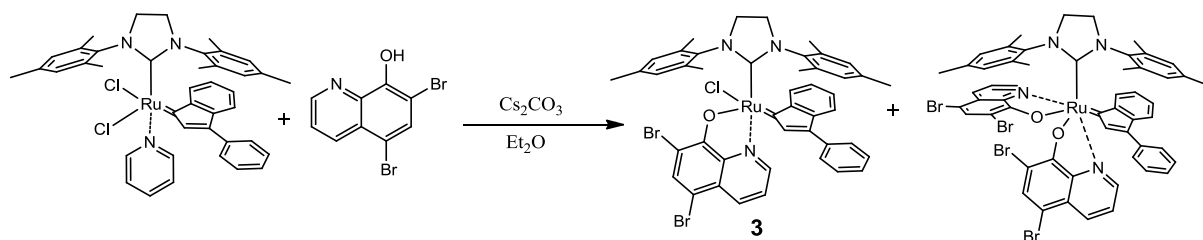


Figure 2: Crystal structure of complex 2

Empirical formula	C ₄₉ H ₄₇ Cl ₄ N ₄ O ₃ Ru	
Formula weight	982.78	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	$a = 11.7075(4)$ Å	$\alpha = 68.854(2)^\circ$
	$b = 13.0761(4)$ Å	$\beta = 76.072(2)^\circ$
	$c = 16.6073(5)$ Å	$\gamma = 73.544(2)^\circ$
Volume	2246.63(12) Å ³	
Z	2	
Density (calculated)	1.453 Mg/m ³	
Absorption coefficient	0.634 mm ⁻¹	
F(000)	1010	
Crystal size	0.18 x 0.12 x 0.04 mm ³	
Theta range for data collection	1.71 to 25.00°	

Index ranges	-13<=h<=13, -15<=k<=15, -19<=l<=19
Reflections collected	27470
Independent reflections	7791 [R(int) = 0.0629]
Completeness to theta = 25.00°	98.5 %
Max. and min. transmission	0.9751 and 0.8944
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7791 / 0 / 558
Goodness-of-fit on F ²	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0727, wR2 = 0.1411
R indices (all data)	R1 = 0.1226, wR2 = 0.1673
Largest diff. peak and hole	1.388 and -1.529 e.Å ⁻³

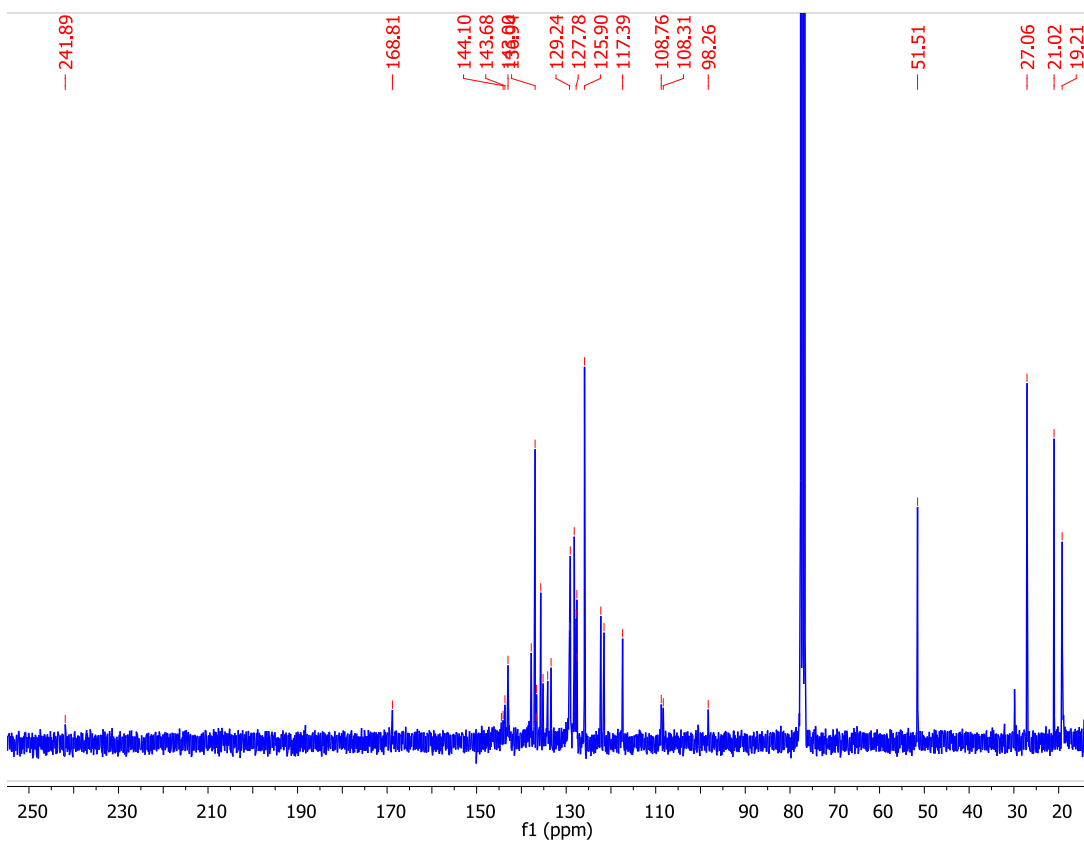
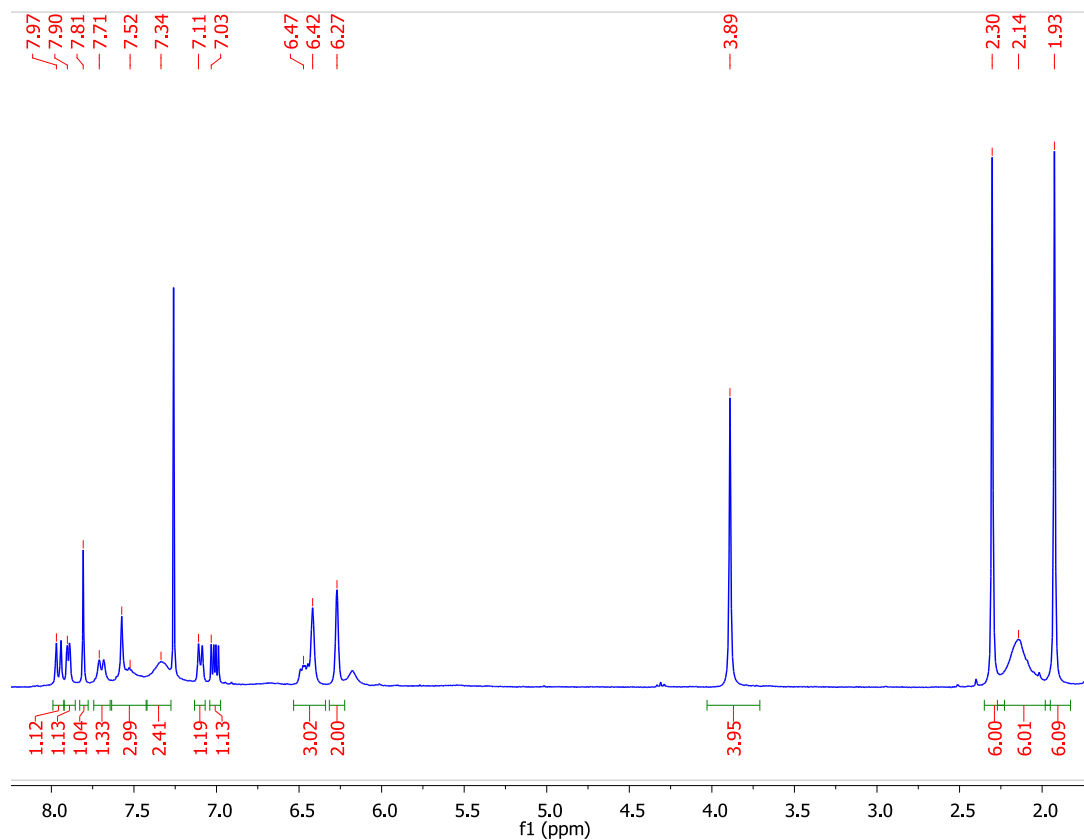
Di-(5,7-dibromo-8-quinolinolate)(isopropylbenzylidene)(1,3-bis(2,4,6-trimethylphenyl) 4,5-dihydroimidazol-2-ylidene)ruthenium (3)



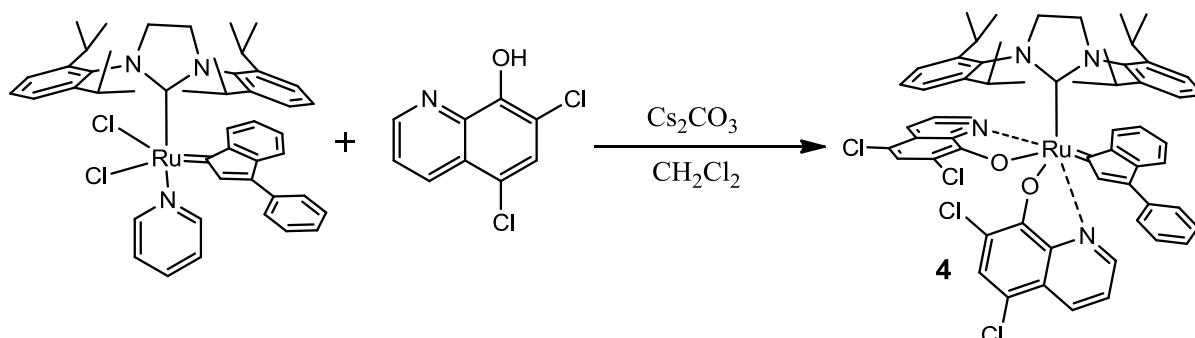
In a Schlenk flask, M31 (160 mg, 0.214 mmol, 1 equiv) was dissolved in degassed Et₂O. 5,7-Dibromo-8-hydroxyquinoline (960 mg, 3.169 mmol, 15 equiv) and Cs₂CO₃ (1g, 3.077 mmol, 14 equiv) were added. The reaction mixture was stirred in a Schlenk flask under argon atmosphere for 12 hours. The reaction progress was followed by TLC (CH/EE 5:1). The insoluble residue was filtered over celite. According to a TLC (CH/EE 5:1) two products were formed. The new formed pre-catalysts were separated by column-chromatography (CH/EE 10:1), however, just the catalyst possessing one 8-quinolinolate was isolated.

3: ¹H-NMR (δ, 20°C, CDCl₃, 300 MHz): 7.97 (d J=8.52, 1H, CH), 7.90 (d J=4.26, 1H, CH), 7.81 (s, 1H, CH^{hq}), 7.71 (d J=8.33, 1H, CH), 7.57 (s), 7.53 (bs, 3H, CH), 7.34 (bs, 3H, CH), 7.11 (d J=7.00, 1H, CH), 7.03 (q, 1H, CH), 6.49 (bs), 6.42 (s, 3H, CH + CH^{mes}), 6.27 (s, 2H, CH^{mes}), 6.18 (1H, bs, CH), 3.89 (s, 4H, CH₂), 2.30 (s, 6H, CH₃), 2.15 (bs, 6H, CH₃), 1.93 (s, 6H, CH₃).

¹³C-NMR (δ, 20°C, CDCl₃, 300 MHz): Ru=C not observed, 241.9 (Ru-C), 168.8, 144.5, 144.1, 143.7, 143.0, 137.8, 137.0, 136.9, 136.6, 135.6, 135.2, 134.2, 133.4, 129.2, 129.1, 128.2, 127.8, 127.6, 127.5, 125.9, 122.6, 121.6, 117.4, 108.7, 108.3, 98.2, 3 C fehlen, 51.5 (2C, CH₂^{mes}), 21.0, 19.2 (18C, CH₃^{mes}).



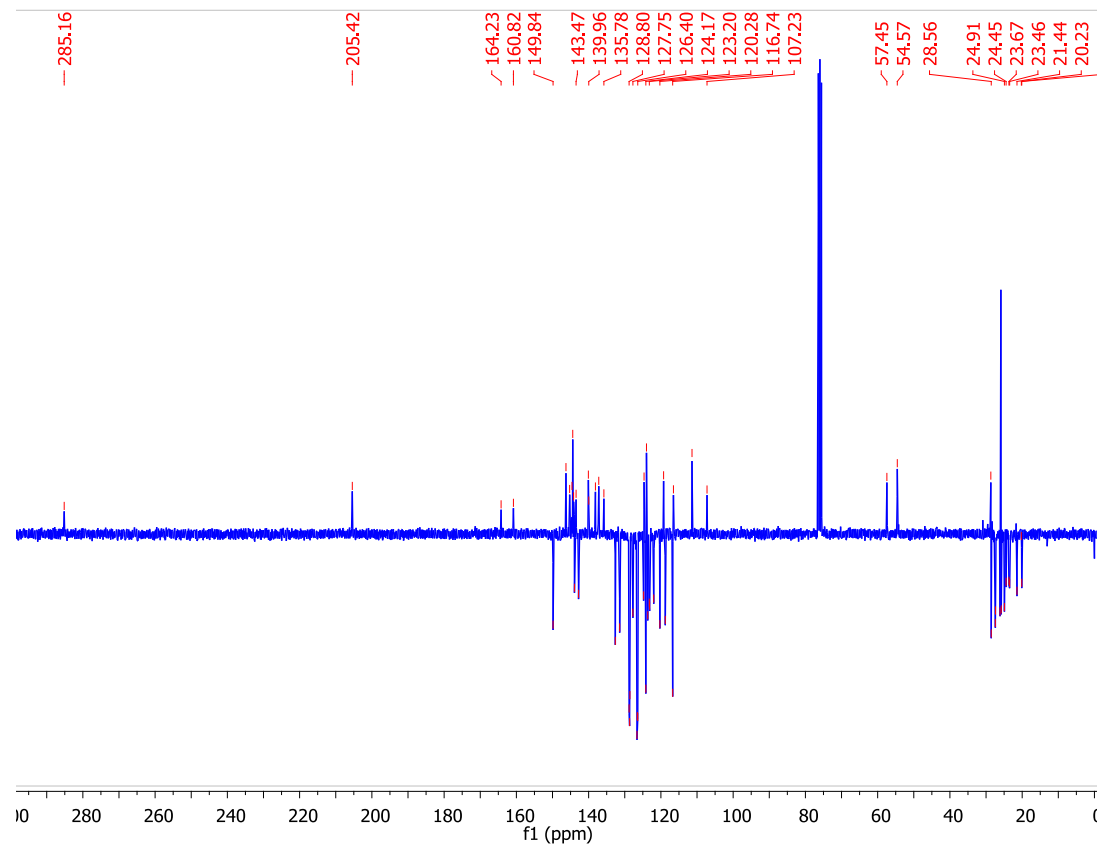
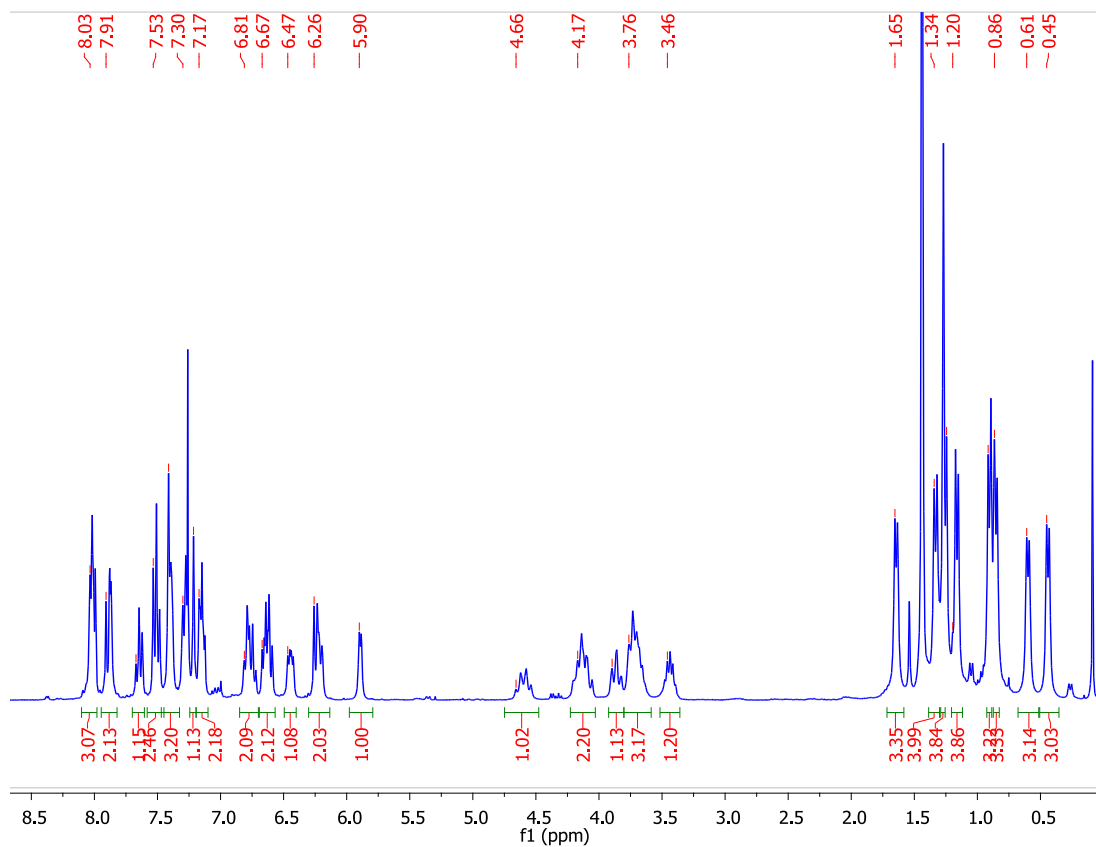
Di(5,7-dichloro-8-quinolinolate)(isopropylbenzylidene)(1,3-bis(2,4,6-trimethylphenyl)-4,5-dihydroimidazol-2-ylidene)ruthenium (4)



In a Schlenk flask, (Py)(H₂IPr)(Cl₂)Ru(3-phenyl-1*H*-inden-1-ylidene) (58 mg, 0,0697 mmol, 1 equiv) was dissolved in degassed CH₂Cl₂ (≈6 mL). Dichlorohydroxyquinoline (136 mg; 0,6355 mmol; 9 equiv) and Cs₂CO₃ (300 mg, 0,9230 mmol, 13 equiv) were added. The reaction mixture was stirred in a Schlenk flask under argon atmosphere overnight. The insoluble residue was filtered over celite. According to a TLC (CH/EE 5:1) two products were formed. The products were separated via column chromatography (CH/EE 5:1). The first derivative was just formed in very low amount and not identified. The second derivative was identified by NMR spectroscopy (¹H, COSY, ¹³C and APT). Yield = 52%.

4: ¹H-NMR (δ, 20°C, CDCl₃, 300 MHz): 8.03 (m, 3H, CH), 7.91 (s + d, 2H, CH), 7.67 (t, 1H, CH), 7.53 (t, 2H, CH), 7.41 (2s, 3H, CH), 7.30 (2s, 2H, CH), 7.21 (s, 1H, CH), 7.16 (m, 2H, CH), 6.79 (m, 2H, CH), 6.65 (m, 2H, CH), 6.47 (q, 1H, CH), 6.26 (m, 2H, CH), 5.9 (d, 1H J=4.51, CH^{hq}), 4.66, 4.17, 3.9, 3.76, 3.48 (8H, CH^{isop} + CH₂), 1.65, 1.34, 1.27, 1.17, 0.91, 0.61, 0.45 (d, 24H, CH₃9).

¹³C-NMR (δ, 20°C, CDCl₃, 300 MHz)ⁱ: 286.2 (Ru=C), 206.6 (1C, Ru-C), 165.4 (1C, C_q), 162.0 (1C, C_q), 151.0 (1C, CH), 147.4, 146.4, 145.8, 145.6, 145.3, 145.2 (6C, C_q), 145.1 (1C, CH), 144.7 (1C, C_q), 144.0 (1C, CH), 141.2, 141.1, 139.3, 138.4, 137.0 (5C, C_q), 133.8, 132.6, 130.0, 129.8, 129.7, 128.9, 127.8, 127.7, 127.6, 126.0 (10C, CH), 125.8 (1C, C_q), 125.3 (1C, CH), 125.2 (1C, C_q), 124.8, 124.4, 124.3, 123.1, 121.5 (5C, CH), 120.4 (1C, C_q), 120.0, 117.9 (2C, CH), 117.7, 112.6, 108.4 (3C, C_q), 58.7, 55.9 (2C, CH₂), 29.7, 28.6, 28.5, 27.3, 26.9, 26.1, 25.6, 24.8, 24.6, 22.0, 21.9, 21.2 (12C, CH^{isop} + CH₃).



2. Product characterization of ROMP products

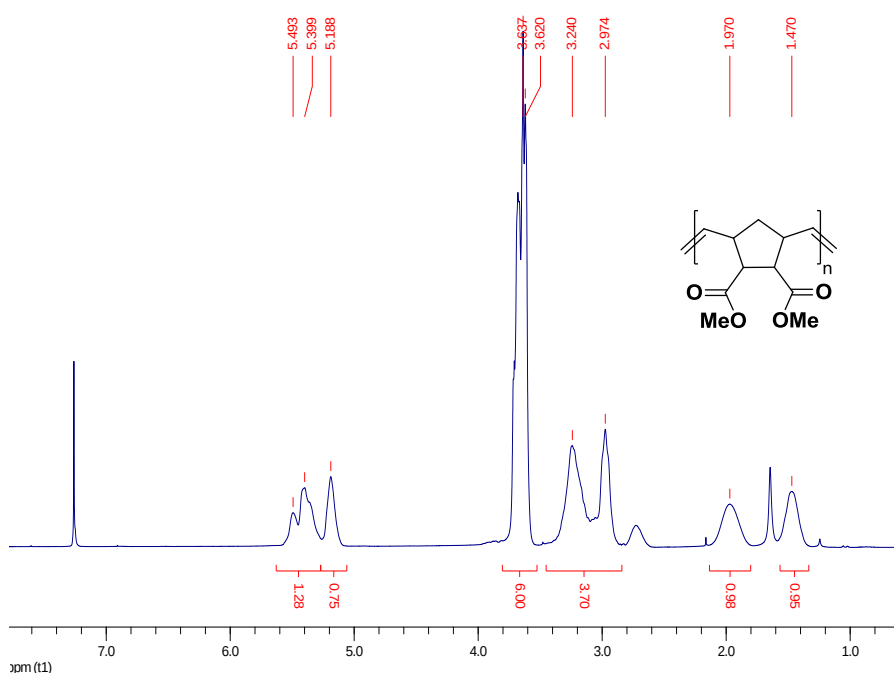
a. Polymerization in a NMR tube

In an NMR tube, catalysts **1–4** (1 equiv) were dissolved in CDCl_3 . **5** (50 equiv) dissolved in CDCl_3 was added. A concentration of 0.1 mol/L **5** was used. ^1H NMR spectra were recorded periodically and until the reaction was complete or no further conversion of the monomers could be observed to obtain conversion time plots

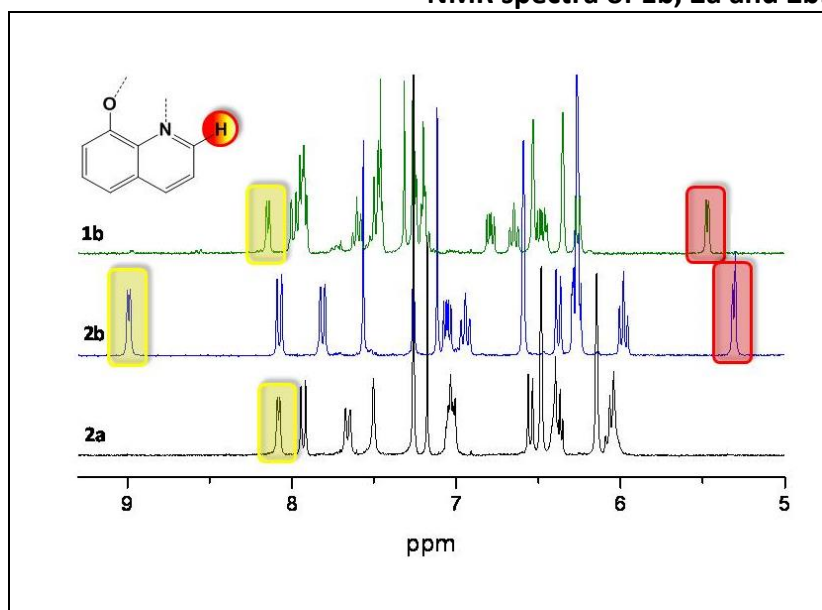
b. Polymerization in a Schlenk tube

Defined solutions of pre-catalyst **1–4** and **5** (300 equiv, 0.1 mol/L) were prepared. The reactions were performed in CH_2Cl_2 for room temperature and in toluene for 80 °C polymerizations. HCl (50 equiv ethereal HCl relative to ruthenium or 2 drops of HCl in aqueous solution) was added to activate the reaction. The reaction was followed by TLC (CH:EE 3:1) and after complete conversion stopped with an excess of ethyl vinyl ether. The polymer was precipitated in vigorously stirred methanol (approx. 50 mL for 100 mg polymer), and the white to yellowish precipitate was sampled and dried in vacuum. Yield: 90–20%.

^1H NMR (δ , 20 °C, CDCl_3 , 300 MHz): 5.50–5.19 (bm, 2H, $\text{CH}=\text{CH}$), 3.63 (bd, 6H, $\text{CH}_3^{5,5'}$), 3.24–2.97 (bd, 4H, $\text{CH}_{2,2',3,3'}$), 1.97, 1.47 (bs, 2H, CH^1).



NMR spectra of 1b, 2a and 2b:



3. STA measurements

For the TGA-DTA measurements, a defined reaction solution of pre-catalyst **1–4** respectively (100 ppm) and DCPD were prepared. The corresponding amount of ethereal HCl (25equiv relative to ruthenium) was added. To avoid polymerization before the measurements starts, the reaction solution was cooled immediately with liquid nitrogen after the HCl was added. A weighted portion of the frozen pre-catalyst/DCPC/HCl mixture was put promptly into the STA and measured with a temperature program of 3 °C/min. The TGA is operated with a helium flow rate of 50 mL/min used in combination with a protective flow of 8 mL/min.

4. Tensile strength tests

To obtain the shoulder-test-bars, the appropriate amount of pre-catalyst was mixed with 28 mL of DCPD. The mixture was shaken, heated or if necessary put into an ultrasonic bath until the catalyst was totally dissolved. Afterwards, the corresponding amount of etherical HCl was added and the mixture put immediately into a cold shoulder-test-bar form. Until complete hardening of the test bar was observable, the form was kept in an at 60 °C temperate dry-box.

5. Computational details

All calculations were performed with the Gaussian09 package Gaussian 09,ⁱⁱ Revision A.1, at the BP86 GGA levelⁱⁱⁱ using the SDD ECP on Ru^{iv} and the split-valence plus one polarization function SVP basis set on all main group atoms during geometry optimizations.^v Furthermore

Figure 1 is an energy profile diagram showing the relative energies (in kcal/mol) of various ruthenium complexes and transition states involved in the reaction of 2a and 2b with H⁺ and H₂O. The diagram illustrates the reaction pathways and the energy barriers for the formation of products 5b and 6b.

Relative Energies (kcal/mol):

- 2a: 2.0
- 2a': -7.9
- 2a'': -2.0
- 2a''': -5.3
- 2b: 0.0
- 2b': -7.3
- 2b'': 4.8
- 2b''': -5.3
- 2c': 4.5
- 2c'': -0.6
- 2c''': -2.0
- 2d': -2.7
- 2d'': -1.3
- 2d''': -9.0
- 2d''bis: -10.1
- 3a: -10.9
- 3b: -13.5
- 3c: -9.0
- 3c': -15.4
- 3c'': -17.5
- 3c''': -17.0
- 4a: -16.3
- 4a': -15.6
- 4b: -17.0
- 4b': -13.4
- 4c: -17.5
- 4c': -15.4
- 4c'': -17.0
- 4c''': -17.0
- 5b: -22.3
- 6b: -33.1

Reaction Pathways and Energy Barriers (kcal/mol):

- 2a → 2a': 13.2
- 2a → 2a'': 10.4
- 2a → 2a''': 4.3
- 2a → 2b: 2.0
- 2a → 2c': 20.1
- 2a → 2c'': 18.9
- 2a → 2c''': 13.2
- 2b → 2b': 14.7
- 2b → 2b'': 26.3
- 2b → 2b''': 16.0
- 2b → 2c': 14.3
- 2b → 2c'': 12.8
- 2b → 2c''': 10.4
- 2b → 2d': 16.6
- 2b → 2d'': 8.8
- 2b → 2d''': 16.6
- 2b → 2d''bis: 8.8
- 2b → 3a: -2.5
- 2b → 3b: -12.0
- 2b → 3c: -5.0
- 2b → 3c': -13.2
- 2b → 3c'': -13.2
- 2b → 3c''': -13.2
- 2b → 4a: -2.5
- 2b → 4a': -13.8
- 2b → 4b: -12.0
- 2b → 4b': -13.4
- 2b → 4c: 8.7
- 2b → 4c': -15.4
- 2b → 4c'': -17.0
- 2b → 4c''': -17.0
- 2b → 5b: -6.8
- 2b → 6b: -11.4

Table S1. coordinate data sets and absolute energies for DFT optimized complexes (in a.u.).

2a				2a'H ⁺				2a'H ⁺ →2a'				2a'			
-4274.4065755				-4274.8260495				-4735.1894584				-4735.2165833			
Ru	0.071128	-0.004208	-0.232504	Ru	0.081438	-0.063396	-0.245671	Ru	0.21358200	-0.03916300	-0.42980700	Ru	0.577672	-0.497936	-0.605352
Cl	1.208657	3.868057	-3.350052	Cl	1.843932	3.766328	-3.303283	Cl	0.42628600	5.00005600	-3.22166400	Cl	-3.943746	3.695461	-3.989504
Cl	1.110459	6.767804	1.263792	Cl	1.347630	6.734781	1.246757	Cl	-1.96246800	6.69461500	1.34807800	Cl	-5.311396	5.260317	1.033264
Cl	-2.239083	-2.822947	3.354055	Cl	-2.490309	-2.151110	3.538982	Cl	-1.43391400	-2.34426500	3.75069800	Cl	-0.268820	-1.769104	4.286053
Cl	-6.475584	0.488380	2.444982	Cl	-6.476339	1.219746	1.987370	Cl	-6.33973900	-0.49391400	2.25720100	Cl	-5.391540	-2.593629	2.611940
O	0.688817	1.516015	-1.503140	O	0.968982	1.491454	-1.520236	O	1.01228200	2.50578000	-1.62402200	O	-1.774413	2.214425	-2.663416
O	-0.937398	-1.250934	1.137549	O	-1.053273	-1.072708	1.138445	O	-0.52903500	-1.10642900	1.16659100	O	0.226773	-1.052233	1.396634
N	0.275264	1.616048	1.140474	N	0.303479	1.624430	1.058837	N	-0.04136900	1.86544400	0.82103900	N	-1.263909	2.088940	0.071249
N	-1.117937	-1.803246	-2.453761	N	-1.194424	-2.196257	-2.130981	N	-0.50931000	-2.51286000	-2.12338300	N	1.366568	-3.246672	-1.262662
N	1.076632	-1.920441	-2.420990	N	0.999916	-2.204125	-2.251812	N	1.66524600	-2.11585500	-2.12498800	N	3.176787	-1.983880	-1.110793
C	4.678985	-0.918926	-2.447475	C	4.438138	-0.781979	-2.693094	C	5.14916800	-0.69998200	-1.98857200	C	5.655370	0.767159	-1.625575
H	5.319292	-0.149838	-2.911638	H	4.939066	0.009931	-3.275781	H	5.76139200	0.05462500	-2.51075800	H	6.038507	1.392559	-2.449408
C	2.474964	-1.869947	-2.092393	C	2.404279	-1.965188	-2.073125	C	3.01559100	-1.82690700	-1.71045300	C	4.137405	-0.951362	-0.836287
C	3.296301	-0.885842	-2.706156	C	3.048182	-0.949994	-2.830996	C	3.81386300	-0.87906500	-2.40513200	C	4.638779	-0.164460	-1.907126
C	4.432820	-2.893415	-1.079417	C	4.554201	-2.648830	-1.168193	C	4.93161600	-2.43697500	-0.33192000	C	5.708536	0.090191	0.693372
H	4.874344	-3.687488	-0.453542	H	5.144470	-3.330084	-0.532920	H	5.37053500	-3.06830600	0.45877300	H	6.137216	0.174044	1.706162
C	3.041439	-2.907627	-1.304916	C	3.163098	-2.852731	-1.262404	C	3.59092100	-2.65211300	-0.70031900	C	6.688041	-0.854814	0.469236
C	2.200934	-4.025390	-0.727737	C	2.531649	-4.018229	-0.534113	C	2.79587200	-3.75397300	-0.04028600	C	4.194263	-1.734543	1.594742
H	2.229749	-4.927578	-1.379088	H	2.763439	-4.977025	-1.047546	H	2.40995300	-4.48571400	-0.78233800	H	4.363251	-2.812546	1.383339
H	1.140475	-3.733010	-0.603887	H	1.431420	-3.927343	-0.462603	H	1.91169600	-3.36055000	0.50224000	H	3.103783	-1.611179	1.765254
H	2.584424	-4.333600	0.265295	H	2.930758	-4.100514	0.496224	H	3.42061600	-4.31132800	0.68464900	H	4.717513	-1.497451	2.541386
C	5.268772	-1.930945	-1.628355	C	5.213215	-1.614865	-1.858983	C	5.72608600	-1.44997900	-0.94798200	C	6.201183	0.917212	-0.334638
C	2.706742	0.161545	-3.618044	C	2.295121	-0.102333	-3.834820	C	3.29857200	-0.10546100	-3.59192400	C	4.111543	-0.326873	-3.312060
H	3.497075	0.820797	-4.027055	H	2.458369	-0.468619	-4.872205	H	3.47224800	-0.67476800	-4.53316200	H	4.572146	0.413483	-3.994965
H	1.966812	0.790769	-3.080058	H	2.660032	0.948012	-3.839844	H	3.83617700	0.85783800	-3.69996200	H	3.008531	-0.205102	-3.351487
H	2.175408	-0.298679	-4.479641	H	1.198363	-0.121748	-3.672329	H	2.21171300	0.10266800	-3.52801900	H	4.338283	-1.337210	-3.718646
C	6.751547	-1.879819	-1.333857	C	6.699948	-1.393682	-1.709140	C	7.14600400	-1.19452600	-0.49621300	C	7.272058	1.950531	-0.065622
H	7.334673	-1.502397	-2.198831	H	7.164293	-1.068792	-2.662314	H	7.17315600	-0.39633900	0.27814700	H	8.020014	1.986473	-0.884625
H	7.135565	-2.886260	-1.070585	H	7.219010	-2.310589	-1.366346	H	7.78885100	-0.85561300	-1.33410500	H	7.809348	1.749310	0.882902
H	6.970295	-1.207099	-0.457474	H	6.904185	-0.598432	-0.959034	H	7.60569800	-2.10066000	-0.05153800	H	6.829044	2.967883	0.010661
C	-0.006090	-1.368433	-1.769181	C	-0.070967	-1.603207	-0.1627304	C	0.46408400	-1.70814300	-1.58104300	C	1.808905	-1.978075	-0.955074
C	-8.005651	-2.577256	-3.763617	C	-0.916070	-3.236239	-3.151053	C	0.02490800	-3.49780300	-3.08931800	C	2.437251	-4.115412	-1.789378
H	-1.052538	-1.985221	-4.581674	H	-1.401971	-2.966410	-1.112223	H	-0.53554100	-3.44875600	-0.40446960	H	2.302526	-4.278642	-2.882197
H	-1.397631	-3.512015	-3.705260	H	-1.342910	-4.208716	-2.827493	H	-0.08898400	-4.52847500	-2.68259400	H	2.411210	-5.107641	-1.293818
C	0.704779	-2.822457	-3.531277	C	0.615866	-3.244017	-3.232778	C	1.48953400	-3.06912000	-3.23937000	C	3.707630	-3.314256	-1.471467
H	0.945570	-3.877441	-3.268892	H	1.061411	-4.222469	-2.954559	H	2.20528600	-3.91265900	-3.15312200	H	4.287410	-3.744540	-0.623091
H	1.277358	-2.568057	-4.447243	H	1.001303	-2.981082	-4.241308	H	1.67993500	-2.55476200	-4.20717600	H	4.395958	-3.234640	-2.337650
C	-4.448795	-2.587745	-0.954407	C	-4.602894	-2.608975	-0.646698	C	-3.43946300	-3.81961300	-0.18585100	C	-1.428625	-4.996112	0.491964
H	-4.885947	-3.316427	-0.251491	H	-5.097956	-3.217749	0.128037	H	-3.62104400	-4.43695900	0.70988300	H	-1.643308	-5.405381	1.493300
C	-3.065420	-2.645029	-1.210079	C	-3.215227	-2.763511	-0.834711	C	-2.10773600	-3.53652700	-0.54616800	C	-0.188990	-4.367668	0.273133
C	-3.325728	-0.749880	-2.775397	C	-3.337328	-1.104537	-2.665462	C	-2.94982100	-2.30541800	-2.51279500	C	-0.854674	-3.969609	-2.076049
C	-6.758243	-1.564686	-1.229698	C	-6.855097	-1.550410	-1.166754	C	-5.95624900	-3.62073100	-0.49076200	C	-3.732490	-5.765430	-0.242738
H	-7.340739	-1.061489	-2.027745	H	-7.391772	-1.206555	-2.973609	H	-6.65934100	-3.63141100	-1.34837000	H	-4.311289	-5.939637	-1.171648
H	-6.919232	-0.992494	-0.289273	H	-7.033184	-0.794250	-0.370477	H	-6.30665900	-2.83410900	0.21377100	H	-4.350362	-5.126673	0.425508
H	-7.189319	-2.574601	-1.070779	H	-7.322132	-2.496217	-0.825394	H	-6.04135300	-4.59166500	0.03893400	H	-3.608681	-6.740958	0.273062
C	-2.507356	-1.691644	-2.104244	C	-2.585876	-1.971440	-1.831349	C	-1.87019100	-2.72747700	-1.69266400	C	0.071893	-3.822898	-1.013992
C	-4.704936	-0.734673	-2.482844	C	-4.721595	-0.985355	-2.431321	C	-4.26362500	-2.61019400	-2.09971400	C	-2.081667	-4.609871	-1.802033
H	-5.344767	0.008554	-2.987976	H	-5.311005	-0.307343	-3.071043	H	-5.10237900	-2.26182200	-2.72594900	H	-2.815159	-4.714202	-2.619217
C	-5.286343	-1.634326	-1.568678	C	-5.375336	-1.719969	-1.422011	C	-4.53642200	-3.35015200	-0.93418700	C	-2.396469	-5.116541	-0.526780
C	-2.205246	-3.706400	-0.564300	C	-2.436244	-3.759180	-0.006687	C	-0.97182500	-4.11563800	0.26404700	C	0.839924	-2.899021	1.376514
H	-2.822954	-4.412274	0.023441	H	-3.108850	-4.316705	0.672635	H	-1.35365400	-4.82062700	1.02769000	H	0.491486	-4.822719	2.281732
H	-1.460261	-3.248850	1.028081	H	-1.668131	-3.249645	0.611490	H	-0.41029700	-3.31512700	0.78834200	H	1.044469	-3.234797	1.657103
H	-1.643332	-4.294346	-1.321720	H	-1.912281	-4.505884	-0.641689	H	-2.24943300	-4.66567500	-0.37521600	H	1.807456	-4.741478	1.068925
C	-2.752724	0.204232	-3.791797	C	-2.700368	-0.361849	-3.818920	C	-2.72979800	-1.59866900	-3.82845900	C	-0.547051	-4.363074	-3.465826
H	-1.708522	0.488745	-3.561189	H	-1.643767	-0.097797	-3.614256	H	-1.84192900						

H	6.210055	1.396129	2.447215	H	6.172034	0.983521	2.709498	H	5.86974000	2.83789300	2.27331600	H	3.272832	5.787153	-0.593717
C	3.584402	-0.790759	2.102863	C	3.444708	-1.061079	2.280501	C	3.63497900	0.23191500	2.16190000	C	2.734037	2.805136	1.023167
C	2.886156	-0.163910	1.006843	C	2.823749	-0.401870	1.149997	C	2.94034900	0.55714700	0.93717100	C	2.241780	2.011036	-0.079463
C	4.628327	1.584911	0.959668	C	4.668026	1.244848	1.152214	C	4.38565700	2.54326500	0.70259500	C	2.495786	3.983145	-1.541890
H	5.040035	2.501076	0.509341	H	5.154710	2.127222	0.710048	H	4.68046300	3.43949300	0.13514900	H	2.400181	4.441566	-2.538222
C	4.771854	-0.217436	2.606433	C	4.642256	-0.541537	2.825260	C	4.68345800	1.05935700	2.62211900	C	3.104445	4.152145	0.817712
H	5.307879	-0.678908	3.447556	H	5.119922	-1.023588	3.688774	H	5.21743100	0.82449300	3.55337200	H	3.480927	4.763620	1.649403
C	3.565626	-2.605334	3.749611	C	3.267529	-2.847000	3.958841	C	3.75961000	-1.26637300	4.09836000	C	3.203755	2.887190	3.428627
H	3.955639	-1.848293	4.468758	H	3.660012	-2.089319	4.673927	H	3.98001600	-0.34921900	4.69216300	H	2.801206	3.925806	3.391820
C	2.405354	-3.354173	4.403109	C	2.035384	-3.512263	4.565482	C	2.67617400	-2.06947400	4.81592900	C	2.561504	2.151529	4.603647
H	1.597886	-2.654529	4.695438	H	1.254497	-2.763024	4.801799	H	1.75714900	-1.46574300	4.94853400	H	1.457947	2.139857	4.508327
H	2.755295	-3.890616	5.308508	H	2.310118	-4.039444	5.501136	H	3.03543900	-2.39182100	5.81441900	H	2.826856	2.647918	5.559177
H	1.975369	-4.096922	3.700174	H	1.604038	-4.254266	3.862834	H	2.40849600	-2.97326800	4.23117100	H	2.912260	1.100089	4.645553
C	4.701158	-3.534161	3.307469	C	4.368822	-3.842673	3.589217	C	5.04725800	-2.06678300	3.87957600	C	4.732429	2.925697	3.518510
H	4.312885	-4.317092	2.623500	H	3.972410	-4.625936	2.910467	H	4.82950400	-2.99300700	3.30898000	H	5.137532	1.895889	3.595440
H	5.153847	-4.037953	4.186471	H	4.750958	-4.344916	4.501331	H	5.49306200	-2.35603700	4.85370200	H	5.051831	3.492499	4.417504
H	5.502258	-2.980271	2.778642	H	5.226263	-3.349451	3.089127	H	5.80322100	-1.48474200	3.31578900	H	5.184999	3.408260	2.629529
				H	1.365662	1.468108	-2.424674	H	0.60794500	2.04651400	-2.46787100	H	-1.052970	1.720851	-2.192598
								CI	-0.09017500	0.68428500	-3.40330000	CI	0.511732	0.083662	-2.930073

2a→3a	3a	3a→4a	4a
-4735.210334	-3339.039572	-3799.823937	-3799.852003
Ru 1.480626 -0.260278 -0.602541	Ru 0.386916 -0.556057 0.584118	Ru -0.883037 0.096629 0.724328	Ru -1.204442 -0.008928 0.806840
Cl -6.193867 1.535036 -4.015983	Cl 1.563840 2.379383 -3.452057	Cl 3.881238 -5.191966 -0.660059	Cl 4.888744 -4.194428 -1.583626
Cl -8.770627 -1.409375 -0.224597	Cl 3.839022 5.573655 0.333675	Cl 0.355914 -2.255390 -3.571964	Cl -0.011495 -2.561629 -3.222070
Cl 2.872533 -2.071161 3.990162	O 0.939742 0.576747 -1.105731	N -1.252989 2.632821 -0.894258	N -1.192857 1.534884 -1.889353
Cl -1.606774 -5.128556 3.429397	N 1.056595 -3.062789 -0.813796	N -3.075631 1.388251 -0.754457	N -3.018538 0.367690 -1.431610
O -3.892486 1.472053 -2.054843	N -1.112310 -2.724570 -1.033190	N 0.253184 -2.205672 1.568474	N 1.415707 -2.278374 1.728958
O 2.133528 -1.046745 1.240685	C -4.612214 -2.186368 0.145963	O -0.509651 -1.179371 -0.923410	O -0.369948 -1.618714 -0.403638
N -3.854844 0.286553 0.323199	H -5.275970 -2.534120 0.955270	O 3.471741 0.418469 -0.395932	O 3.252884 1.103707 0.676065
N 4.172722 -0.398726 -1.767288	C -2.441714 -2.196761 -0.931851	C -1.752488 1.453075 -0.385673	C -1.800807 0.763467 -0.926630
N 3.881141 1.657076 -1.021963	C -3.288232 -2.660858 0.109092	C -2.270689 3.436157 -1.603004	C -2.055480 1.726974 -3.079617
C 2.283314 5.007520 -0.649651	C -4.241419 -0.848970 -1.835221	H -2.423132 4.405754 -1.079928	H -2.425844 2.777381 -3.110888
H 1.793089 5.765594 -1.283234	H -4.613644 -0.145404 -2.598726	H -1.933355 3.668913 -2.635934	H -1.485707 1.542816 -4.012935
C 3.345048 2.841869 -0.417792	C -2.906220 -1.293219 -1.920404	C -3.515288 2.538217 -1.567081	C -3.181494 0.707400 -2.856614
C 2.727618 3.813980 -1.247124	C -1.995192 -0.809511 -3.025355	H -3.829768 2.193354 -2.576714	H -3.052084 -0.202923 -3.484551
C 3.063444 4.269573 1.518351	H -1.644590 -1.645638 -3.668767	H -4.392571 3.031618 -1.097295	H -4.192173 1.119862 -3.055314
H 3.200162 4.448808 2.597937	H -1.086709 -0.313800 -2.621490	C 0.051101 3.227262 -0.794199	C -0.079296 2.437800 -1.763811
C 3.524164 3.054242 0.971798	H -2.518836 -0.086736 -3.681005	C 0.344145 4.106771 0.280205	C -0.239002 3.660828 -1.050262
C 4.176647 2.007187 1.845085	C -5.109058 -1.279607 -0.812950	C 1.579963 4.786104 0.262835	C 0.814211 4.593401 -1.086310
H 5.192916 1.740060 1.483455	C -2.774272 -3.617975 1.158054	H 1.816638 5.466991 1.097634	H 0.690646 5.543145 -0.538732
H 3.588755 1.064359 1.863753	H -3.565247 -3.860493 1.894444	C 2.504064 4.640065 -0.788736	C 1.997491 4.369417 -1.820033
H 4.279480 2.368663 2.886967	H -1.905918 -3.189152 1.704888	C 2.170296 3.771719 -1.7849324	C 2.119231 3.155029 -2.518312
C 2.443216 5.257317 0.729116	H -2.428906 -4.575971 0.711819	H 2.871229 3.651807 -2.693045	H 3.031399 2.958789 -3.107699
C 2.539429 3.563795 -2.724741	C -6.531021 -0.771443 -0.724250	C 0.956344 3.060897 -1.877503	C 1.097969 2.180880 -2.510680
H 3.512444 3.462201 -3.253566	H -7.246523 -1.594088 -0.515406	C -0.636169 4.326407 1.405150	C -1.505584 3.979526 -0.297762
H 1.990119 4.399092 -3.201306	H -6.848356 -0.270727 -1.660869	H -0.229117 5.035953 2.151853	H -1.498057 5.027671 0.060105
H 1.976535 2.622635 -2.907655	H -6.636330 -0.036151 0.103409	H -1.597326 4.746387 1.036072	H -2.406298 3.844640 -0.933473
C 1.952829 6.554332 1.333920	C 0.030471 -2.212570 -0.487439	H -0.885116 3.374019 1.921273	H -1.645878 3.311085 0.580246
H 2.386178 7.434741 0.813162	C 0.615619 -4.240805 -1.586814	C 3.820690 5.384701 -0.783048	C 3.084391 5.421028 -1.862352
H 2.216355 6.632620 2.407513	H 0.783712 -5.175972 -1.008236	H 3.831543 6.190365 -0.022240	H 2.698278 6.381951 -2.265386
H 0.848334 6.642232 1.246586	H 1.193438 -4.325604 -2.531706	H 4.667581 4.701304 -0.554412	H 3.479655 5.638518 -0.846989
C 3.285172 0.434585 -1.133741	C -0.880189 -3.952295 -1.823694	H 4.035037 5.842113 -1.771673	H 3.935762 5.107699 -2.499161
C 5.404190 0.290908 -2.200832	H -1.118012 -3.773694 -2.895899	C 0.634706 2.127356 -3.021984	C 1.257272 0.915243 -3.319061
H 5.439008 0.371097 -3.310232	H -1.539490 -4.772915 -1.469879	H -0.312062 2.403158 -3.533678	H 0.922655 1.060683 -4.371062
H 6.303781 -0.272199 -1.874933	C 4.611955 -1.944391 -1.177870	H 1.440115 2.140682 -3.782146	H 2.319816 0.602561 -3.366781
C 5.273472 1.666039 -1.519240	H 5.225680 -1.369124 -1.891554	H 0.505092 1.078727 -2.676041	H 0.663335 0.079988 -2.902669
H 5.985463 1.794642 -0.671823	C 3.242534 -2.117807 -1.457834	C -4.041080 0.337168 -0.544109	C -4.073998 -0.307664 -0.713019
H 5.434298 2.512438 -2.218755	C 3.045040 -3.479885 0.602375	C -4.963743 0.451572 0.528033	C -5.076560 0.488450 -0.090663
C 4.208415 -4.084750 -1.122294	C 6.682161 -2.255286 0.263432	C -5.957277 -0.539032 0.654035	C -6.121423 -0.162616 0.590564
C 4.493313 -4.775903 -0.311214	H 7.107307 -3.050142 0.909017	H -6.668487 -0.465535 1.494033	H -6.891346 0.453162 1.085252
C 4.375788 -2.700802 -0.916850	H 6.825591 -1.288715 0.795263	C -6.069184 -1.609325 -0.253793	C -6.209414 -1.566722 0.661821
C 3.560384 -2.310996 -3.224074	H 7.284620 -2.204435 -0.666687	C -5.164957 -1.661017 -1.332087	C -5.237119 -2.323165 -0.017413
C 3.496225 -6.094456 -2.507395	C 2.453211 -2.851094 -2.573442	H -5.247281 -2.477643 -2.069214	H -5.305142 -3.424042 -0.007436
H 3.644874 -6.409506 -3.560412	C 4.421092 -3.272173 0.831334	C -4.151609 -0.699657 -1.506800	C -4.175484 -1.724980 -0.727349
H 2.658792 -6.381049 -2.225514	H 4.884159 -3.748271 1.712069	C -4.892453 1.587035 1.520078	C -5.033602 1.995892 -0.140166
H 4.182186 -6.686009 -1.867738	C 5.218374 -2.495800 -0.031189	H -5.742125 1.543608 2.229502	H -5.995282 2.429424 0.197918
C 3.995648 -1.815016 -1.963753	C 2.643995 -1.548670 -2.721323	H -3.947653 1.547226 2.104367	H -4.228502 2.370069 0.528886
C 3.412853 -3.705020 -3.371766	H 3.435378 -1.160168 -3.391678	H -4.921979 2.580801 1.022951	H -4.825003 2.378784 -1.161128
H 3.061961 -4.095065 -4.342096	H 1.948525 -0.714559 -2.486554	C -7.114160 -2.685721 -0.063244	C -7.306710 -2.237570 1.056777
C 3.710317 -4.607730 -2.331851	H 2.066532 -2.311617 -3.285240	H -7.447191 -3.111771 -1.031764	H -7.533069 -3.252138 1.407629
C 4.960229 -2.187659 0.376694	C 2.245519 -4.356424 1.534456	H -6.706892 -3.526976 0.540216	H -7.006410 -3.351476 2.521842
H 5.111555 -3.014128 0.960146	H 1.474315 -3.760030 2.703055	H -8.006595 -2.302486 0.472171	H -8.243798 -1.644075 1.445162
H 4.174374 -1.711926 1.001503	H 2.904114 -4.832244 2.287339	C -3.206442 -0.790622 -2.679763	C -3.222481 -2.585540 -1.518429
H 5.746518 -1.424204 0.200036	H 1.715823 -5.167250 0.990439	H -2.172806 -1.011548 -2.339367	H -2.169548 -2.266687 -1.394895
C 3.286709 -1.389570 -4.387465	N 1.465862 1.069846 1.491342	H -3.520131 -1.592066 -3.377023	H -3.302256 -3.646612 -1.209758
H 2.541173 -0.612112 -4.114581	C 1.739959 1.241607 2.789539	H -3.162974 0.158128 -3.257279	H -3.461280 -2.545413 -2.604838
H 2.893166 -1.956646 -5.253680	H 1.378576 0.443513 3.460197	C 0.856091 0.722834 0.487855	C 0.508843 0.715411 0.856053
H 4.211420 -0.872137 -4.724679	C 2.446934 2.378601 3.253949	H 1.216633 0.884661 -0.551282	H 1.126917 0.606932 -0.005859
N -0.048625 -1.709091 -0.193870	H 2.650221 2.483201 4.330110	C 1.978123 0.723736 1.437063	C 1.267349 1.211640 2.003157
C -1.080270 -2.046374 -0.977072	C 1.550084 1.693930 -0.810018	C 3.332874 0.600929 0.943595	C 2.697548 1.398025 1.884495
H -1.150683 -1.496476 -1.930943	C 2.594413 3.185723 0.957866	C 4.418773 0.630114 1.845668	C 3.448584 1.828249 3.000409
C -2.011422 -3.041053 -0.588416	C 1.879168 1.998601 0.568063	H 4.534527 0.535368 1.481122	H 4.534527 1.972812 2.020595
H -2.843840 -2.390366 -1.262816	C 2.866172 3.346226 2.347661	C 4.192958 0.774972 3.224955	C 2.815674 2.078982 4.230003
C 1.309404 -1.919428 1.757187	H 3.410358 4.243788 2.679304	H 5.056933 0.795907 3.909104	H 3.423313 2.417933 5.085053
C -0.779229 -3.336384 1.495154	C 1.950854 2.662232 -1.767739	C 2.885237 0.888260 3.728409	C 1.429388 1.896647 4.370805
C 0.137133 -2.332920 1.018198	C 2.968161 4.099439 -0.072250	H 2.711400 1.006938 4.809179	H 0.934811 2.088808 5.335356
C -1.868611 -3.675689 0.640363	C 2.645312 3.837978 -1.405096	C 1.801605 0.850777 2.842960	C 0.677078 1.459586 3.274673
H -2.582355 -4.444513 0.973556	H 2.932521 4.552303 -2.189611	H 0.769521 0.947851 3.215475	H -0.407315 1.302013 3.367563
C 1.488425 -2.536526 3.023670	O -2.940938 2.373572 -0.261192	C 4.773607 0.216491 -1.000039	C 4.677047 1.234522 0.452496
C -0.518879 -3.908728 2.775776	C -1.250358 0.317948 0.400989	H 5.375237 -0.432741 -0.323046	H 5.211219 0.833591 1.345733
C 0.591910 -3.508371 3.521187	H -1.333661 0.847195 -0.572801	C 4.521314 -0.536137 -2.304520	C 4.997672 0.351091 -0.751520
H 0.780549 -3.953572 4.508483	C -2.609441 0.019956 2.536304	H 3.884246 0.064422 -2.985588	H 4.448906 0.708216 -1.646918
C -5.013464 0.180839 -0.384034	H -1.914140 -0.775585 2.845266	H 5.482015 -0.744851 -2.817692	H 6.083971 0.381987 -0.972330
C -6.059291 -1.128506 1.381717	C -4.545752 1.419343 2.941375	H 4.009436 -1.499118 -2.110368	H 4.708637 -0.701930 -0.565212
H -6.920724 -1.679232 1.789728	H -5.398740 1.717903 3.572613	C 2.448960 1.553638 -1.212017	C 5.064836 2.698566 0.224830
H -4.869726 -1.011821 2.091416	C -3.239821 1.732818 0.899587	H 5.629821 2.103210 -0.259754	H 4.788235 3.339052 1.085470
H -4.756054 -1.471992 3.084693	C -2.353648 0.657471 1.292729	H 6.489997 1.387337 -1.662136	H 6.159909 2.768781 0.068571
C -5.002965 0.832652 -1.668931	C -3.685977 0.384484 3.351653	H 4.900494 2.197024 -1.896617	H 4.547353 3.090873 -0.673359
C -7.313256 0.065998 -1.992900	H -3.854376 -0.134272 4.308044	C 0.717038 -2.520934 2.784678	C 2.232133 -2.485041 2.769072
H -8.202614 0.031953 -2.637268	C -4.327914 2.090182 1.727077	H 0.124440 -2.151091 3.636936	H 1.815717 -2.239167 3.757301
C -7.323515 -0.562287 -0.751726	H -5.011292 2.898672 1.433034	C 1.868057 -3.324442 2.947474	C 3.526530 -2.999303 2.558146
C -3.784506 -0.290651 1.517429	C -3.642989 3.569381 -0.677752	H 2.240748 -3.547391 3.957487	H 4.199550 -3.155240 3.412920
H -2.827742 -0.191541 2.059250	H -3.917935 4.150740 0.232204	C 2.478447 -3.858520 1.817924	C 3.910093 -3.328481 1.261520
C -6.161404 0.760932 -2.452269	C -2.642174 4.381643 -1.498504	H 3.346245 -4.530101 1.905756	H 4.900587 -3.763773 1.058720
C -6.172247 -0.526175 0.095900	H -1.749972 4.634831 -0.892526	C 1.991673 -3.551327 0.513233	C 3.028596 -3.310666 0.158157
O -0.106872 2.430189 2.676203	H -3.108038 5.324887 -1.849734	C 0.878632 -2.634198 0.421037	C 1.734534 -2.532735 0.425217
C 0.855732 1.147855 0.449260	H -2.304202 3.806115 -2.384528	C 0.373710 -2.129952 -0.845551	C 0.746351 -2.227950 -0.608882
H 1.197637 1.055632 1.502781	C -4.905629 3.205170 -1.463861	C 0.938621 -2.748757 -1.999918	C 1.125500 -2.727100 -1.903050
C -0.651975 2.657893 -0.947513	H -4.636282 2.654887 -2.388723	C 1.983843 -3.692647 -1.928750	C 2.368226 -3.325567 -2.182023
H -0.319844 2.123377 -1.850830	H -5.458228 4.122544 -1.754605	H 2.391625 -4.108260 -2.861271	H 2.587507 -3.642066 -3.211645
C -2.001402 4.353942 0.136444	H -5.588074 2.565226 -0.869834	C 2.525099 -4.073547 -0.699168	C 3.325066 -3.502645 -1.180597
H -2.730822 5.178534 0.082870	Cl 0.208318 -1.760527 2.665810	Cl -1.556777 1.118480 2.752963	Cl -2.439705 1.521862 2.107639

4a→5b				5b→II				II				2a→2c'			
-3799.8259731				-2403.6594089				-2403.6916615				-4735.1742699			
Ru	1.492630	0.679710	0.869864	Ru	0.244579	0.445391	0.442201	Ru	-0.147873	0.501707	-0.043609	Ru	-0.04204400	-0.09887200	0.27285300
Cl	-7.826643	0.783893	-0.534500	N	0.318450	-2.444810	-0.453058	N	0.721178	-2.431875	0.006600	Cl	0.16716300	4.35404200	2.29155200
Cl	-3.423534	-1.031391	-3.162144	N	2.312105	-1.519850	-0.182773	N	-1.464141	-2.125052	-0.010992	Cl	3.01968700	6.62364700	-1.70700400
N	2.599277	-0.272532	-1.821351	O	-2.005513	3.072740	-0.575281	O	-0.039941	2.847635	-0.109849	Cl	-0.48675500	-4.99941000	-1.08086500
N	2.616565	1.918802	-1.491643	C	0.953722	-1.260266	-0.141734	C	-0.251321	-1.457446	-0.003516	Cl	4.68519800	-4.45260900	-2.71388500
N	-3.044013	1.467293	1.313751	C	1.265344	-3.512023	-0.835832	C	0.173186	-3.799047	0.114941	O	0.17047100	1.93822200	0.62865800
O	-1.890213	0.198582	-0.796619	H	1.243637	-3.674628	-1.938638	H	0.363462	-4.211943	1.132407	O	-0.15827300	-2.14925100	-0.14139600
O	-0.895823	-3.131991	0.996106	H	0.989126	-4.469879	-0.350013	H	0.660007	-4.476020	-0.617251	N	1.08949000	1.78690600	-2.12104800
C	2.277165	0.713210	-0.926759	C	2.608004	-2.954558	-0.350731	C	-1.320459	-3.584376	-0.161310	N	0.54609900	-0.65920200	3.08938000
C	3.246317	0.262889	-3.039599	H	2.924336	-3.403054	0.618819	H	-1.608867	-3.898971	-1.190225	N	-1.64406400	-0.52546000	2.81766900
H	4.309328	-0.063577	-3.077016	H	3.432102	-3.101671	-1.078331	H	-1.977757	-4.122569	0.552672	C	-4.93192000	1.05161000	2.02732200
H	2.746251	-0.124566	-3.951895	C	-1.082948	-2.719710	-0.594533	C	2.146272	-2.281455	0.067519	H	-5.39444600	2.05272800	2.04546700
C	3.103923	1.787999	-2.876843	C	-1.711348	-2.506906	-1.850192	C	2.789356	-2.185316	1.328281	C	-2.98464300	-0.36006700	2.33077100
H	2.368580	2.227740	-3.588052	C	-3.071051	-2.850912	-1.980774	C	4.195927	-2.090265	1.347526	C	-3.57623700	0.93004400	2.37900900
H	4.064355	2.327946	-3.013546	H	-3.568405	-2.681462	-2.950743	H	4.705619	-2.002924	2.321991	C	-5.09304300	-1.32930900	1.63088900
C	2.500872	-1.699169	-1.674541	C	-3.810490	-3.395876	-0.910456	C	4.964265	-2.094632	0.165593	H	-5.68519100	-2.21366200	1.34142200
C	3.574706	-2.422155	-1.089092	C	-3.149472	-3.601311	0.316830	C	4.287766	-2.188953	-0.168465	C	-3.73562000	-1.50726900	1.96622200
C	3.482031	-3.825740	-1.046915	H	-3.708176	-4.032522	1.164624	H	4.869138	-2.180964	-2.006021	C	-3.09371500	-2.87303800	1.89810400
H	4.308311	-4.394188	-0.587498	C	-1.789489	-3.277512	0.500925	C	2.884393	-2.287086	-1.144237	H	-2.63906900	-3.17118500	2.86723400
C	2.379056	-4.521310	-1.583485	C	-0.958582	-1.876573	-0.300043	C	1.992923	-2.125497	2.610946	H	-2.27719500	-2.90035800	1.14331800
C	1.348644	-3.771428	-2.180756	H	-1.612024	-1.763181	-3.886870	H	2.663600	-2.060547	3.489903	H	-3.83752400	-0.364768200	1.62782500
H	0.488977	-4.296474	-2.629921	H	-0.079050	-2.481658	-3.308265	H	1.351839	-3.022969	2.745855	C	-5.71097000	-0.64414900	1.65616700
C	1.383668	-2.362713	-2.242792	H	-0.574008	-0.871303	-2.723482	H	1.314279	-1.244559	2.625340	C	-2.76199300	2.31318300	2.78328500
C	4.787981	-1.717119	-0.532091	C	-5.279414	-3.719094	-1.068968	C	6.474931	-2.028578	0.218541	H	-3.30439400	3.06830400	2.65342200
H	5.524913	-2.447927	-0.145522	H	-5.509769	-4.088672	-2.089114	H	6.919421	-3.048384	0.200155	H	-1.82953800	2.21417900	2.18739900
H	5.300509	-1.104452	-1.305407	H	-5.904612	-2.814224	-0.902326	H	6.831717	-1.533978	1.144470	H	-2.45308400	2.08040200	3.85079900
H	4.165303	-1.023955	0.292723	H	-5.611633	-4.485413	-0.340066	H	6.891954	-1.479104	-0.650068	C	-7.17206800	0.10609200	1.30420700
C	2.314039	-0.630814	-1.511097	C	-1.113413	-3.501020	1.832995	C	2.176809	-2.343220	-2.477769	H	-7.30523400	0.85201100	0.49216700
H	1.509935	-6.438697	-2.155930	H	-0.231557	-4.171006	1.740802	H	1.562456	-3.263560	-2.581162	H	-7.75619900	0.47415500	2.17539300
H	3.272957	-6.495230	-1.822503	H	-1.810622	-3.964116	2.558416	H	2.902598	-2.328747	-3.314250	H	-7.62885400	-0.84695100	0.917130400
H	2.147164	-6.372569	-0.471871	H	-0.741575	-2.545274	2.626971	H	1.483486	-1.482794	-2.600155	C	-0.44493300	-0.56492100	1.25138400
C	0.256516	-1.594984	-2.890188	C	3.406071	-0.590572	-0.049763	C	-2.783791	-1.547139	-0.027218	C	0.02571200	-0.71582300	4.46912400
H	0.626969	-0.852717	-3.628288	C	3.924413	0.012203	-1.228749	C	-3.464500	-1.365024	1.211480	H	0.29937100	0.20855500	5.02601400
H	-0.430733	-2.280883	-3.421967	C	5.015108	0.891618	-1.105088	C	-4.758515	-0.811666	1.186738	H	0.46156200	-1.57896500	5.01286900
C	-0.355319	-1.025671	-2.154295	H	5.410225	1.373293	-2.015360	H	-5.283042	-0.657761	2.144962	C	-1.48838900	-0.84262700	4.25664000
C	2.285878	3.209746	-0.945166	C	5.614542	1.170201	0.139802	C	-5.406541	-0.471201	-0.018428	H	-1.86983200	-0.86701600	4.46609000
C	3.312133	3.988325	-0.344681	C	5.121777	0.499941	1.274671	C	-4.742337	-0.752565	-1.226010	H	-2.07558900	-0.13248200	4.87029100
C	2.974422	5.262959	0.148213	H	5.603010	0.668738	2.252810	H	-5.251803	-0.547722	-2.182915	C	-3.82753700	-2.36621300	2.55885900
H	3.762947	5.868815	0.625696	C	4.037437	-0.400055	1.207795	C	-3.448163	-1.313103	-1.261599	H	4.20772100	-3.38522900	2.37518400
C	1.668345	5.783117	0.049076	C	3.337456	-0.288746	-2.587424	C	-2.846837	-1.792518	2.520612	C	2.34707400	-2.17585600	2.66643600
C	0.687522	4.999498	-0.588483	H	3.961575	0.148554	-3.391324	H	-3.586890	-1.728805	3.342496	C	2.84708800	0.23234700	3.05860000
C	-0.334545	5.399280	-0.699304	H	2.317236	0.139671	-2.673087	H	-1.980257	-1.146577	2.778102	C	6.22917300	-1.54019000	2.55209600
C	0.967953	7.317861	-1.101543	H	3.259005	-1.381099	-2.737371	H	-2.477055	-2.839079	2.475809	H	6.54401500	-2.47872300	3.05356600
H	4.725124	3.469894	-0.228732	C	6.747169	2.165830	0.251131	C	-6.777407	0.167390	-0.007224	H	6.82256500	-0.70586700	2.97688700
H	5.381872	4.218483	0.256096	H	7.379665	1.970860	1.140632	H	-7.294867	0.047340	-0.980299	H	6.51153500	-1.63829500	1.48064100
H	4.751402	2.537365	0.374747	H	6.353800	3.201857	0.348559	H	-6.706197	1.258726	0.195949	C	1.95603600	-0.85669900	2.88617300
H	5.164731	3.231955	-1.221499	H	7.397607	2.150059	-0.647463	H	-7.423787	-0.265287	0.784240	C	4.23130500	-0.10665500	2.95653900
C	1.331442	7.138590	0.629010	C	3.630293	-1.176809	2.434803	C	-2.864540	-1.739212	-2.588332	H	4.93021900	0.82721600	3.98571500
H	1.161703	7.067815	1.726046	H	2.530078	-1.219017	2.563867	H	-1.759919	-1.730270	-2.583793	C	4.74316100	-1.30229400	2.69703100
H	2.255973	7.865348	0.476601	H	4.056868	-0.717215	3.351333	H	-3.194909	-1.065724	-3.403386	H	1.49225100	-3.35342200	2.59497800
C	-0.401387	7.561088	0.179539	H	4.013096	-2.221158	2.391760	H	-3.215805	-2.763918	-2.847253	H	2.02753700	-4.27124600	2.28362300
C	-0.109183	2.920492	-1.796799	C	-1.543264	0.299694	0.076632	C	1.675362	0.797323	-0.044151	H	0.66059200	-2.17868400	1.88318200
H	-0.444112	2.041888	-1.201235	H	-1.961615	-0.529579	-0.530041	H	2.442181	0.001922	-0.000074	H	1.03456900	-3.56074000	3.58791000
H	-1.001583	3.548598	-1.986951	C	-2.532388	1.180816	0.751303	C	2.190192	2.151959	-0.131239	C	2.33527100	1.62009300	3.35793300
H	0.232659	2.520833	-2.774449	C	-2.751556	2.558862	0.439083	C	1.268577	3.241906	-0.168925	H	1.47522300	1.88882700	2.71247000
C	0.943708	-1.080575	0.921970	C	-3.717609	3.291597	1.169911	C	1.720963	4.568406	-0.270145	H	3.12965800	2.77882800	3.21620500
H	0.232018	-1.300167	0.089892	H	-3.896310	4.351893	0.944420	H	1.016914	5.411008	-0.300577	H	1.98998200	1.70993300	4.41195700
C	1.028886	-2.107939	1.949199	C	-4.465601	2.674895	2.185276	C	3.106186	4.815559	-0.333076	N	2.03785500	-0.62080200	-0.34083500
C	0.071583	-3.189705	1.946821	H	-5.209426	3.269227	2.739980	H	3.457948	5.856528	-0.413025	C	1.38227000	0.15385000	-0.37382900
C	0.162360	-4.209910	2.919918	C	-4.278299	1.315545	2.484981	C	4.036509	3.760137	-0.292218	H	3.02755900	1.16299900	0.05398000
H	-0.555145	-5.041731	2.922832	H	-4.869704	0.826858	3.274459	C	5.115887	3.971356	-0.338852	C	4.35048500	-0.28264100	-0.94011200
H	-1.168169	-4.169601	3.899548	C	-3.321426	0.585135	1.766603	C	3.577648	2.439813	-0.192075	H	5.21503400	0.39759300	-0.94578600
H	1.216580	-4.974331	4.650524	H	-3.154320	-0.478983	1.996180	H	4.287393	1.597334	-0.161633	C	0.88931400	-2.66858100	-0.72229900
C	2.099417	-3.115233	3.928419	C	-2.228034	4.421649	-1.050926	C	-1.124587	3.835467	-0.004401	C	3.30046500	-2.41757600	

Cl	-0.067247	1.961950	2.156218				C	-2.69538900	0.83428900	-0.97896200
							C	-3.37400600	3.13445800	-1.56587900
							H	-3.22770300	4.22059700	-1.46245400
							C	-4.58812100	1.24196400	-2.52209800
							H	-5.39339600	0.87332500	-3.17226300
							C	-4.70517000	-1.64003500	-2.92034400
							H	-4.70835900	-0.99663600	-3.83000200
							C	-4.03584500	-2.97145400	-3.25735200
							H	-3.00524100	-2.80723600	-3.62672900
							H	-4.61484200	-3.50725400	-4.03715100
							H	-3.97591800	-3.61713400	-2.35743200
							C	-6.13381500	-1.80628700	-2.39366500
							H	-6.13941800	-2.46176600	-1.49863000
							H	-6.77839200	-2.27152200	-3.16808100
							H	-6.58427700	-0.83434100	-2.10981300
							H	-0.13064400	0.42382500	-2.57515400
							Cl	-0.61283000	-0.54444100	-3.37863200

2c'	2c'→3a			3a→4a'	4a'						
-4735.2017062	-4735.1838533			-3799.8426415	-3799.8451169						
Ru -0.215338	-0.164989	-0.047750	Ru -0.480669	0.443578	-0.053971	Ru -0.710749	-0.045981	-0.718013	Ru -0.711252	-0.033474	-0.719843
Cl 0.862630	3.960946	2.242420	Cl 3.484576	-2.935267	3.159617	Cl 3.037118	5.906238	-0.269385	Cl 3.197697	5.836499	-0.402355
Cl 4.547795	6.166797	-1.061605	Cl 6.890734	-5.100964	-0.490137	Cl 0.284873	2.957273	3.372380	Cl 0.335229	3.091336	3.307028
Cl -1.912858	-4.851806	-0.949951	Cl -4.579929	1.258219	-2.814920	N -1.165155	-2.887385	0.385519	N -1.248449	-2.863221	0.376026
Cl 3.220535	-5.826947	-2.498762	Cl -5.267723	-4.130968	-2.371130	N -3.036960	-1.732200	0.355800	N -3.085815	-1.653850	0.374381
O 0.606516	1.841292	0.151991	O 2.152249	-1.676404	0.711412	N 0.272928	1.681036	-1.585051	N 0.338314	1.642338	-1.606471
O -0.855741	-2.121541	-0.250352	O -2.255381	0.803576	-0.959129	O -0.616262	1.365551	0.975933	O -0.589011	1.438857	0.967040
N 1.860258	1.963381	-2.417353	N 2.878087	-2.143579	-1.883393	O 3.441614	-0.258955	1.019134	O 3.384678	-0.300527	1.142566
N 0.726328	-0.433635	2.838051	N -2.275411	0.764474	2.455037	C -1.687494	-1.637835	0.123016	C -1.737483	-1.596693	0.126149
N -1.420411	0.074056	2.739998	N -0.509168	2.073560	2.521789	C -2.177634	-3.884022	0.794120	C -2.286740	-3.836032	0.776959
C -4.765043	1.661070	2.219627	C 3.198469	2.547758	2.572671	H -2.180108	-4.742065	0.088363	H -2.334361	-4.671809	0.046205
H -5.207109	2.671487	2.227960	H 4.103286	1.973559	2.835566	H -1.939353	-4.287930	1.802809	H -2.043507	-4.277831	1.768059
C -2.804525	0.233215	2.381139	C 0.787082	2.657276	2.327205	C -3.483436	-3.081982	0.761032	C -3.563683	-2.988600	0.793779
C -3.375056	1.532401	2.407124	C 1.947115	1.914080	2.681868	C -3.993103	-3.034396	1.747751	H -4.033757	-2.925367	1.799455
C -5.004714	-0.735125	2.032968	C 2.158069	4.608219	1.863556	H -4.217404	-3.479587	0.027824	H -4.339272	-3.357290	0.089287
H -5.640377	-1.627211	1.901819	H 2.236462	5.664433	1.554771	C 0.199120	-3.331690	0.458305	C 0.103665	-3.347217	0.423683
C -3.620722	-0.920623	2.211469	C 0.879561	4.018317	1.937216	C 0.762000	-4.071071	-0.617058	C 0.628642	-4.102631	-0.660110
C -3.029852	-2.307972	2.202320	C -0.336817	4.840656	1.572616	C 2.051638	-4.610433	-0.447754	C 1.914797	-4.658871	-0.518432
H -2.361997	-2.481213	3.072187	H -0.331183	5.818017	2.099145	H 2.498310	-5.174315	-1.284053	H 2.333691	-5.231837	-1.362902
H -2.414650	-2.473297	1.289962	H -1.283567	4.317929	1.804555	C 2.777831	-4.466611	0.751506	C 2.671843	-4.521409	0.661858
H -3.825342	-0.078018	2.227038	H -0.341204	5.055057	0.482693	C 2.176473	-3.756021	1.808239	C 2.100156	-3.809927	1.734292
C -5.599912	0.543061	2.034064	C 3.329523	3.891685	2.163780	H 2.717037	-3.648534	2.763751	H 2.660283	-3.715512	2.767970
C -2.519908	2.750212	2.648934	C 1.866874	0.484422	3.160131	C 0.892447	-3.189014	1.690352	C 0.821453	-3.226587	1.645465
H -3.024070	3.668841	2.290412	H 2.677037	0.265733	3.883986	C 0.001674	-4.293551	-1.901325	C -0.165486	-4.333779	-1.922419
H -1.539982	2.656421	2.142158	H 1.982582	-0.246706	2.326256	H 0.644620	-4.779801	-2.661107	H 0.460470	-4.817944	-2.697664
H -2.313485	2.894287	3.734002	H 0.899698	0.256413	3.649619	H -0.878635	-4.955753	-1.744103	H -1.033846	-5.004974	-1.738276
C -7.088698	0.705556	1.824639	C 4.692897	4.529693	2.025893	H -0.384286	-3.338898	-2.317852	H -0.567700	-3.383170	-2.332401
H -7.456783	1.670578	2.227607	H 5.411048	4.130596	2.771100	C 4.161939	-5.060956	0.889321	C 4.056747	-5.120659	0.764542
H -7.661231	-0.112386	2.308690	H 4.645828	5.631266	1.444440	H 4.186484	-6.117485	0.548794	H 4.092539	-6.114436	0.302722
H -7.343769	0.682595	0.742334	H 5.118570	4.324464	1.018709	H 4.898956	-4.507692	0.267190	H 4.798187	-4.508329	0.205681
C -0.321409	-0.222065	1.959837	C -1.151956	1.128737	1.748893	H 4.519246	-5.031950	1.938086	H 4.400912	-5.182834	1.816485
C 0.378711	-0.090630	4.234528	C -2.448402	1.516537	3.717585	C 0.272286	-2.444202	2.850091	C 0.228533	-2.495436	2.827459
H 0.829767	0.888670	4.512344	H -2.645505	0.823683	4.561652	H -0.698515	-2.889190	3.156805	H -0.736576	-2.943176	3.148290
H 0.765661	-0.858987	4.933495	H -3.325261	2.197569	3.631643	H 0.940495	-2.455785	3.733194	H 0.915131	-2.522473	3.695996
C -1.148363	-0.029492	4.188561	C -1.123944	2.272777	3.848896	H 0.061414	-1.383799	2.593019	H 0.015280	-1.430866	2.592358
H -1.631152	-0.944113	4.605109	H -1.252454	3.353693	0.466664	C -0.404032	-0.704487	0.408386	C -4.068965	-0.603564	0.35198
H -1.564473	0.844260	4.729480	H -0.461705	1.851245	4.639419	C -4.934912	-0.545940	-0.682054	C -4.963739	-0.427366	-0.649290
C 3.302318	-3.111180	2.429504	C -5.557062	-0.550432	1.225172	C -5.981404	0.386327	-0.550274	C -5.990469	0.524636	-0.511030
H 3.340574	-4.210626	2.349508	H -6.450226	-0.182468	0.693138	H -6.669489	0.529121	-1.400686	H -6.681077	0.681102	-1.357021
C 2.045565	-2.489088	2.537340	C -4.491322	0.345772	1.449022	C -6.168801	1.143247	0.622394	C -6.152061	1.288644	0.661304
C 3.189466	-0.305642	2.671073	C -3.289763	-1.469390	2.622592	C -5.277319	0.939957	1.693323	C -5.255286	1.070749	1.724564
H 5.838806	-3.080275	2.305174	C -6.651992	-2.842624	1.353590	H -5.409257	1.517843	2.623914	H -5.367534	1.653524	2.654741
H 6.686332	-2.408758	2.548824	H -6.853298	-3.524531	2.205731	C -4.213310	0.022046	1.613958	C -4.212427	0.128622	1.639442
H 5.987903	-4.545263	1.265298	H -6.409908	-3.478868	0.473823	C -4.754271	-1.327127	-1.961391	C -4.797593	-1.204959	-1.932537
H 5.902619	-3.968909	2.967552	H -7.589005	-2.299885	1.116295	H -5.472571	-0.989584	-2.734063	H -5.529190	-0.870710	-2.694027
C 1.997408	-1.069320	2.622179	C -3.339835	-0.143054	2.118219	H -3.274789	-1.210141	-2.362852	H -3.774978	-1.077899	-2.347966
C 4.425629	-0.980106	2.577719	C -4.377449	-2.324362	2.363754	H -4.920051	-2.417297	-1.812311	H -4.950393	-2.297007	-1.784556
H 5.354604	-0.385269	2.607057	H -4.335843	-3.361438	2.737061	C -7.271402	2.174074	0.714020	C -7.234841	2.339979	0.758518
C 4.507469	-2.377336	2.444049	C -5.516984	-1.890304	1.655327	H -7.608484	2.324333	1.760001	H -7.513832	2.547056	1.811704
C 0.786200	-3.319242	2.615108	C -4.584944	1.777437	0.975487	H -6.919086	3.160388	0.338687	H -6.892171	3.300654	0.314230
H 1.009386	-4.392871	2.462766	H -5.615305	2.019782	0.650804	H -8.152700	1.889300	0.103592	H -8.151256	2.038082	0.210803
H 0.034216	-3.011915	1.861870	H -3.899849	1.950299	0.118607	C -3.262948	-0.150660	2.776999	C -3.257080	-0.062058	2.756729
H 0.302127	-3.216304	3.612090	H -4.299937	2.500322	1.768565	H -2.265737	0.283249	2.549532	H -2.255675	0.359979	2.594744
C 3.158787	1.193627	2.840488	C -2.124682	-1.946642	3.549799	H -3.651282	0.354487	3.683246	H -3.632793	0.443347	3.707212
H 2.325358	1.633784	2.420001	H -1.149987	-1.631001	0.303947	H -3.096304	-1.219170	3.029693	H -3.101335	-1.133630	3.041953
H 4.032437	1.671434	2.353138	H -2.122733	-3.050846	3.545723	C 0.998865	-0.648282	-0.239414	C 0.976946	-0.673525	-0.191737
C 2.200109	1.480954	3.915079	H -2.178530	-1.540980	4.954333	H 1.156353	-0.752280	0.854882	H 1.100812	-0.755930	0.909036
N 1.691918	-1.254949	-0.480337	N -1.372116	-1.570530	-0.017400	C 2.246861	-0.719582	-0.988411	C 2.248780	-0.776123	-0.955193
C 2.936582	-0.788222	-0.600028	C -0.876965	-2.722208	0.444437	C 3.508705	-0.554154	-0.306805	C 3.490544	-0.617000	-0.176733
H 3.110937	0.239454	-0.245368	H 0.068848	-2.650411	1.007721	C 4.718038	-0.659165	-1.028755	C 4.720661	-0.747706	-0.857967
C 3.990987	-1.562682	-1.147124	C -1.507825	-3.965041	0.180768	H 5.685102	-0.536490	-0.522068	H 5.672997	-0.626893	-0.323531
H 4.997195	-1.125045	-1.229101	H -1.067187	-4.889181	0.584442	C 4.698217	-0.915366	-2.410660	C 4.740642	-1.027269	-2.235545
C 0.032034	-2.944756	-0.745978	C -2.909592	-0.286978	-1.299870	H 5.654554	-0.991950	-2.953353	H 5.712390	-1.123312	-2.746903
C 2.422288	-3.398796	-1.443428	C -3.192733	-2.791540	-1.128172	C 3.479917	-1.068563	-0.3096031	C 3.542534	-1.179836	-2.955984
C 1.409377	-2.531989	-0.895611	C -2.494943	-1.576325	-0.803353	H 3.740448	-1.271418	-4.178184	H 3.565025	-1.402415	-4.034099
H 3.736388	-2.861673	-1.567829	C -2.660635	-0.401545	-0.594979	C 2.276999	-0.960718	-2.388426	C 2.319325	-1.044109	-2.288863
H 4.528214	-3.492920	-1.998988	H -3.167933	-4.950866	-0.824920	H 1.306808	-1.083865	-2.895772	H 1.363540	-1.163686	-2.823905
-0.269141	-4.275136	-1.133987	C -0.403402	-0.269588	-2.146344	C 4.630809	0.058749	1.782790	C 4.553489	-0.004623	1.944416
C 2.031006	-4.716749	-1.822022	C -4.343243	-2.684793	-1.963902	H 5.319563	0.641766	1.128778	H 5.276121	0.561934	1.312763
C 0.711479	-5.141925	-1.663456	C -4.749705	-1.450159	-2.468311	C 4.169298	0.952090	2.932598	C 4.071912	0.901411	3.076095
H 0.421923	-6.160534	-1.958197	H -5.627754	-1.383874	-3.126186	H 3.442413	0.416008	3.576441	H 3.317234	0.379848	3.699669
C 2.137351	2.876554	-1.442150	C 3.609460	-2.699434	-0.874759	H 5.035297	1.251441	3.557526	H 4.923133	1.189250	3.726192
C 3.764215	3.851394	-3.017337	C 5.055259	-3.658426	-2.609139	H 3.678897	1.868352	2.549325	H 3.607906	1.823854	2.675354
H 4.517232	4.621073	-3.245209	H 5.927552	-4.269140	-2.889403	C 5.327136	-1.217699	2.263603	C 5		

C	-5.259144	-0.459518	-2.924443	C	0.577186	5.644896	-2.965873		
H	-5.193938	0.222437	-3.803255	H	1.289391	5.401963	-3.787228		
C	-4.897733	-1.875679	-3.370152	C	-0.833353	5.736910	-3.545878		
H	-3.884997	-1.895074	-3.818313	H	-1.116944	4.786512	-4.039453		
H	-5.627592	-2.242070	-4.120833	H	-0.889706	6.554491	-4.293226		
H	-4.901103	-2.570889	-2.505917	H	-1.572433	5.945274	-2.744933		
C	-6.650908	-0.362101	-2.292476	C	1.018548	6.927995	-2.255258		
H	-6.721336	-1.040274	-1.417170	H	0.301732	7.189419	-1.449380		
H	-7.431049	-0.656848	-3.024625	H	1.053367	7.774194	-2.972352		
H	-6.873917	0.668671	-1.950159	H	2.024250	6.821436	-1.801486		
Cl	-0.155968	-0.139245	-2.637168	Cl	0.365893	-0.473978	-2.228259		
H	1.073653	1.220934	-2.285209	H	2.010182	-1.566073	-1.635093		

4a ⁺ →5b				2a→2c ⁺				2c ⁺				2c ⁺ →3b			
-3799.8261078				-4735.1738349				-4735.2086666				-4735.1871175			
Ru	-1.133887	0.024220	0.839864	Ru	0.22008200	-0.18282000	-0.23935100	Ru	-0.167885	-0.501138	-0.239859	Ru	-0.690562	-0.458793	-0.135859
Cl	4.867908	-4.464121	-1.141208	Cl	3.82020400	2.56797100	-2.57520700	Cl	-3.417712	-4.345408	0.231593	Cl	-5.498707	-1.929909	-0.505750
Cl	0.417699	-2.300671	-3.349814	Cl	2.64329400	6.18950500	1.29863300	Cl	-2.416442	-3.722329	5.553703	Cl	-5.351484	-1.669732	4.938208
N	-1.468299	2.294865	-1.182703	Cl	-3.65880100	-1.26623200	2.33628200	Cl	2.025657	3.572051	-1.355493	Cl	4.221080	2.793819	-1.048442
N	-3.262654	1.030995	-0.895545	Cl	-6.06381600	3.47937300	1.31152300	Cl	6.063252	3.669530	2.273798	Cl	8.006267	0.353410	1.986622
N	1.071578	-2.323948	1.733946	O	1.78247400	0.80881000	-1.11211600	O	-1.637854	-1.909781	-0.054499	O	-2.640007	-0.950050	-0.304138
O	-0.454020	-1.818097	-0.535919	O	-1.76522600	-0.48778600	0.18911900	O	1.599214	0.768422	-0.425553	O	2.475129	0.388416	-0.277616
O	3.312767	0.821419	-0.013703	N	0.32445000	1.51980900	1.00571000	N	-0.320371	-0.643809	1.892293	N	-1.275890	-0.427661	1.920479
C	-1.949674	1.191490	-0.512472	N	-0.79978600	-2.47716900	-2.14626400	N	0.679154	-1.126432	-3.172884	N	-0.259499	-1.815283	-2.873429
C	-2.503578	2.966595	-1.998634	N	1.39362200	-2.45267100	-1.94505700	N	-1.147301	0.092902	-3.106841	N	-0.810987	0.298665	-3.117518
H	-2.725377	3.970787	-1.573519	C	4.86711500	-1.09717300	-2.26376000	C	-4.750103	0.627350	-2.271784	C	-2.880882	3.396400	-2.847648
H	-2.143895	3.119941	-3.038070	H	5.42925900	-0.42876600	-2.93671900	H	-5.654958	0.021547	-2.095152	H	-3.945956	3.677487	-2.789460
C	-3.698904	2.009166	-1.909217	C	2.77332400	-2.15950700	-1.64221500	C	-2.372280	0.749277	-2.743521	C	-1.172133	1.679230	-2.947014
H	-3.910545	1.492638	-2.872130	C	3.50349500	-1.31594700	-2.52503500	C	-3.538928	-0.037657	-2.534044	C	-2.546451	2.030115	-2.888133
H	-4.636127	2.511191	-1.589616	C	4.79829000	-2.58949000	-0.36987100	C	-3.686435	2.780877	-2.517334	C	-0.549466	0.422840	-2.977577
C	-0.206754	2.981092	-1.108136	H	5.30653400	-3.11094800	0.45911100	H	-3.743210	3.882545	-2.527427	H	0.232375	4.799297	-3.028823
C	-0.015617	4.009523	-0.144859	C	3.42931100	-2.85251000	-0.59389700	C	-2.446541	2.166047	-2.786321	C	-0.158803	2.669217	-3.022102
C	1.149727	4.794037	-0.235331	C	2.74813500	-3.90536100	0.25367900	C	-1.246577	3.016290	-3.134650	C	1.296853	2.286753	-3.135911
H	1.301502	5.594318	0.508611	H	3.25233600	-4.88796400	0.12862500	H	-1.244699	3.282603	-4.215587	H	1.483392	1.624984	-4.008821
C	2.103971	4.612617	-1.256918	H	1.68056600	-4.03376900	-0.00450400	H	-0.292435	2.502965	-2.909509	H	1.660323	1.737242	-2.239423
C	1.881148	3.586747	-2.194775	H	2.80146600	-3.65039600	1.33251700	H	-1.260187	3.969303	-2.569423	H	1.932652	3.184419	-3.259317
H	2.608734	3.428853	-3.008974	C	5.53156000	-1.70421900	-1.17780900	C	-4.845920	2.034428	-2.240882	C	-1.900508	4.401994	-2.882212
C	0.737604	2.764308	-2.144310	C	2.84307300	-0.68668800	-3.72461100	C	-3.488958	-1.543603	-2.604700	C	-3.618946	0.967856	-2.874070
C	-1.033440	4.275358	0.934696	H	2.34231300	-1.44290500	-4.36675100	H	-4.508637	-1.974647	-2.574328	H	-4.622423	1.418209	-2.743663
H	-0.732950	5.139459	1.558876	H	3.58508200	-0.15432800	-4.35022300	H	-2.908782	-1.962580	-1.755429	H	-3.453534	0.231063	-2.060677
H	-2.035797	4.500626	0.510569	H	2.06970500	0.04210400	-3.41227900	H	-2.998526	-1.894290	-3.537923	H	-3.638175	0.962742	-3.826146
H	-1.170395	3.392080	1.594111	C	6.98885800	-1.40815900	-0.90173700	C	-6.154192	2.711251	-1.901498	C	-2.294789	5.867064	-2.799625
C	3.318117	5.511056	-1.341401	H	7.43257700	-2.14275500	-0.20005100	H	-7.019534	2.176674	-2.345193	H	-3.206661	6.078896	-3.395659
H	3.023287	6.580361	-1.404820	H	7.11031700	-0.39981500	-0.44859100	H	-6.178692	3.762102	-2.254279	H	-1.485110	6.533204	-3.159816
H	3.960174	5.410684	-0.440202	H	7.59069100	-1.41459100	-1.83450600	H	-6.311594	2.726070	-0.800395	H	-2.521503	6.155889	-1.749721
H	3.941282	5.280389	-2.228591	C	0.24470600	-1.81660000	-1.53770500	C	-0.210443	-0.535025	-2.314170	C	-0.500637	-0.657451	-2.181397
C	0.542259	1.683629	-3.178207	C	-0.35882200	-3.57395700	-3.04333900	C	0.348032	-0.938200	-4.602903	C	-0.483506	-1.690380	-3.311185
H	-0.397160	1.853373	-3.776614	H	-0.65333300	-3.35338300	-4.09155000	H	0.148728	-1.923492	-0.507894	H	-1.352108	-2.313935	-4.638720
H	1.375242	1.637733	-3.885585	H	-0.85567800	-4.52241400	-2.74873000	H	1.205990	-0.479936	-1.537913	H	0.403122	-2.058235	-4.888435
H	0.412465	0.682277	-2.712935	C	1.15968600	-3.60245600	-2.84402800	C	-0.885704	-0.030874	-4.556656	C	-0.731577	-0.188740	-4.511521
C	-4.170510	-0.044409	-0.576834	H	1.52266800	-4.54069500	-2.36879200	H	-0.701585	0.970317	-5.003613	H	0.093274	0.324704	-5.054452
C	-5.166506	0.159179	0.413258	H	1.72606100	-3.47221800	-3.79003300	H	-1.768653	-0.467117	-5.071116	H	-1.674543	0.036080	-5.052195
C	-6.082359	-0.884037	0.653581	C	-4.14211100	-3.17699100	-0.61141000	C	4.209847	-2.312791	-2.830275	C	2.055482	-4.626352	-2.058257
H	-6.848705	-0.739967	1.433771	H	-4.54705400	-3.68300000	0.28044300	H	5.230352	-1.892885	-2.845445	H	3.141659	-4.819715	-2.301416
C	-6.051498	-2.092662	-0.066583	C	-2.74724100	-3.10528500	-0.76648900	C	3.115086	-1.432889	-2.961179	C	1.607562	-3.333060	-2.389518
C	-5.087488	-2.232394	-1.083998	C	-3.08961600	-1.92638100	-2.90546100	C	1.599679	-3.380012	-2.808108	C	-0.721739	-4.127316	-2.143927
H	-5.063244	-1.580466	-1.683595	C	-6.52704100	-2.67325700	-3.27873000	C	5.226061	-4.627629	-2.534829	C	1.664368	-7.046184	-1.757426
C	-4.147344	-1.224327	-1.365532	H	-7.09059000	-2.46418500	-2.25923600	H	5.122639	-5.539466	-3.159555	H	1.034580	-7.851463	-1.807138
C	-5.262602	1.446991	1.194393	H	-6.84277000	-1.92063900	-0.57239500	H	5.323275	-4.970995	-1.481222	H	1.645710	-7.180593	-0.271132
H	-6.145892	1.435725	1.862672	H	-6.84726000	-3.66513400	-0.94584900	H	6.177233	-4.129041	-2.810456	H	2.708767	-7.210312	-1.709984
H	-4.354581	1.601139	1.815734	C	-2.22293100	-2.43760200	-1.90713700	C	1.810872	-1.981428	-2.921643	C	0.211294	-3.097380	-2.417050
H	-5.356395	2.333712	0.530567	C	-4.48281300	-2.00868900	-2.69145300	C	2.725845	-4.214532	-2.700033	C	-0.220871	-5.401247	-1.814040
C	-7.010224	-3.216412	0.255747	H	-5.15690900	-1.59037300	-3.45833900	H	2.568140	-5.301749	-2.599560	H	-0.939398	-6.207030	-1.586581
H	-7.270947	-3.807261	-0.646226	C	-5.03239000	-2.61931200	-1.55185700	C	4.039258	-3.703318	-2.697924	C	1.160445	-5.673391	-1.763770
H	-6.555767	-3.920761	0.987163	C	-1.84142400	-3.71423100	0.27410100	C	3.343378	0.047099	-3.164212	C	2.588328	-2.220574	-2.674160
H	-7.950258	-2.838593	0.706731	H	-2.39650400	-4.42865000	0.91301700	H	4.369147	0.335256	-2.859118	H	3.631252	-2.593726	-2.646264
C	-3.143933	-1.407665	-2.487819	H	-1.42795200	-2.91935600	0.92855100	H	2.620638	0.651835	-2.582462	H	2.490072	-1.396625	-1.933316
H	-2.108861	-1.479876	-2.087669	H	-0.98309700	-4.25359000	-0.78111900	H	3.237691	0.334432	-4.234942	H	2.427234	-1.764739	-3.357168
H	-3.353584	-2.334202	-3.048422	C	-2.58236600	-1.36373500	-4.21235100	C	0.205458	-3.956077	-2.758136	C	-2.209114	-3.868317	-2.184926
H	-3.159748	-0.562688	-3.200327	H	-1.53586400	-1.01447900	-4.17470500	H	-0.318288	-3.629057	-1.834706	H	-2.489056	-2.956088	-1.573924
C	0.602325	0.707194	0.648031	H	-3.19910600	-0.50396700	-4.54343400	H	0.233437	-5.063163	-2.762568	H	-2.773821	-4.743390	-1.808333
H	1.045102	0.589297	-0.367156	H	-2.64462400	-2.12819200	-5.01947100	H	-0.417973	-3.629172	-3.617735	H	-2.567144	-3.668710	-3.219370
C	1.601028	1.039522	1.652461	N	-1.72377200	1.98650300	-1.18459600	N	3.289648	-0.605657	1.379443	N	3.313216	-1.706364	1.288388
C	3.009069	1.086512	1.287251	C	-1.65624800	3.20996400	-1.71807700	C	4.020481	-1.309952	2.250140	C	3.606255	-2.776249	2.038552
C	3.987237	1.368572	2.267133	H	-0.83881800	3.38545400	-2.43701300	H	3.751703	-2.374053	2.336983	H	2.798003	-3.515908	2.141045
H	5.052179	1.397060	2.000139	C	-2.59168600	4.23690400	-1.44314400	C	5.055705	-0.685457	2.975025	C	4.882805	-2.882179	2.628395
C	3.614908	1.612733	3.599045	H	-2.47585800	5.22321900	-1.91652800	H	5.647316	-1.266910	3.696220	H	5.125704	-3.758433	3.245959
H	4.398129	1.830270	4.343498	C	-2.67837400	0.41539700	0.41013000	C	2.570402	1.363605	0.157449	C	3.654742	0.410603	0.183837
C	2.261680	1.576344	3.977437	C	-3.74759200	2.67882300	0.02056600	C	4.546920	1.409226	1.803257				

	C	0.36764000	-3.23359800	4.71979800	C	-1.406678	5.120317	1.253317	C	1.131060	4.797913	1.703710
	H	0.51587300	-2.57261200	5.60491500	H	-1.878925	5.188015	2.260153	H	0.593447	5.153155	2.612749
	C	-1.10550600	-3.62928400	4.64524400	C	0.048779	5.568682	1.365144	C	2.517433	4.307513	2.113343
	H	-1.74712300	-2.73173400	4.54644200	H	0.586413	4.971246	2.128066	H	2.440962	3.502368	2.870954
	H	-1.40306200	-4.18143100	5.55978700	H	0.100336	6.637457	1.657033	H	3.104127	5.142236	2.548482
	H	-1.28923600	-4.28218700	3.76730000	H	0.571196	5.437408	0.395929	H	3.064234	3.911871	1.234006
	C	1.30765900	-4.44028000	4.80766300	C	-2.214032	5.946746	0.247486	C	1.174790	5.912069	0.654145
	H	1.14642500	-5.11585200	3.94221300	H	-1.725774	5.924149	-0.748789	H	1.725157	5.564850	-0.244074
	H	1.11319500	-5.01529800	5.73657400	H	-2.279747	7.004486	0.576606	H	1.693819	6.805648	1.058672
	H	2.37264700	-4.13283900	4.81274000	H	-3.245528	5.556469	0.136315	H	0.156456	6.218203	0.340640
	H	-0.84422700	1.21244700	-2.66450800	Cl	1.416670	-2.544603	0.251473	Cl	0.463101	-2.536932	0.721243
	Cl	-0.28860600	1.25321300	-3.88931800	H	2.525363	-1.188483	0.842723	H	2.331939	-1.677089	0.867600

4b ⁺	2a ⁺ H ⁺			2a ⁺ H ⁺ →2a ⁺	2a ⁺						
-3799.84340738	-4274.8311272			-4735.1929981	-4735.208667						
Ru 1.008631	0.105106	0.742062	Ru 0.077931	-0.032362	-0.207696	Ru -0.16696800	-0.13602100	0.12735200	Ru -0.058526	-0.144576	-0.023238
Cl -4.798549	-4.858054	-1.412922	Cl 1.195770	3.738351	-3.360624	Cl -0.19710400	3.93716100	3.14885300	Cl -0.779113	4.181913	2.640768
Cl -0.221324	-2.559277	-3.179006	Cl 1.158776	6.742111	1.178865	Cl 0.25118600	6.66830300	-1.54415600	Cl -0.969520	6.475157	-2.294313
N 1.631819	1.589959	-1.932213	Cl -2.442292	-2.888933	3.318125	Cl 2.54450800	-4.24688700	-3.02577600	Cl 3.866755	-4.654886	-1.673745
N 3.153693	0.151459	-1.214097	Cl -6.551481	0.604211	2.422654	Cl 6.39732800	-0.44115400	-3.30122100	Cl 6.132327	-0.165203	-3.673187
N -1.664543	-2.255600	1.767111	O 0.674901	1.437303	-1.468634	O -0.11357400	1.48957500	1.36415400	O -0.220744	1.636343	1.093005
O 0.028104	-1.490425	-0.387141	O -1.087430	-1.340752	1.157643	O 1.33291100	-2.47624300	-0.92412200	O 2.126469	-2.849547	-0.198171
O -2.299475	2.318075	2.442998	N 0.267888	1.601565	1.177977	N 0.01180000	1.45663600	-1.30977700	N -0.161004	1.366559	-1.588048
C 1.937894	0.719655	-0.915760	N -1.055977	-1.858053	-2.445651	N 0.91339100	-1.87716100	2.46011100	N 1.167112	-1.282234	2.557000
C 2.729793	1.698083	-2.920904	N 1.139952	-1.937308	-2.391331	N -1.14793300	-2.43944000	1.93126400	N -0.495354	-2.566461	1.875011
H 3.258659	2.670996	-2.796301	C 4.718699	-0.850765	-2.418196	C -4.81259400	-1.72983700	2.02645700	C -4.178002	-3.093195	1.423063
H 2.323889	1.657886	-3.954897	H 5.344470	-0.077866	-2.894998	H -5.51302000	-1.08701100	2.58582300	H -5.121208	-2.671568	1.809900
C 3.616546	0.495865	-2.572011	C 2.537512	-1.846952	-2.057568	C -2.53562500	-2.43472400	1.55462100	C -1.743500	-3.062914	1.351815
H 3.345986	-0.362830	-3.263290	C 3.338326	-0.852519	-2.684608	C -3.43665800	-1.61573800	2.29112700	C -2.962031	-2.534977	1.863984
H 4.699158	0.735472	-2.571264	C 4.514855	-2.814971	-1.027714	C -4.39891100	-3.45800700	0.38810600	C -2.997596	-4.718592	0.091266
C 0.554653	2.539761	-2.019043	H 4.974680	-3.596412	-0.399829	H -4.77373800	-4.18927700	-0.34790300	H -3.004112	-5.590152	-0.585456
C 0.625691	3.757648	-1.288939	C 3.124959	-2.865177	-1.260485	C -3.00624600	-3.37724500	0.60495400	C -1.751711	-4.193059	0.490782
C -0.423005	4.687282	-1.447315	C 2.319822	-4.012761	-0.690700	C -2.06629800	-4.24905200	1.08899600	C -0.490408	-4.862194	0.003008
H -0.377607	5.630094	-0.876376	H 2.456805	-4.936030	-1.295760	H -1.14471500	-4.50327800	0.37037000	H 0.391179	-4.635186	0.627499
C -1.502674	4.464487	-2.322922	H 1.234752	-3.793825	-0.660108	H -1.73669800	-3.70912500	-1.10718900	H -0.242436	-4.508503	-1.022124
C -1.504936	3.276576	-3.079202	H 2.650266	-4.256721	-0.339093	H -2.56226800	-5.18917400	-0.50277100	H -0.622083	-5.962710	-0.040735
H -2.326368	3.090328	-3.791584	C 5.329486	-1.813111	-1.584557	C -5.31717300	-2.65100800	1.08454600	C -4.221246	-4.183314	0.536362
C -0.489245	2.309788	-2.953722	C 2.737054	0.156996	-3.631800	C -2.93500600	-0.66447300	3.35169800	C -2.983521	-1.460899	2.925907
C 1.799533	0.484091	-0.400345	H 3.513035	0.844094	-4.020629	H -3.74737500	0.00022800	3.70372200	H -3.945566	-0.912865	2.918576
H 1.730208	5.124210	-0.025630	H 1.951786	0.762395	-3.135812	H -2.10643900	-0.03237700	2.97485600	H -2.171122	-2.732455	2.975123
H 2.761762	3.988554	-0.948070	H 2.266456	-0.337888	-4.509275	H -2.54639600	-1.21018400	4.24024500	H -2.870405	-1.905802	3.040228
H 1.873757	3.401749	0.476440	C 6.814182	-1.760391	-1.310317	C -6.80796000	-2.78099500	0.86284500	C -5.537041	-4.803346	0.116494
H -2.630907	5.463843	-2.449640	H 7.393709	-1.603303	-2.243565	H -7.27861100	-1.79257900	0.67785500	H -5.771998	-5.697276	0.736008
H -2.355215	6.450468	-2.026147	H 7.178934	-2.690767	-0.831999	H -7.31004300	-3.21112800	1.75695700	H -5.513923	-5.143069	-0.393458
H -3.536152	5.110545	-1.908813	H 7.060576	-0.914191	-0.632750	H -7.04011900	-3.43829000	0.00154900	H -6.380918	-4.094110	0.233947
H -2.927508	5.614023	-3.508657	C 0.044564	-1.397633	-1.768750	C -0.13921100	-1.55216700	1.63303300	C 0.186674	-1.398216	1.593303
C -0.506192	1.800357	-3.830870	C -0.724955	-2.695131	-3.623048	C 0.06963900	-3.06390800	3.30683400	C 1.266306	-2.473589	3.428026
H 0.115457	1.228174	-4.742965	H -1.054368	-2.188987	-4.555920	H 0.83993000	-2.81658200	4.37480000	H 1.354539	-2.169655	4.491106
H -1.532541	0.853313	-4.181166	H -1.257952	-3.666848	-3.555062	H 1.35090700	-3.88876300	3.03231800	H 2.168849	-0.765757	3.164450
H -0.111271	0.186455	-3.311099	C 0.799257	-2.831810	-3.522683	C -0.80626100	-3.40029200	3.00151900	C -0.031126	-3.222476	3.117478
C 3.961018	-0.678385	-0.350001	H 1.128958	-3.869710	-3.300576	H -0.94541300	-4.44215300	2.64454900	H 0.121739	-0.347666	2.947972
C 4.982288	-0.055716	0.421426	H 1.328565	-2.505880	-4.441722	H -1.47568600	-3.25494400	3.87504200	H -0.797399	-3.110748	3.918102
C 5.786993	-0.869499	1.246000	C -4.922297	-2.512125	-1.112782	C 4.57810000	-1.09997200	2.57107000	C 4.130708	0.968404	3.083354
H 6.568610	-0.388939	1.852666	H -5.001413	-3.240338	-0.458910	H 5.52663400	-1.53012000	2.20660700	H 5.216128	0.969453	2.884564
C 5.622286	-2.266962	1.304166	C -3.101433	-2.635274	-1.370966	C 3.37536700	-1.76016000	2.25152400	C 3.374881	-0.150509	2.672891
C 4.647005	-2.855127	0.477751	C -3.191452	-0.689100	-2.829067	C 2.15121200	-0.05446900	3.55517200	C 1.376144	0.909918	3.653188
H 4.526250	-3.951548	0.479686	C -6.738708	-1.388364	-1.498578	C 5.91408000	0.78070500	3.63502800	C 4.372955	3.275756	4.130091
C 3.820023	-2.091743	0.709681	H -7.253504	-0.872384	-2.333224	H 6.71101800	0.06089100	3.91571200	H 4.263064	4.091716	3.381845
C 5.210506	1.435012	0.379373	H -6.942828	-0.804333	-0.574007	H 5.81040800	1.51719500	4.45687500	H 5.452944	3.033671	4.196093
H 1.636591	1.706420	0.923115	H -7.211964	-2.381845	-1.362538	H 6.28057800	1.33045900	2.74025400	H 4.051677	3.691992	5.107146
H 4.355920	1.959289	0.860487	C -2.451662	-1.690787	-2.146102	C 2.15380500	-1.19112200	2.70284300	C 1.975915	-0.142195	2.906098
H 5.301968	1.819537	-0.658728	C -4.580055	-0.614695	-2.605063	C 3.38374600	0.57141100	3.83742400	C 2.172333	2.005264	0.403972
C 6.458341	-3.107037	2.242906	H -5.159310	0.163368	-3.129924	H 3.38418300	1.46196000	4.48857600	H 1.698713	2.831355	4.589401
H 6.989588	-4.137550	1.857762	C -5.252253	-1.509004	-1.745755	C 4.60686000	0.07821500	3.34283800	C 3.550298	2.067223	3.741807
H 5.9565381	-3.193312	3.236442	C -2.363710	-3.798882	-0.688137	C 3.42317800	-3.06582400	1.49090300	C 4.086393	-1.335072	2.061845
H 7.458929	-2.660125	2.413951	H -2.693030	-3.972744	0.363396	H 4.26988000	-3.07666000	0.77576400	H 4.887646	-1.007886	1.368621
C 2.859072	-2.779054	-1.308580	H -1.267254	-3.650557	-0.682397	H 2.49245900	-3.25684000	0.92447200	H 3.397472	-1.998877	1.509214
H 1.848355	-2.328145	-1.275567	H -2.572565	-4.740539	-1.234617	H 3.58796800	-3.91900200	2.18701000	H 4.581608	-1.939466	2.854450
H 2.765764	-3.854040	-0.105793	C -2.521374	0.256878	-3.799845	C 0.87872700	0.45742200	4.18327700	C -0.066013	0.828949	4.086448
H 3.215003	-2.719273	-2.361193	H -1.502862	0.546360	-3.471672	H 0.23222000	0.94760600	3.42692500	H -0.736767	0.845729	3.260200
C -0.411403	1.296857	0.773027	H -3.122560	1.766611	-3.940710	H 1.10310200	1.19869400	4.97451500	H -0.333350	1.684882	4.735747
H -0.197723	2.213459	1.364518	H -2.419422	-0.207578	-4.805998	H 0.29254000	-0.36659000	4.64185200	H -0.267413	-0.106083	4.650623
C -1.829098	1.165097	0.426200	N -2.037015	0.766444	-0.197099	N 2.23613600	0.02022300	-0.17169000	N 2.066717	0.039955	-0.362202
C -2.801147	1.759607	1.309506	C -2.469190	1.855744	-0.841155	C 2.77513800	1.14222300	0.30962400	C 2.401737	1.334693	-0.185694
C -4.176542	1.983664	0.994848	H -1.781699	2.280049	-1.589315	H 2.18736600	1.66925100	1.07591800	H 1.793225	1.880461	0.548542
H -4.923902	2.146632	1.664476	C -3.733573	2.445235	-0.592578	C 4.02367900	1.66242600	-0.11293400	C 3.426827	2.010706	-0.881984
C -4.603495	1.057134	-0.181000	H -4.025412	3.348039	-1.148846	H 4.39743700	2.59770200	0.32881000	H 3.581989	3.083957	-0.699214
H -5.680831	1.018870	-0.410239	C -2.351668	-0.919013	1.473915	C 2.43145300	-1.98708500	-1.51241200	C 2.942458	-2.178937	-1.034324
C -3.671850	0.476561	-1.058726	C -4.163059	0.716220	1.056529	C 4.21539500	-0.22805100	-1.61640600	C 4.014258	-0.103601	-1.890108
H -4.008399	-0.012191	-1.985782	C -2.852027	0.204872	0.755501	C 2.95351200	-0.71064200	-1.09259600	C 2.967851	-0.736527	-1.103952
C -2.06189	0.533130	-0.747318	C -4.585401	1.875100	0.344643	C 4.73057100	0.99193100	-1.09802400	C 4.189106	1.304981	-1.794726
H -1.560779	0.109657	-1.431658	H -5.576379	2.302555	0.556808	H 5.68785200	1.37202000	-1.48517300	H 4.968348	1.786987	-2.402787
C -3.142441	3.016424	3.388480	C -3.131786	-1.526497	2.455081	C 3.14207900	-2.69428400	-2.49996600	C 3.884113	-0.912209	-1.778639
H -4.083023	2.432462	3.523305	C -4.939107	0.040798	2.056557	C 4.87844600	-1.00457700	-2.61845500	C 4.902122	-0.917429	-2.665636
C -3.471314	4.424573	2.882906	C -4.435039	-1.057073	2.748433	C 4.35030400	-2.20904800	-3.06076600	C 4.847102	-2.300374	-2.612537
H -2.538808	5.012337	2.756495	H -5.036256	-1.557600	3.519713	H 4.86835100	-2.80069800	-3.82793100	H 5.545013	-2.919633	-3.19171

	C	3.594292	-2.566336	3.807902	C	-4.93143000	-0.10420600	-3.16641200	C	-5.262847	-0.434014	-2.783672
	H	4.012095	-1.816189	4.516585	H	-5.28504600	0.91632800	-3.44208300	H	-5.734558	0.562755	-2.945427
	C	2.457669	-3.313901	4.500400	C	-4.16167800	-0.70056200	-4.34296500	C	-4.608550	-0.888714	-4.086950
	H	1.674564	-2.612004	4.850530	H	-3.33743000	-0.02890000	-4.65308400	H	-3.863109	-0.144958	-4.431354
	H	2.844269	-3.866147	5.380312	H	-4.83976300	-0.85310200	-5.20744300	H	-5.374634	-1.013304	-4.879071
	H	1.993844	-4.049445	3.810686	H	-3.71018300	-1.67211800	-4.05835500	H	-4.088553	-1.857698	-3.942567
	C	4.705062	-3.493455	3.310483	C	-6.11776200	-0.96450400	-2.72290100	C	-6.303946	-1.426443	-2.258459
	H	4.288507	-4.275106	2.642001	H	-5.76938600	-1.98245600	-2.45342400	H	-5.839104	-2.421415	-2.104280
	H	5.193782	-4.000521	4.167391	H	-6.85942000	-1.05261800	-3.54354700	H	-7.133684	-1.536120	-2.987034
	H	5.485680	-2.939234	2.752732	H	-6.63114600	-0.53082600	-1.84123800	H	-6.737092	-1.095018	-1.293537
	H	-0.808591	-2.091550	1.732204	H	0.52112600	-2.45577400	-1.60118800	H	1.190201	-2.546335	-0.423406
					Cl	-0.83578400	-1.87753400	-2.58370300	Cl	-0.115800	-1.912837	-1.746317

2a ⁺ →3b				3b→4b ⁺				4b ⁺ →5b				2b ⁺ H ⁺			
-4735.209666				-3799.8231279				-3799.8243664				-4274.8440066			
Ru	-0.392321	-0.177560	0.088176	Ru	-0.714918	-0.196891	0.588565	Ru	1.248002	1.164948	-0.883755	Ru	-0.064659	-0.057504	0.195316
Cl	-0.117407	4.177291	2.73818	Cl	2.870001	6.037827	-0.587123	Cl	-8.038500	-2.004028	-0.071862	Cl	4.988582	1.396142	-0.538816
Cl	0.852702	6.395787	-2.106914	Cl	-0.473754	2.854536	-3.458330	Cl	-3.822558	-1.480114	3.339792	Cl	5.004622	-2.964600	-3.807361
Cl	3.835189	-4.832192	-2.402946	N	-1.062751	-2.705477	-1.069811	N	2.026087	0.679585	2.059980	Cl	0.517255	6.541661	-2.100088
Cl	6.877085	-0.385751	-3.005025	N	-2.969045	-1.708653	-0.556648	N	1.325631	2.714763	1.535407	Cl	-0.450456	4.299155	2.764367
O	-0.167190	1.569227	1.222481	N	0.314337	2.049310	1.551838	N	-3.486944	-0.059838	-1.576662	N	-1.359047	-1.667724	2.512381
O	2.092670	-3.143282	-0.771183	O	-0.619018	1.233148	-0.951777	O	-2.385483	-0.351711	0.875584	N	0.830608	-1.598046	2.705702
N	0.087864	1.276069	-1.427896	O	3.291928	-1.143897	1.950899	O	3.214110	-2.800431	-2.056066	N	0.856247	-1.609440	-0.911631
N	0.454863	-1.682985	2.616654	C	-1.604763	-1.615412	-0.430731	C	1.589663	1.462830	1.025071	N	0.111253	1.387733	-1.391377
N	-1.418903	-2.534232	1.821074	C	-2.089140	-3.644059	-1.568874	C	2.186781	1.458680	3.307831	O	2.239103	0.470528	0.154412
C	-5.067372	-2.331312	1.008232	H	-2.082591	-4.580770	-0.967740	H	3.267278	1.655812	3.495440	O	-0.391598	1.698419	1.229912
H	-5.948678	-1.741823	1.312719	H	-1.883391	-3.919744	-2.624050	H	1.787548	0.898118	4.176737	O	-3.485663	-1.569303	-2.326272
C	-2.681208	-2.770929	1.175482	C	-3.389186	-2.847112	-1.396525	C	1.403145	2.743954	3.007298	C	-0.217437	-1.194151	1.920831
C	-3.817670	-2.018029	1.578997	H	-3.800912	-2.478129	-2.363369	H	0.382516	2.730638	3.454723	C	-1.108487	-2.425946	3.761769
C	-4.087231	-4.137748	-0.256343	H	-4.189987	-3.424683	-0.890898	H	1.917871	3.661106	3.358969	H	-1.514426	-3.455564	3.673285
H	-4.189871	-4.981508	-0.960297	C	0.308751	-2.993915	-1.370336	C	2.453209	-0.691596	2.035228	H	-1.628728	-1.936862	4.612590
C	-2.812079	-3.861791	0.276051	C	1.013524	-3.948461	-0.591405	C	3.774963	-1.011358	1.632657	C	0.420993	-2.391414	3.888565
C	-1.655629	-4.768438	-0.077838	C	2.319657	-4.295454	-0.994376	C	4.171869	-2.364139	1.680418	H	0.772770	-1.899470	4.820103
H	-0.685494	-4.365644	0.262989	H	2.881055	-5.028435	-0.390617	H	5.196917	-2.622631	1.365668	H	0.882720	-3.400729	3.851366
H	-1.583980	-4.903520	-1.175525	C	2.923806	-3.741333	-2.139288	C	3.312523	-3.380928	2.136750	C	-2.738386	-1.419713	2.184237
H	-1.801637	-5.776771	0.369170	C	2.182905	-2.813569	-2.901706	C	2.020121	-3.016486	2.565322	C	-3.492312	-2.429727	1.532737
C	-5.262186	-3.384881	0.087268	H	2.634278	-2.375775	-0.890898	H	1.335960	-3.795041	2.942625	C	-4.865443	-2.200499	1.308899
C	-3.724580	-0.953001	2.647433	C	0.877640	-2.431746	-2.545604	C	1.566046	-1.684715	2.530403	H	-5.455349	-2.976689	0.793743
H	-4.583580	-0.256399	2.591193	C	0.390499	-4.567050	0.637605	C	4.746861	0.057030	1.191337	C	-5.505752	-1.024460	1.738839
H	-2.795300	-0.358617	2.565877	H	1.149664	-5.108696	-1.235546	H	5.729209	-0.386099	0.935520	C	-4.734857	-0.064160	2.429806
H	-3.738713	-1.407642	3.663468	H	-0.398103	-5.304821	0.369079	H	4.921579	0.805754	1.994628	H	-5.224637	0.850586	2.803009
C	-6.578688	-3.718385	-0.503618	H	-0.087201	-3.799664	1.286113	H	4.379922	0.622294	0.307896	C	-3.362905	-0.238628	2.678257
H	-6.845526	-4.782384	-0.328224	C	4.332430	-4.115784	-2.543298	C	3.754116	-4.826891	2.183143	C	-2.876023	-3.741506	1.099476
H	-6.589619	-3.567028	-1.604694	H	4.716862	-4.969109	-1.949679	H	4.824630	-4.939788	1.919470	H	-3.226719	-0.310176	0.807655
H	-7.382559	-3.091389	-0.069174	H	5.028976	-3.261866	-2.396795	H	3.162044	-5.447463	1.475730	H	-3.171225	-4.567352	1.783344
C	-0.502843	-1.523012	1.634584	H	4.387325	-4.393249	-3.617138	H	3.604073	-5.264790	3.192880	H	-1.769390	-3.702054	1.086845
C	0.279167	-2.938365	3.383613	C	0.091304	-1.458002	-3.390967	C	1.880348	-1.340340	3.025420	C	-6.977594	-0.790375	1.490697
H	0.433935	-2.753651	4.465579	H	-0.840168	-1.920253	-3.784272	H	0.211523	-0.625470	3.876401	H	-7.461835	-1.667977	1.019083
H	1.019499	-3.699856	3.053352	H	0.685703	-1.113988	-4.259832	H	-0.343576	-2.248010	3.382253	H	-7.134062	-0.085173	0.824823
H	-1.153275	-3.338987	3.033468	H	-0.223546	-0.564552	-2.810653	H	-0.465139	-0.880839	2.247263	H	-7.515344	-0.571662	2.437249
H	-1.262118	-4.420047	2.814118	C	-3.996844	-0.791649	-1.289792	C	0.766088	3.811872	0.787874	C	-2.586699	0.795718	3.455727
H	-1.885447	-3.079372	3.833015	C	-4.727082	-1.081971	1.052471	C	1.623133	4.869836	0.376616	H	-2.027667	0.341004	4.301203
C	3.773562	-0.718577	3.490757	C	-5.790984	-0.226669	1.398305	C	1.056833	5.943176	-0.337333	H	-3.264738	1.561671	3.878788
H	4.845279	-0.404800	3.370766	H	-6.354896	-0.436395	2.322830	H	1.717706	6.761364	-0.669533	H	-1.838649	1.310036	2.816686
C	2.827988	-1.065763	2.946923	C	-6.150830	0.881026	0.606670	C	-1.319059	6.003051	-0.635046	C	2.224933	-1.265365	2.596251
C	1.033302	0.370124	3.580254	C	-5.424881	1.114751	-0.576997	C	-1.145956	4.966342	-0.161381	C	3.130094	-2.217227	2.064657
C	4.340081	1.961433	4.712175	H	-5.699921	1.966645	-1.221727	H	-2.231677	5.011500	-0.350294	C	4.507052	-1.905324	2.066149
H	4.642784	2.763760	3.971579	C	-4.351504	0.293335	-0.971470	C	-0.636748	3.870672	0.563473	H	5.217010	-2.643277	1.656603
H	5.392585	1.455592	4.930429	C	-4.368176	-2.252297	1.933701	C	3.099110	4.855241	0.690991	C	5.001244	-0.696560	2.590023
H	4.084367	2.463735	5.639246	H	-5.090609	-2.355949	2.767088	H	5.377476	5.804778	0.380453	C	4.070739	0.220873	3.129492
C	1.450122	-0.754085	3.084549	H	-3.349153	-2.121686	2.360987	H	5.988847	4.018886	0.156198	H	4.438012	1.161574	3.573564
C	2.018772	1.233880	4.364286	H	-4.359584	-3.212748	3.742522	H	3.292664	4.716850	1.776039	C	2.687476	-0.403565	3.162802
H	1.695057	2.114979	4.942433	C	-7.266555	1.810013	1.030274	C	-0.888491	7.140573	-1.452395	C	2.664620	-0.359709	1.547630
C	3.395343	0.994160	4.182020	H	-7.769308	2.274127	0.157241	H	-1.949460	7.338597	-1.197481	H	3.303922	-3.911788	0.713608
C	3.299755	-2.341058	2.899918	H	-6.871162	2.639006	1.658108	H	-0.852142	6.901229	-2.538236	H	1.615513	-3.528587	1.195540
H	4.319849	-2.218280	1.874774	H	-8.034292	1.282805	1.632532	H	-0.315071	8.078664	-1.306842	H	2.727065	-4.336461	2.341635
H	2.632346	-2.668245	1.469495	C	-3.593925	0.589007	-2.243628	C	-1.575164	2.826917	1.120107	H	6.479682	-0.383536	2.582718
H	3.385223	-3.169071	3.031984	H	-2.567565	0.951406	-2.202681	H	-1.337627	1.794498	0.790993	H	6.730424	0.321409	1.760628
C	-0.422838	0.611366	4.162444	H	-4.110273	1.369223	-3.783497	H	-2.618026	3.036685	0.812304	H	7.091743	-1.295316	2.436658
H	-0.973392	0.895265	3.244340	H	-3.488105	-0.308277	-2.889443	H	-1.560839	2.816378	2.315557	H	6.797738	0.097874	3.529906
H	-0.537839	1.432120	4.895940	C	1.020008	-0.908280	0.442116	C	1.909840	-0.551866	-1.143977	H	1.372920	0.940174	3.799196
H	-0.905229	-0.296644	4.583000	H	1.200977	-1.820918	1.046266	H	2.897417	-0.570900	-1.654002	H	0.987737	1.335890	3.076137
N	2.457545	-0.373942	-0.202673	C	2.275918	-0.315741	-0.023093	C	1.296442	-1.859430	-1.003434	H	2.281478	1.799317	4.230898
C	2.772485	0.860430	4.188748	C	3.471028	-0.517400	0.785824	C	1.993173	-3.021730	-1.506178	H	1.154409	4.070060	4.623019
H	2.709926	1.330682	0.905242	C	4.713584	-0.031563	0.295572	C	1.384214	-4.294248	-1.428042	C	-1.790748	-0.535796	-0.395917
C	3.916547	1.570255	-0.259681	H	5.628349	-0.179679	0.886164	H	1.906028	-5.187311	-1.799129	H	-1.993292	-1.620200	-0.527891
H	4.092264	2.597647	0.091634	C	4.789974	0.655576	-0.928068	C	0.103297	-4.431386	-0.867759	C	-2.880597	0.261017	-0.928618
C	3.111640	-2.451596	-1.298184	H	5.767745	1.029819	-1.272356	H	-0.352282	-5.433817	-0.815408	C	-3.784144	-0.314328	-1.899467
C	4.536419	-0.402148	-1.526559	C	3.637869	0.866485	-1.705468	C	-0.594606	-3.310324	-0.380234	C	-4.870494	0.446642	-2.383242
C	3.340111	-1.049154	-1.015236	H	3.702872	1.397246	-2.667478	H	-1.597806	-3.419857	0.058535	H	-5.563630	0.027573	-3.124894
C	4.780669	0.946641	-1.143045	C	2.402550	0.391356	-1.246366	C	-0.000830	-2.046999	-0.455945	C	-5.076330		

C	-5.104297	0.499922	-3.232720			H	0.624511	2.049309	-4.678598
H	-5.294521	1.565871	-3.497324			C	0.482968	3.571227	-3.134895
C	-4.447292	-0.194451	-4.423988			H	0.632698	4.426622	-3.810800
H	-3.508180	0.320019	-4.708102			C	0.284509	3.818114	-1.745825
H	-5.130781	-0.188238	-5.297210			C	0.086862	2.672921	-0.895871
H	-4.202780	-1.247179	-4.174613			C	-0.154226	2.787225	0.517500
C	-6.408767	-0.170972	-2.793857			C	-0.158770	4.095217	1.055759
H	-6.221376	-1.232705	-2.534172			C	0.051918	5.234540	0.243537
H	-7.155641	-0.136531	-3.613735			H	0.038166	6.231099	0.707040
H	-6.850646	0.326120	-1.907177			C	0.266190	5.106742	-1.129333
H	1.212231	-2.651899	-0.892002			H	2.870316	1.019740	0.675968
Cl	-0.469591	-1.978439	-1.549772						

2b ⁺ H ⁺ →2b ⁺				2b ⁺				2b ⁺ →3b				2b ⁺ →2d ⁺			
-4735.1870134				-4735.2002086				-4735.1907826				-4735.1646116			
Ru	-0.052958	0.117795	0.166158	Ru	0.051060	-0.447976	-0.158643	Ru	-0.600778	-0.309453	-0.174537	Ru	0.07734800	0.22899900	-0.22030800
Cl	4.707870	1.600510	-2.921348	Cl	4.443608	1.240469	3.852679	Cl	4.478889	-2.764855	3.751408	Cl	-4.83785500	0.28333600	-0.10868500
Cl	5.718167	-3.706223	-2.409819	Cl	4.723172	5.285250	0.281059	Cl	7.739611	-0.293669	0.183623	Cl	-5.00024400	-4.45671300	2.54182300
Cl	-2.493941	5.674789	-3.376592	Cl	-1.897464	-2.982051	0.680254	Cl	-4.297497	-1.092248	5.711319	Cl	-2.05381900	4.47241200	4.92320200
Cl	-2.299333	4.318115	1.895561	Cl	-2.664369	-4.574434	0.928578	Cl	-5.571699	-0.864484	0.419482	Cl	0.03183700	5.26036300	-0.04404800
N	-0.708669	-1.394826	2.792205	N	-1.038085	-0.514464	-3.059193	N	-0.889289	0.757156	-3.068452	N	1.81594700	0.20827600	-2.79700900
N	1.300122	-0.488182	2.902682	N	0.808213	-1.711792	-2.935796	N	-0.888215	-1.450645	-3.054080	N	-0.34653500	0.23555500	-3.26539500
N	1.388688	-1.486208	-0.443278	N	1.680300	1.093488	-0.574781	N	2.558129	-0.567193	-0.480189	N	-0.61735100	-2.58793000	0.41079700
N	-0.549333	1.136376	-1.683913	N	-0.163775	-0.245172	1.981131	N	-0.746131	-0.290327	1.965446	N	-0.52547300	0.54494900	1.82616300
O	2.119237	0.931352	-1.605273	O	2.850132	-0.094625	1.924852	O	2.334011	-1.212177	1.885045	O	-1.93411800	-0.39765800	-0.54279400
O	-1.118553	1.729716	0.851461	O	-1.257996	-1.971755	0.260659	O	-2.598381	-0.389967	0.058726	O	0.21850400	2.23494100	-0.09366100
O	-2.473442	-2.906671	-1.982788	O	-1.725955	3.715777	0.107340	O	1.615273	3.536764	0.589209	O	3.40702700	-2.40159700	1.37475900
C	0.201880	-0.614249	2.095322	C	-0.047320	-0.944570	-2.185630	C	-0.793005	-0.352353	-2.240276	C	0.55588300	0.22999800	-2.22869300
C	-0.244340	-1.766491	4.149482	C	-0.895245	-1.048255	-4.432370	C	-1.080710	0.409861	-4.496442	C	1.77519200	0.03856500	-4.26874800
H	-0.283298	-2.868180	4.287275	H	-0.888222	-0.220870	-5.173944	H	-0.267754	0.845659	-5.117431	H	2.11200100	-0.98389300	-4.54552700
H	-0.913346	-1.316989	4.915562	H	-1.760431	-1.701460	-4.679858	H	-2.037941	0.837013	-4.865680	H	2.45379200	0.76673400	-4.75841600
C	1.179125	-1.202807	4.193906	C	0.429410	-1.809591	-4.365405	C	-1.074340	-1.122168	-4.485426	C	0.29858300	0.27153400	-4.59695200
H	1.346619	-0.497377	5.035042	H	0.340964	-2.875497	-4.863037	H	-2.021456	-1.568415	-4.857669	H	0.10797800	1.25571000	-5.08197500
H	1.958397	-1.992290	4.261539	H	1.227499	-1.358387	-4.994823	H	-0.247430	-1.560982	-5.083985	H	-0.13199000	-0.51299200	-5.25182900
C	-2.116970	-1.594075	2.553993	C	-2.312065	0.105974	-2.788512	C	-1.182037	2.129731	-2.734502	C	3.10361900	0.51043900	-2.22072400
C	-2.599656	-2.876292	2.179414	C	-2.527650	1.462960	-3.149587	C	-0.198202	3.133495	-2.929710	C	4.09779800	-0.50071100	-1.23405200
C	-3.990667	-3.058623	2.034218	C	-3.813025	2.013939	-2.968734	C	-0.547194	4.478507	-2.686298	C	5.37596200	-0.15140200	-1.65120300
H	-4.363579	-4.051061	1.728822	H	-3.975975	3.071853	-3.235599	H	0.222880	5.256176	-2.824850	H	6.14114800	-0.94204900	-1.57200600
C	-4.910639	-2.024548	2.278004	C	-4.888882	1.257013	-2.473561	C	-1.839985	4.856815	-2.285940	C	5.70600200	1.16355700	-1.27819600
C	-4.404746	-0.789600	2.733180	C	-4.662550	-0.108626	-2.206011	C	-2.814417	3.843946	-2.173037	C	4.72257900	2.15723300	-1.45045200
H	-5.109028	0.021094	2.984756	H	-5.503506	-0.737120	-1.867877	H	-3.848651	4.181155	-1.904982	H	4.97009500	3.20726000	-1.21973600
C	-3.028684	-0.554262	2.902540	C	-3.403888	-0.713072	-2.576571	C	-2.522935	2.489071	-2.408980	C	3.43403500	1.86703500	-1.93724500
C	-1.689316	-4.059166	1.928824	C	-1.436978	2.345749	-3.714347	C	1.215577	2.817829	-3.361695	C	3.84015700	-1.91944800	-2.58167600
H	-1.590000	-4.262196	0.840299	H	-0.967441	2.959730	-2.915489	H	1.898067	2.783693	-2.484678	H	4.50221500	-2.63049000	-2.04851600
H	-2.107474	-4.978234	2.388720	H	-1.852931	3.049471	-4.463745	H	1.602688	3.601872	-4.044087	H	4.05585100	-2.04111900	-3.66725700
H	-0.671018	-3.908236	2.343414	H	-0.628397	1.767141	-4.012030	H	1.295535	1.842214	-3.878299	H	2.79176400	-2.23691000	-2.42049600
C	-6.392819	-2.220912	2.060175	C	-6.244394	1.880115	-2.233193	C	-2.182695	6.297115	-1.981358	C	7.06467700	1.50478700	-0.70957400
H	-6.672019	-3.293839	2.060446	H	-6.375248	2.817494	-2.810655	H	-1.433595	6.997397	-2.402555	H	7.82367700	3.73896800	-0.96805200
H	-6.700405	-1.796848	2.107954	H	-6.372057	2.131072	-1.157104	H	-2.218284	6.467007	-0.882944	H	7.02348300	1.56954300	0.40014200
H	-6.993230	-1.705965	2.838203	H	-7.068240	1.188068	-2.504071	H	-3.719265	6.574438	-2.383229	H	7.42749300	2.48751200	-1.07581200
C	-2.551773	0.762814	3.460249	C	-3.243352	-2.195157	-2.145647	C	-3.618141	1.456046	-2.324617	C	2.46327800	2.99139000	-2.19449900
H	-1.867001	0.620347	4.323091	H	-2.797978	-2.703016	-3.027906	H	-3.647478	0.809273	-3.227149	H	2.00860200	2.91113900	-3.20429400
H	-3.407235	1.372972	3.809073	H	-4.225000	-2.668839	-1.950495	H	-6.091010	1.940526	-2.226714	H	2.97440300	3.97175200	-2.12921500
H	-2.000574	1.349672	2.695516	H	-2.580157	-2.403898	-1.880077	H	-3.475168	0.781319	-1.454751	H	1.63030800	2.98876600	-1.46295700
C	2.473836	0.342632	2.776888	C	1.919805	-2.567436	-2.583921	C	-0.943052	-2.863718	-2.753405	C	-1.77094500	0.49590100	-3.28020400
C	3.717252	-0.229388	2.418319	C	3.248802	-2.122467	-2.673787	C	0.224409	-3.653181	-2.894766	C	-2.67724900	-0.55354200	-3.57479300
C	4.861234	0.595542	2.424856	C	4.294774	-3.046301	-2.554968	C	0.110407	-5.046608	-2.735601	C	-4.04156600	-0.24002300	-3.72900100
H	5.827825	0.158954	2.120620	H	5.335381	-2.701608	-2.589072	H	1.019749	-5.664058	-2.829869	H	-4.74680300	-1.06073400	-3.94545800
C	4.809222	1.941832	2.826525	C	4.053324	-4.383310	-2.196653	C	-1.118543	-5.668475	-2.443455	C	-4.52942900	1.07303800	-3.60998600
C	3.567381	2.460135	3.241823	C	2.712636	-4.798458	-2.057153	C	-2.607896	-4.853387	-2.330561	C	-3.59895200	2.09624200	-3.34889400
H	3.502492	3.511101	3.568463	H	2.495877	-5.842860	-1.775840	H	-3.237062	-5.317928	-2.111705	H	-3.94493600	3.13942200	-2.73408500
C	2.390425	1.692946	3.222936	C	1.635040	-3.918915	-2.248240	C	-2.204148	-3.455543	-2.491712	C	-2.22236100	1.84081100	-3.19594200
C	3.873013	-1.699667	2.105130	C	3.586479	-0.694306	-3.120075	C	1.576539	-3.025764	-3.120639	C	-2.23910300	-1.99076700	-3.71517800
H	2.913088	-2.177304	1.834888	H	2.771919	-0.188380	-3.673937	H	1.555617	-2.210097	-3.872960	H	-2.59606200	-2.42607200	-4.67262300
H	4.287539	-2.248922	2.980103	H	4.508929	-0.642182	-3.733020	H	2.319190	-3.778429	-3.450984	H	-2.67302100	-2.61034900	-2.90156200
H	4.582241	-1.857493	1.268064	H	3.767365	-0.096602	-2.200982	H	1.936453	-2.580875	-2.168664	H	-1.14326800	-2.11354700	-3.65681000
C	6.037698	2.821351	2.784032	C	5.190088	-5.347698	-1.942417	C	-1.202074	-7.162402	-2.224003	C	-6.00720600	1.36667700	-3.73299000
H	6.044654	3.434837	1.856256	H	5.339912	-5.503539	-0.851445	H	-0.100549	-7.415849	-1.158843	H	-6.53381300	1.11458500	-2.78633000
H	6.673285	2.226327	2.795064	H	6.147695	-4.974312	-2.357784	H	-0.453222	-7.709802	-2.832317	H	-6.48018200	0.76477700	-4.53653600
H	0.650500	3.283818	3.638776	H	4.987199	-6.345270	-2.385001	H	-2.207420	-7.558887	-2.473031	H	-6.19864900	-0.37493800	-3.94481500
C	1.076792	2.303079	3.640361	C	0.216394	-4.384693	-2.034501	C	-3.454977	-2.621444	-2.362762	C	-1.27040800	2.99027000	-2.97082100
H	0.1419452	2.436242	2.755322	H	-0.241064	-3.854905	-1.719099	H	-3.380747	-1.914889	-1.510417	H	-1.707708700	2.93343200	-1.97957700
H	1.232135	3.298244	4.099795	H	0.182748	-5.471655	-1.826411	H	-4.342937	-3.262188	-2.198774	H	-1.80354400	3.95902200	-3.02849700
H	0.529372	1.671004	4.371722	H	-0.433511	-4.190921	-2.915438	H	-3.647802	-2.010811	-3.271757	H	-0.45935300	3.01092800	-3.73022300
C	-1.455985	-1.055787	-0.231416	C	-1.138870	1.034419	-0.321215	C	-0.187726	1.526382	-0.111886	C	1.77225600	-0.37903400	0.30000400
H	-1.225516	-2.141767	-0.172820	C	-0.790268	1.877387	-0.961036	H	0.722412	1.760371	-0.711479	H	2.14688200	-1.20311400	-0.34612600
C	-2.773398	-0.850752	-0.826402	C	-2.324560	1.434927	0.428239	C	-0.574535	2.625407	0.759924	C	2.57612100	-0.16569600	-1.49560000
C	-3.308656	-1.864386	-1.701882	C	-2.634113	2.833178	0.609879	C	0.351735	3.682597	1.079518	C	3.44695600	-1.19223600	0.20132600
C	-4.599844	-1.718781	-2.249474	C	-3.795009	3.216427	1.314953	C	-0.061195	4.763647</					

H	-0.490324	1.192710	-5.069872	H	0.405053	1.498558	4.831253	H	0.764277	-0.156626	4.993682	H	-1.53613700	-0.69105200	4.81930200
C	-1.242166	2.815250	-3.836133	C	-0.535381	-0.458342	4.771383	C	-1.357091	-0.524529	4.711390	C	-1.55282500	1.42077800	4.31635800
H	-1.501085	3.480782	-4.673354	H	-0.658756	-0.558700	5.860087	H	-1.597339	-0.630282	5.779789	H	-1.96241300	1.76422700	5.27785200
C	-1.487672	3.254918	-2.505082	C	-1.004439	-1.503322	3.924637	C	-2.403437	-0.653854	3.751467	C	-1.23835400	2.38394000	3.31346500
C	-1.133494	2.352336	-1.442280	C	-0.816239	-1.335200	2.508085	C	-2.039759	-0.519148	2.367733	C	-0.71110600	1.88881500	2.07099300
C	-1.378780	2.647341	-0.055989	C	-1.341299	-2.263419	1.541276	C	-3.001244	-0.585237	1.306453	C	-0.30622400	2.75951400	1.00644900
C	-1.963290	3.900142	0.229729	C	-1.998724	-3.406821	2.051613	C	-4.347622	-0.807693	1.669484	C	-0.46679700	4.14805700	1.21016200
C	-2.287642	4.821141	-0.793853	C	-2.144961	-3.622731	3.440514	C	-4.727360	-0.970178	3.021734	C	-1.01152900	4.65706300	2.41150900
H	-2.729980	5.789584	-0.521450	H	-2.655137	-4.530841	3.790960	H	-5.784292	-1.151057	3.262342	H	-1.12757000	5.74363800	2.52794400
C	-2.060689	4.508899	-2.133140	C	-1.666322	-2.690679	4.360814	C	-3.779851	-0.895098	4.043119	C	-1.39000100	3.79771100	3.44281100
H	2.181115	1.773648	-0.832376	H	2.443203	-0.776683	1.262038	H	1.604942	-2.174122	1.174560	H	0.04928800	-2.83494100	-1.23498200
Cl	1.827874	2.835100	0.309759	Cl	1.768530	-2.236371	0.436967	Cl	-0.076331	-2.719199	0.272631	Cl	0.59778000	-3.55329400	-2.24338700

2d"	2d"→2d"bis			2d"bis	2d"bis→3b						
-4735.206600	-4735.1926596			-4735.2254131	-4735.2116757						
Ru -0.257136	0.310571	0.314015	Ru 0.301601	-0.128163	-0.354061	Ru 0.481761	-0.375502	0.091676	Ru -0.775449	-0.200854	0.300530
Cl 2.035482	2.170049	0.123469	Cl -0.303247	1.833294	-1.140319	Cl -3.458996	1.114923	-2.118392	Cl 5.259992	2.120093	0.340493
Cl 6.666148	0.962394	-2.455331	Cl -6.869549	0.758469	2.547745	Cl -7.331556	1.106048	1.686343	Cl 8.230156	-1.680616	-2.194187
Cl -2.287727	5.823272	-3.501182	Cl -0.332713	6.762918	0.669985	Cl -1.521838	6.282288	-0.833111	Cl 1.567968	6.168499	-1.455696
Cl -2.995162	4.353103	1.697213	Cl 1.396569	3.689143	-3.485610	Cl 0.029592	2.298099	-4.213988	Cl -1.268164	4.227247	2.772751
N -1.194996	-1.365546	2.738136	N 1.977725	-2.146175	-2.008449	N 2.095615	-2.694038	-1.131377	N -2.577712	-1.874762	2.189783
N 0.826836	-0.556991	3.058046	N -0.154047	-2.222993	-2.554117	N -0.060949	-3.126282	-1.173068	N -0.492627	-1.707235	2.878596
N 3.166242	-2.666726	-1.232474	N -2.635513	-2.183372	2.051383	N -2.690517	-1.026733	2.499288	N 3.152886	-2.235780	-1.368251
N -0.426101	1.356043	-1.538031	N -0.167579	1.546349	0.865264	N -0.052591	1.559817	0.839283	N 0.140923	1.161910	-1.059586
O 1.428203	-0.829148	-0.255347	O -1.723333	-0.713718	-0.068756	O -1.828315	-0.410972	-0.049567	O 2.943769	0.159614	-0.130020
O -1.509685	1.847522	0.857163	O 0.826444	1.386335	-1.591484	O 0.392042	0.710305	-1.666247	O -1.035158	1.586273	1.307840
O -1.644342	-2.909511	-2.327768	O 2.680053	-0.962206	3.198660	O 4.077929	0.471707	2.620767	O -3.615832	-0.870837	-3.060666
C -0.219640	-0.579221	2.172920	C 0.746785	-1.604801	-1.725678	C 0.860390	-2.171097	-0.814677	C -1.355869	-1.335647	1.881691
C -0.769076	-2.000837	4.005400	C 1.901968	-3.272732	-2.966701	C 2.038589	-4.080519	-1.640823	C -2.559377	-2.697797	3.419922
H -0.641909	-3.094920	3.861113	H 2.051682	-4.238102	-2.434728	H 2.469698	-4.786665	-0.896622	H -2.750268	-3.766016	3.174653
H -1.537047	-1.845520	4.791290	H 2.692930	-3.178519	-3.738162	H 2.629551	-4.174404	-2.575636	H -3.357024	-2.367449	4.118200
C 0.559037	-1.297459	4.310082	C 0.485443	-3.134532	-3.527892	C 0.537355	-4.297042	-1.850574	H -1.142161	-2.462873	3.968730
H 0.492003	-0.585794	5.164232	H 0.463177	-2.676913	-4.543777	H 0.546200	-4.302435	-2.925601	H -1.136365	-1.866117	4.908463
H 1.382636	-2.007236	4.528115	H -0.060442	-4.097612	-3.581245	H 0.164800	-5.240196	-1.400836	H -0.594509	-3.406747	4.172061
C -2.558810	-1.562506	2.322571	C 3.286368	-1.760388	-1.550365	C 3.385920	-2.066395	-1.105839	C -3.836800	-1.662090	1.537120
C -2.967916	-2.818281	1.797546	C 3.965116	-2.564155	-0.596307	C 4.312336	-2.415151	-0.088976	C -4.355441	-2.665223	0.680257
C -4.325997	-2.984204	1.454827	C 5.282708	-2.207072	-0.243395	C 5.610062	-1.868903	-0.152933	C -5.643847	-2.476158	0.139167
H -4.642748	-3.949862	1.025901	H 5.807539	-2.818756	0.509998	H 6.331513	-2.125587	0.641053	H -6.055377	-3.250472	-0.530270
C -5.282218	-1.971225	1.649037	C 5.945764	-1.108674	-0.821952	C 6.011085	-1.013820	-1.196547	C -6.415392	-1.334299	0.427815
C -4.855906	-0.770699	2.251884	C 5.259719	-0.366161	-1.083989	C 5.737466	-0.712394	-2.205832	C -5.865742	-0.357597	1.284413
H -5.595664	0.019033	2.467300	H 5.769592	0.478954	-2.296777	H 5.371575	-0.055607	-3.040351	H -6.453148	0.545611	1.520800
C -3.514193	-0.549202	2.615190	C 3.943232	-0.675822	-2.194050	C 3.764443	-1.226977	-2.189709	C -4.587763	-0.498151	1.855262
C -2.014947	-3.978173	1.639326	C 3.320288	-3.780699	0.025142	C 3.923225	-3.334139	1.046729	C -3.541288	-3.890934	0.330404
H -2.400635	-4.702222	0.895503	H 3.841216	-4.064279	0.960993	H 4.609109	-3.209266	1.907603	H -3.994021	-4.439383	-0.515223
H -1.911771	-4.537415	2.596637	H 3.383669	-4.661812	-0.652923	H 3.973882	-4.404925	0.746637	H -3.481132	-4.603651	1.186487
H -0.992861	-3.687986	3.178171	H 2.247459	-3.622590	0.267756	H 2.888285	-3.137620	1.396230	H -2.498624	-3.621407	0.061158
C -6.719676	-2.158447	1.220386	C 7.344039	-0.723425	-0.394017	C 7.400266	-0.417178	-1.234290	C -7.791100	-1.141192	-0.710767
H -7.008118	-3.229131	1.204706	H 7.889419	-1.581308	0.048932	H 8.085664	-0.924907	-0.526296	H -8.129524	-2.041354	-0.721792
H -6.8777430	-1.760682	0.193361	H 7.314720	0.081372	0.373269	H 7.375781	0.660934	-0.963521	H -7.800941	-0.681588	-0.881206
H -7.421640	-1.619724	1.889587	H 7.941070	-0.336766	-1.245628	H 7.844485	-0.483107	-2.249452	H -8.546565	-0.914917	0.611051
C -3.125507	0.721156	3.332027	C 3.260803	0.115994	-3.281814	C 2.788484	-0.892999	-3.290327	C -4.023926	0.558844	2.773425
H -2.496703	0.512115	4.223505	H 2.842371	-0.547163	-0.469055	H 2.344581	-1.809161	-3.735490	H -3.726173	0.131937	3.755251
H -4.026482	1.267793	3.673017	H 3.969945	0.814665	-3.767263	H 3.284365	-0.326170	-4.102318	H -4.767213	1.357257	2.964281
H -2.547328	1.395441	2.667424	H 2.413611	0.707712	-2.876694	H 1.941745	-0.283396	-2.907053	H -3.111833	1.026873	2.344236
C 2.012653	0.252745	3.024928	C -1.564902	-1.986194	-2.721208	C -1.498945	-3.066796	-1.203656	C 0.887853	-1.317127	3.020748
C 3.261897	-0.360971	2.754456	C -2.481866	-2.935724	-2.200304	C -2.237894	-3.765409	-0.217175	C 1.906981	-2.230298	2.641811
C 4.423756	0.435356	2.838564	C -3.853554	-2.740554	-2.456140	C -3.643508	-3.791443	-0.332769	C 3.248434	-1.848250	2.837747
H 5.398989	-0.030351	2.617395	H -4.574419	-3.471057	-2.050793	H -4.227587	-4.326697	0.435439	H 4.046330	-2.545578	2.531262
C 4.378778	1.793118	3.206547	C -4.328782	-1.654111	-3.217228	C -4.317096	-3.172541	-1.403115	C 3.599690	-0.613873	3.416409
C 3.121371	2.359767	3.500218	C -3.384665	-0.751220	-3.743061	C -3.544570	-2.515410	-2.382049	C 2.560613	0.236206	3.842390
H 3.063064	3.418895	3.803891	H -3.731093	0.096992	-4.357261	H -4.050243	-2.030753	-3.233677	H 2.812371	1.916568	4.332431
C 1.929585	1.616274	3.419008	C -2.001419	-0.897677	-3.517833	C -2.140788	-2.448045	-2.308433	C 1.202669	-0.092619	2.627168
C 3.689483	-1.832985	2.429446	C -2.013239	-4.126157	-1.398579	C -1.550309	-4.475991	0.926154	C 1.575462	-3.585099	2.060153
H 4.323255	-2.051892	1.910159	H -2.877361	-4.698367	-1.005539	C -2.292967	-4.871109	1.647911	H 2.499587	-4.163701	1.861672
H 2.532699	-2.203459	1.802139	H -1.365279	-3.830763	-0.543017	H -0.854060	-3.797427	1.463484	H 1.006536	-3.485475	1.110719
H 3.371432	-2.447485	3.357882	H -1.416441	-4.831867	-2.018579	H -0.949084	-5.343077	0.572888	H 0.950931	-4.191594	2.751880
C 5.637077	2.630583	3.269584	C -5.810279	-1.450190	-3.445616	H -5.826421	-3.195301	-1.501617	C 5.043329	-0.194690	3.564781
H 6.547170	2.000907	3.332863	H -6.372308	-2.403284	-3.370995	H -6.254363	-2.191992	-1.285599	H 5.295584	0.573164	3.801158
H 5.629093	3.314540	4.143490	H -6.014696	-1.006066	-4.441468	H -6.275323	-3.911003	-0.783865	H 5.738146	-1.047731	3.430910
H 5.739393	3.627878	2.633604	H -6.238191	-0.757085	-2.688782	H -6.164390	-3.474736	-2.521711	H 5.237734	0.259184	4.559097
C 0.601330	2.263845	3.733951	C -1.022910	0.085428	-4.115996	C -1.349773	-1.715801	-3.364018	C 0.125626	0.829674	4.191941
H -0.046159	2.345610	2.834127	H -0.497832	0.676796	-3.336602	H -0.906457	-0.782379	-2.954969	H -0.453255	1.284082	3.360650
H 0.745858	3.282931	4.142674	H -1.539456	0.793737	-4.792690	H -1.993019	-1.442297	-4.222663	H 0.566946	1.651924	4.787947
H 0.020475	1.680048	4.478940	H -0.231454	-0.424603	-4.705771	H -0.068898	-2.326191	-3.752222	H -0.599088	0.294555	4.842292
C -1.342624	-1.052829	-0.349194	C 1.857370	-0.384582	0.645309	C 2.268836	-0.081735	0.603321	C -2.345109	-0.323151	-0.686115
H -0.940746	-2.075468	-0.173312	H 1.960850	-1.456648	0.919200	H 2.689898	-0.851349	1.281195	C -2.626351	-1.355344	-0.980514
C -2.490605	-0.996397	-1.239747	C 2.749461	0.518029	1.361866	C 3.134369	1.092400	0.528057	C -3.169361	0.694890	-1.329525
C -2.680032	-2.045140	-2.209845	C 3.238143	0.154422	2.666804	C 4.100169	1.338690	1.571052	C -3.861309	0.366463	-2.552236
C -3.853776	-2.077565	-2.992992	C 4.191581	0.965423	3.318178	C 4.965563	2.451041	1.488243	C -4.696474	1.323222	-3.169119
H -4.014824	-2.880261	3.726309	H 4.573124	0.692271	4.312158	H 5.699414	2.652373	2.281014	H -5.223714	1.086867	-4.103629
C -4.818763	-1.064539	-2.851971	C 4.652784	2.142150	2.700846	C 4.891787	3.324589	0.388848	C -4.854489	2.597802	-2.598224
H -5.725167	-1.099600	3.478174	H 5.393983	2.766649	3.225625	H 5.573557	4.189572	0.345711	H -5.508707	3.330503	-3.097982
C -4.637567	-0.014941	-1.932283	C 4.179443	2.523128	1.432813	C 3.962934	3.102129	-0.641965	C -4.188227	2.938890	-1.408529
H -5.500641	0.771294	-1.826348	H 4.550291	3.440934	0.951361	H 3.912374	3.782543	-1.505794	H -4.318622	3.935951	-0.960918
C -3.481317	0.014328	-1.141680	C 3.235343	1.717142	0.781095	C 3.097231	2.003948	-0.559444	C -3.351816	1.997434	-0.796293
H -3.338255	0.798868	-0.385399	H 2.883152	1.978100	-0.226358	H 2.382925	1.798827	-1.366937	H -2.838728	2.236510	0.144211
C -1.729528	-4.122894	-3.118252	C 3.119663	-1.515535	4.460348	C 4.950278	0.640967	3.760526	C -4.217278	-1.314622	-4.998184
C -2.273336	-3.892735	-4.063682	H 3.305919	-0.677359	5.171975	H 5.033851	1.729904	3.983247	H -4.228976	-0.457630	-5.011751
C -2.470906	-5.206762	-2.332272	C 4.404529	-2.326700	4.268248	C 6.39532	0.062268	3.473			

H	0.318463	1.534443	-4.840190	H	-1.300568	2.746438	3.826567	H	-0.782375	3.523415	3.502726	H	1.790198	1.638324	-3.979307
C	-0.777842	3.062679	-3.754460	C	-0.737311	3.996614	2.143174	C	-0.919795	4.169706	1.434179	C	1.404597	3.204875	-2.526152
H	-0.910298	3.735791	-4.614668	H	-0.961417	4.953991	2.636712	H	-1.261417	5.190918	1.660743	H	1.899784	4.006382	-3.094601
C	-1.319395	3.442970	-2.491037	C	-0.239326	4.007573	0.806703	C	-0.739829	3.791457	0.070666	C	0.816125	3.517235	-1.266973
C	-1.131594	2.528782	-1.396511	C	0.044046	2.733629	0.205903	C	-0.293210	2.445518	-0.181918	C	0.182096	2.440223	-0.556024
C	-1.662964	2.765403	-0.079373	C	0.563104	2.596948	-1.124304	C	-0.053982	1.934833	-1.509484	C	-0.457136	2.618216	0.721221
C	-2.346802	3.989115	0.113788	C	0.774223	3.788957	-1.853518	C	-0.274516	2.840564	-2.576530	C	-0.452456	3.928890	1.251243
C	-2.525145	4.915005	-0.939670	C	0.492282	5.055035	-1.290911	C	-0.726539	4.159443	-2.355407	C	0.173366	5.003633	0.577756
H	-3.067714	5.850369	-0.743196	H	0.669698	5.957741	-1.892221	H	-0.892591	4.820101	-3.218027	H	0.158073	6.003260	1.034170
C	-2.030872	4.649412	-2.217747	C	-0.000960	5.167278	0.010491	C	-0.957874	4.630148	-1.061189	C	0.797376	4.806435	-0.653723
H	2.228477	-3.101279	-0.685562	H	-1.621087	-2.432813	1.640907	H	-1.690393	-1.236302	2.176983	H	2.258627	-1.829615	-0.976860
Cl	1.227932	-4.301990	0.076573	Cl	0.020339	-3.220102	1.516456	Cl	0.273470	-1.597557	2.255637	Cl	0.037215	-2.213151	-0.846338

2b→2d*	2d*			2d*→3c	3c
-4735.1822894	-4735.2153304			-4735.1821947	-3339.0358833
Ru -0.09828800 -0.09430600 0.22202900	Ru 0.345265 0.063008 -0.258317	Ru 0.703379 0.251518 -0.413655	Ru 0.248736 -0.458410 0.626616		
Cl 0.11533000 4.02107700 2.73945000	Cl -4.664931 0.895657 -1.208155	Cl -3.519980 2.851780 -1.861317	Cl 3.831624 1.909423 3.401028		
Cl 2.89822200 6.69824300 -1.03217300	Cl -2.938417 6.032176 -1.773550	Cl -0.206370 7.114834 -1.149716	Cl 4.746913 4.540097 -1.280210		
O -0.20892700 1.91338800 0.71332500	Cl -4.932210 -5.663687 -0.512308	Cl -7.392951 -3.880808 -1.114357	N -1.446380 -2.309535 -1.226424		
N 0.69893400 2.06719100 -2.04691400	Cl -0.670960 -3.863082 2.273430	Cl -3.279853 -4.048072 2.457263	N 0.708727 -2.788492 -1.111110		
N 0.43081900 -1.23665900 2.88359600	N 1.526617 -0.520228 2.493688	N 1.048933 -1.217423 2.230252	N 1.104340 0.814996 -0.770776		
N -1.74855200 -0.91759900 2.66640700	N -0.534604 0.272119 2.649334	N -0.515401 0.351033 2.318307	O 1.681175 0.480666 1.796049		
C -4.86486500 1.06968600 2.11349600	N 0.266878 2.107618 -0.461106	N 1.268134 2.189411 -0.154617	O -2.986800 2.619223 -0.347777		
H -5.21680600 2.10531800 2.25397100	N -1.887552 -1.925801 -2.367809	N -2.936937 -1.375311 -1.912614	C -0.258885 -1.921512 -0.654697		
C -3.07671700 -0.56752500 2.23997800	O -1.785927 0.367023 -0.421371	O -1.153473 1.267935 -0.785530	C -1.303322 -3.477200 -2.125446		
C -3.53365100 0.76443900 2.44212200	O -0.157696 -2.075098 -0.122354	O -1.868424 -2.244822 0.428977	H -1.583527 -3.200716 -3.166342		
C -5.28921700 -1.22001800 1.47703300	O 4.573838 0.922782 -1.720828	O 5.079622 -0.236953 -1.612842	H -1.986371 -4.293102 -1.808717		
H -5.97756700 -2.00140200 1.11309100	C 0.482852 0.010460 1.757261	C 0.505415 -0.154833 1.540457	C 0.183630 -3.853117 -1.986866		
C -3.96144200 -1.57996800 1.78939800	C 1.143960 -0.817692 3.890776	C 0.397353 -1.423945 3.542249	H 0.333787 -4.852185 -1.521335		
C -3.53492800 -3.02344100 1.64098100	H 1.922276 -0.461444 4.597084	H 1.071284 -1.077918 4.361129	H 0.720804 -3.856023 -2.959442		
H -4.05915500 -3.67502000 2.37347600	H 1.037135 -1.916705 4.026707	H 0.181858 -2.497925 3.703912	C -2.778221 -1.846675 -0.938000		
H -2.44647500 -3.15522900 1.78969900	C -0.193827 -0.085675 4.042466	C -0.874782 -0.586137 3.408095	C -3.405813 -0.914709 -1.801510		
H -3.79094100 -3.40667300 0.63113900	H -0.988612 -0.723286 4.481595	H -1.737012 -1.212635 3.091545	C -4.735812 -0.532763 -1.527849		
C -5.75923000 0.09684100 1.61886000	C -0.120807 0.832798 4.668043	H -1.139771 -0.302026 4.328664	H -5.224859 0.196234 -2.195727		
C -2.60956900 1.81924000 2.98797900	C 2.925506 -0.668686 2.173983	C 2.211450 -0.2013061 1.945376	C -5.452833 -1.055779 -0.438174		
H -3.13612200 2.78453600 3.11652900	C 3.784371 0.442110 2.267192	C 3.505331 -1.480079 2.197516	C -4.816550 -2.026085 0.369970		
H -1.74206400 1.98374800 2.31490900	C 5.174732 0.270600 2.408295	C 4.626606 -2.305568 1.987778	H -5.371526 -2.468581 1.211179		
H -2.19226900 1.52937300 3.97677800	H 5.835510 1.134188 2.453822	H 5.631441 -1.888172 2.169703	C -3.496599 -2.445222 0.136334		
C -7.17532300 0.47330000 1.24650200	C 5.742249 -0.969958 1.917531	C 4.500997 -3.646109 1.575270	C -2.702412 -0.313797 -2.996951		
H -7.64521600 1.11129800 2.02397100	C 4.868885 -2.051647 1.760492	C 3.203060 -4.157446 1.389097	H -2.426181 0.743915 -2.796621		
H -7.81545800 -0.42008700 1.10204000	H 5.285911 -3.034315 1.422718	H 3.078544 -5.209646 1.082298	H -3.363105 -0.313058 -3.888444		
H -7.19155900 1.05564700 0.29946300	C 3.470750 -1.934885 1.832305	C 2.046450 -3.372624 1.568665	H -1.775720 -0.860674 -3.256519		
C -0.54207000 -0.80089700 2.01000800	C 3.230487 1.788166 2.808701	C 3.695920 -0.083540 2.740704	C -6.858206 -0.593868 -0.126511		
C -0.09047100 -1.50672100 4.23748600	H 4.045600 2.513419 2.999343	H 4.733613 0.269312 2.578577	H -7.343358 -0.125750 -1.006702		
H 0.26134900 -0.72328900 4.94599100	H 2.608447 1.728781 3.726916	H 3.506459 -0.048919 3.836768	H -6.848475 0.160673 0.690661		
H 0.27861700 -2.48468200 4.60886500	H 2.575085 2.210333 2.018716	H 3.000717 0.641615 2.1277253	C -7.498857 -1.432423 0.216368		
C -1.61085900 -1.47665900 4.02809400	C 7.237605 -1.137828 1.766303	C 5.717457 -4.505719 1.316632	C -2.871496 -3.505710 1.006603		
C -2.07312600 -2.48856000 4.07835100	H 7.793051 -0.280107 2.195921	H 6.617777 -4.110889 1.829411	H -2.465312 -4.348558 0.406967		
H -2.13815900 -0.83409100 4.76327100	H 7.525044 -1.218777 0.965286	H 5.944312 -4.546628 0.228468	H -3.614764 -3.924852 1.712681		
C 3.77779700 -2.80281300 2.20770300	H 7.595669 -2.062983 2.624286	H 5.559010 -5.551137 1.652904	H -0.226271 -3.090404 1.595785		
H 4.19536400 -3.80129300 2.05767900	C 2.597765 -3.143877 1.269964	C 0.682128 -3.992652 1.388610	C 2.113819 -2.749511 -0.958721		
C 2.38057700 -2.67187400 2.42188100	H 2.333099 -3.614595 2.602551	H 0.321292 -4.443107 2.340987	C 3.017660 -2.083255 -1.656041		
C 2.70200100 -0.25632600 2.83296200	H 3.123591 -3.912522 1.030111	H 0.722349 -4.819997 0.651766	C 4.382214 -2.040655 -1.307989		
C 6.13472600 -1.84400500 2.15955700	H 1.647448 -2.883103 1.126789	H -0.094289 -3.269261 1.065339	H 5.080458 -1.503098 -1.971887		
H 6.43910500 -1.31955300 2.12798600	C -1.717631 1.087523 2.497330	C -1.126587 1.654386 2.293606	C 4.878854 -2.675203 -0.154283		
H 6.44079200 -2.90512400 2.06867500	C -1.601327 2.497666 2.652723	C 3.973476 2.756489 2.823109	C 3.973487 -3.414864 0.631308		
H 6.71363900 -1.38710400 2.98984200	C -2.775172 3.277746 2.594321	C -0.101253 4.021496 2.852369	H 4.348403 -3.968089 1.508573		
C 1.84855600 -1.38069900 2.66637900	H -2.681965 4.373761 2.675310	H -0.443002 4.877097 3.253092	C 2.598372 -3.487179 0.334570		
C 4.08540900 -0.44229000 2.67409200	C -4.052537 2.701002 2.475391	C -2.333158 4.219987 2.401094	C 2.584416 -1.499393 -2.981467		
H 4.74767400 0.43317700 2.77585800	C -4.134801 1.298009 2.396438	C -3.047586 3.096473 1.948616	H 3.007863 -0.487138 -3.138334		
C 6.46581900 -1.70233900 2.37733400	H -5.124651 0.820066 2.307178	H -4.089114 3.222415 1.609163	H 1.485723 -1.423982 -3.069760		
C 1.51445900 -3.91051500 2.36506800	C -2.993328 0.474387 2.406284	C -2.478030 1.806519 1.895412	H 2.950236 -2.134883 -3.818114		
H 1.81100500 -4.56594600 1.52128200	C -0.265257 3.171703 2.832841	C 0.987599 2.581257 3.400779	C 6.336187 -2.567269 0.232048		
H 0.44173400 -3.66947500 2.24359900	H -0.374762 4.273571 2.824455	H 1.337115 3.517383 3.878547	H 6.495348 -1.711812 0.924928		
H 1.62478900 -4.51327400 3.29378000	H 0.464262 2.895821 2.046928	H 1.729433 3.205317 2.624682	H 6.985198 -2.398502 -0.651109		
C 2.14435700 1.09975000 3.18022200	H 0.190486 2.892249 3.808169	H 1.013261 1.777192 4.166911	H 6.690134 -3.478756 0.755312		
H 1.36684400 1.42217300 2.46034300	C -5.301342 3.550575 2.414147	C -2.946335 5.602065 2.393702	C 1.693844 -4.345778 1.181525		
H 2.94098600 1.86768900 3.18827100	H -5.765078 3.492114 1.045650	H -2.517950 6.217587 1.572418	H 1.043129 -3.717111 1.298956		
H 1.66961500 1.10307000 4.18589500	H -5.085158 4.617155 2.623005	H -2.745255 6.144553 3.341391	H 2.288836 -5.016156 1.832121		
C 0.97265400 3.05233900 -1.12864000	H -6.066745 3.204563 3.140702	H -4.043899 5.563352 2.245056	H 1.021410 -4.977987 0.564921		
C 2.25785300 4.28113900 -2.84847400	C -3.154761 -1.015747 2.259903	C -3.312856 0.635627 1.444205	C -1.312243 0.556936 0.399493		
H 2.85638100 5.15628800 -3.14226100	H -3.170557 -1.269154 1.179367	H -4.022476 0.948212 0.653532	C -1.369723 1.121787 -0.561547		
C 1.99620300 3.24873900 -3.72902300	H -4.109175 -1.362520 2.704291	H -3.914022 0.230748 2.288903	C -2.385916 0.977416 1.293200		
H 2.38011400 3.25446300 -4.76007200	H -2.321578 -1.586773 2.711545	H -2.684389 -0.183399 1.048531	C -3.246678 2.062731 0.871482		
C 0.48044400 2.92788300 0.24581600	C 2.231326 -0.007069 -0.573458	C 2.497637 -0.399861 -0.613881	C -4.283230 2.516145 1.716049		
C 1.45540900 5.18804500 0.70537800	H 2.868372 0.818205 -1.049590	C 3.312240 0.297371 -0.316103	H -4.945319 3.333030 1.397588		
H 1.61639000 5.99945400 1.42838200	C 3.009305 -0.849767 -1.439483	C 3.082535 -1.512180 -1.350939	C -4.481338 1.930656 2.977443		
C 1.96876700 5.27187700 -0.58026500	C 4.239528 -0.365799 -2.013841	C 4.434820 -1.412674 -1.851356	H -5.293225 2.305648 3.621797		
C 1.19580700 2.17049300 3.27997700	C 4.999794 -1.197852 -2.864761	C 5.005331 -2.480667 -2.577292	C -3.648564 0.886072 3.414315		
H 0.94614100 1.35524300 -3.97935500	H 5.940854 -0.842164 -3.306809	H 6.030632 -2.412131 -2.966548	H -3.793717 0.434014 4.407595		
C 0.73162100 4.04384000 1.09503200	C 4.552965 -2.495502 -3.166174	C 4.259470 -3.646720 -2.820096	C -2.621085 0.428559 2.583089		
C 1.74517700 4.22352300 -1.52216400	H 5.160866 -3.128867 -3.832812	H 4.720962 -4.466448 -3.394714	H -1.949859 -0.375220 2.921110		
O -3.87011400 -1.34173900 -2.05052400	C 3.344171 -2.980970 -2.635373	C 2.944322 -3.772284 -2.393976	C -3.616915 3.854990 -0.760079		
C -1.88760900 -0.33709100 -0.38097900	H 2.994710 -3.995262 -2.883559	H 2.365971 -4.689342 -2.529164	H -3.787718 4.480094 0.145899		
H -2.25258100 -1.38324900 -0.46823400	C 2.584752 -2.157017 -1.797690	C 2.375175 -2.716059 -1.620740	C -4.951384 3.576157 -1.458885		
C -2.79876500 1.97229200 -0.89205800	H 1.632409 -2.507474 -1.373249	H 1.348645 -2.797968 -1.240513	H -4.786468 2.976741 -2.378056		
H -2.00875700 2.38171000 -0.24949600	C 5.697823 1.571797 -2.356845	C 6.405671 0.018899 -2.130880	H -5.441951 4.527837 -1.750936		
C -4.73032500 2.25596400 -2.32379300	H 5.764518 1.208462 -3.408024	H 6.480733 -0.432093 -3.146887	H -5.648751 3.016201 -0.804541		
H -5.46711100 2.90439900 -2.82543000	C 6.999072 1.257915 -1.612178	C 7.471623 -0.586126 -1.211968	C -2.611875 4.568240 -1.664112		
C -3.86915900 0.00986700 -1.88861800	H 6.937408 1.619416 -0.565109	H 7.413755 -0.128289 -2.020758	H -1.659659 4.749163 -1.127456		
C -2.83151600 0.56001900 -1.04592600	H 7.858921 1.757439 -2.104790	H 8.486432 -0.398768 -1.620021	H -3.018681 5.544814 -1.997285		
C -3.72946400 2.81463600 -1.50932300	H 7.203748 0.169086 -1.587105	H 7.343686 -1.681264 -1.100836	H -2.392751 3.958935 -2.565396		
C -3.67243500 3.90409100 -1.36170600	C 5.370409 3.064527 -2.376222	C 6.524028 1.536588 -2.261972	C 0.729226 1.021752 -2.044731		
C -4.80384200 0.86562100 -2.51168500	H 4.417703 3.248562 -2.911158	H 5.728221 1.936603 -2.920989	H -0.096454 0.399640 -2.414770		
H -5.59612500 0.45542100 -3.15287300	H 6.176318 3.630369 -2.886523	H 7.508543 1.809974 -2.693041	C 1.353444 1.980919 -2.877752		
C -4.70583600 -1.98119800 -3.04334500	H 5.273613 3.456068 -1.342113	H 6.432660 2.024158 -1.269256	H 1.004330 2.093379 -3.914943		
H -4.80773100 -1.29112000 -3.91150000	C 1.295593 2.974327 -0.463525	C 2.483396 2.646490 0.201105	C 2.398061 2.755927 -2.385550		
C -3.95059300 -3.22971600 -3.49777500	H 2.292544 2.556227 -0.699970	H 3.214809 1.895485 0.534583	H 2.909069 3.502751 -3.012119		
H -2.95121400 -2.95765300 -3.88951200	C 1.131707 4.351202 -0.741433	C 2.822969 4.017483 0.171201	C 2.808511 2.588358 -1.031186		
H -4.51537700 -3.75384000 -4.29568400	H 2.017846 5.003208 -0.726919	H 8.387561 4.317278 0.473585	C 2.111826 1.608187 -0.242983		
H -3.81324000 -3.93443500 -2.65140000	C -0.126661 4.855274 -1.037924	H 7.887619 4.958899 -0.238047	C 2.893939 1.374420 1.148134		
C -6.08822300 -2.29808100 -2.46421900	H -0.284869 5.919056 -1.268866	H 1.252977 6.031792 -0.279566	C 3.429158 2.147452 1.721004		
H -5.99623700 -3.00678800 -1.61515000	C -1.242541 3.969518 -1.059847	C			

C	3.86243500	-0.90263400	-1.19332900	H	-4.412813	-2.486933	-4.525636	H	-5.005758	-0.739073	-4.483012	
C	4.41432500	-2.06637400	-1.77256400	C	-4.097962	-3.528574	-2.639569	C	-5.470802	-1.996492	-2.768500	
C	3.64947800	-3.22432300	-1.91496700	H	-4.977983	-4.183092	-2.733089	H	-6.487204	-2.252329	-3.106055	
C	2.28943900	-3.26496100	-1.48278400	C	-3.290189	-3.658288	-1.473207	C	-5.015668	-2.540303	-1.531570	
C	1.75006600	-2.06495000	-0.90038500	C	-2.133240	-2.795903	-1.346814	C	-3.680655	-2.187668	-1.109226	
C	1.42797800	-4.39461200	-1.58459200	C	-1.217375	-2.807805	-0.205384	C	-3.038115	-2.627791	0.135463	
C	0.12645800	-4.29684600	-1.10827000	C	-1.604098	-3.759569	0.796090	C	-3.900352	-3.472227	0.921905	
C	-0.33035200	-3.08542900	-0.54078300	C	-2.715702	-4.620517	0.689253	C	-5.201001	-3.842245	0.528673	
H	5.45997600	-2.05383300	-2.11108200	H	-2.925887	-5.321115	1.509659	H	-5.790645	-4.495129	1.188705	
H	1.81194800	-5.32162300	-2.03554800	C	-3.553402	-4.580904	-0.422338	C	-5.761950	-3.392891	-0.673534	
H	-0.56481100	-5.15096500	-1.16456600	Cl	0.183178	0.096683	-2.825211	Cl	0.092928	-0.764538	-2.530205	
H	-1.35826700	-2.99346300	-0.16587700	H	-1.040275	-1.250066	-2.330034	H	-1.953409	-1.165805	-1.601155	

3c→4c	4c	4c→5b	2b ⁺ H ⁺
-3799.8051594	-3799.8498625	-3799.8345064	-4274.8328261
Ru -0.843410 -0.119006 0.621480	Ru 0.616047 -0.661336 -0.275674	Ru -0.686415 -0.341209 0.300333	Ru 0.141023 -0.058640 -0.168491
Cl 2.351425 -2.937191 3.417428	Cl -2.915013 -1.878202 -3.173387	Cl 4.284613 3.643468 2.446018	Cl -4.519074 2.139853 -0.429490
Cl 4.446958 -4.720411 -1.277322	Cl -7.410390 -0.809205 -0.315336	Cl 8.452851 1.476187 -0.325109	Cl -5.641120 -1.528107 3.431542
N -1.655635 2.641015 -0.438957	N 3.498563 0.401758 -0.396472	N -3.006325 -2.272512 0.469156	Cl -0.196959 6.771907 1.551522
N -3.390345 1.289393 -0.310483	N 3.311406 -1.772840 -0.056233	N -1.001260 -3.213034 0.413071	Cl 0.860808 4.115398 -3.097859
N -0.059930 -2.126148 -1.038139	N -2.698728 -0.674544 1.816848	N 3.524076 0.254417 -1.318110	N 1.248782 -1.913834 -2.355057
O 0.299112 -1.632745 1.665703	O -1.471691 -1.278201 -0.603828	O 2.579368 1.886935 0.615579	N -0.944597 -2.065758 -2.283114
O 3.306961 0.838691 -0.926125	O -0.714967 3.376798 1.251284	O -3.646523 2.936105 -1.112237	N -0.976108 -1.238808 1.092056
C -2.020778 1.337912 -0.164868	C 2.586072 -0.601847 -0.165530	C -1.663672 -1.998209 0.331579	N 0.144601 1.572253 1.253052
C -2.789072 3.494322 -0.854642	C 4.897404 -0.075847 -0.362151	C -3.281692 -3.722956 0.540167	O -1.816665 0.779815 -0.479693
H -2.707683 3.748385 -1.937179	H 5.405300 0.277680 0.565389	H -3.724574 -4.080160 -0.418764	O 0.769453 1.675468 -1.336840
H -2.782492 4.449035 -0.289707	H 5.467731 0.321275 -1.226554	H -4.010236 -3.941420 1.347305	O 3.288561 -1.966775 2.522293
C -4.001188 2.616911 -0.537391	C 4.734392 -1.601274 -0.400957	C -1.893568 -4.318051 0.804650	C 0.127468 -1.453934 -1.697562
H -4.539392 2.951496 0.377054	H 9.422211 -2.020846 -1.411496	H -1.747515 -4.577621 1.877956	C 0.943110 -2.822605 -3.483256
H -4.737888 2.568465 -1.365323	H 5.385095 -2.129273 0.326433	H -1.684678 -5.226028 0.202218	H 1.524719 -3.763234 -3.395172
C -0.362845 3.265610 -0.501340	C 3.297857 1.824240 -0.416290	C -4.146250 -1.406962 0.348623	H 1.230968 -2.344318 -4.445532
C 0.347295 3.257656 -1.730323	C 3.261334 2.529719 0.814664	C -4.686750 -1.149122 -0.938370	C -0.569211 -3.031232 -3.344944
C 1.529837 4.017554 -1.828812	C 3.203393 3.937464 0.778549	C -5.897249 -0.433666 -1.020735	H -1.132453 -2.811435 -2.975088
H 2.081265 4.016278 -2.784139	H 3.185826 4.490619 1.733191	H -6.328871 -0.241729 -2.017613	H -0.837394 -4.062082 -3.028655
C 2.012485 4.788332 -0.754230	C 3.187007 4.652655 -0.434962	C -6.573199 0.027102 0.127642	C 2.623133 -1.531881 -2.183721
C 1.277256 4.781282 0.448554	C 3.225972 3.918959 -1.637273	C -5.990932 -0.223212 1.385686	C 3.504530 -2.405173 -1.489281
H 1.634887 5.807585 1.302815	H 3.217260 4.459085 -2.599253	H -6.944743 0.142386 2.296296	C 4.861583 -2.043818 -1.384161
C 0.087005 4.045541 0.598705	C 3.292915 2.511827 -1.658666	C -4.787686 -0.944239 1.526145	H 5.544519 -2.712429 -0.834002
C -0.142152 2.447794 -2.909000	C 3.274514 1.791899 2.134033	C -3.968235 -1.599610 -2.189841	C 5.373603 -0.866333 -1.962203
H 0.499585 2.608825 -3.797193	H 3.250055 2.499935 2.985520	H -2.975570 -1.108138 -2.280610	C 4.485985 -0.055080 -2.698386
H -1.183895 2.707335 -3.193261	H 4.182813 1.162356 2.249208	H -4.556633 -1.356136 -3.095835	H 4.874153 0.848513 -3.198372
H -0.141893 1.359579 -2.681857	H 2.405165 1.105329 2.228552	H -3.779339 -2.694186 -2.194143	C 3.123148 -0.375345 -2.841002
C 3.276489 5.609935 -0.876490	C 3.119577 6.163950 -0.456639	C -7.905394 0.735358 0.014227	C 3.033599 -3.716854 -0.902217
H 3.714576 5.543537 -1.892168	H 3.352404 6.599854 0.535779	H -7.981684 1.324180 -0.922599	H 3.512714 -3.906416 0.078515
H 4.047287 5.271985 -0.150977	H 2.105948 6.517313 -0.747186	H -8.080804 1.420138 0.868518	H 3.308261 -4.567760 -1.563868
H 3.083911 6.682435 -0.659678	H 8.305011 6.592676 -1.193553	H -8.744400 0.004574 0.005392	H 1.936269 -3.744613 -0.760270
C -0.691577 4.099736 1.889024	C 3.375435 1.766010 -2.968105	C -4.201404 -1.211566 2.891434	C 6.823267 -0.477060 -1.793662
H -1.688142 4.572792 1.745459	H 4.357336 1.256361 -3.085846	H -4.123012 -2.300802 3.100027	H 7.470569 -1.362228 -1.633345
H -0.150740 4.692167 2.652537	H 3.258961 2.458422 -3.824880	H -4.828982 -0.763912 3.686566	H 6.949279 0.187397 -0.910694
O -0.880803 3.081444 2.291553	H 2.595386 0.977176 -3.034750	H -3.172536 -0.799989 2.977180	H 7.204896 0.076319 -2.675191
C -4.277567 0.157323 -0.374018	C 2.815631 -3.069162 0.330305	C 0.399740 -3.467178 0.200581	C 2.258588 0.469534 -3.752588
C -4.396816 -0.530634 -1.608872	C 2.826416 -3.402689 1.716607	C 0.833540 -3.771597 -1.119892	H 1.174362 0.291682 -3.599848
C -5.330812 -1.576533 -1.710828	C 2.360596 -4.671774 2.104910	C 2.191048 -4.080881 -1.324314	H 2.460951 0.236144 -4.820833
H -5.416437 -2.122748 -2.665713	H 2.353725 -4.925940 3.178363	H 2.529586 -4.322034 -2.346492	H 2.481900 1.551658 -3.640323
C -6.152999 -1.945031 -0.627682	C 1.911034 -5.622508 1.166515	C 3.119457 -4.114262 -0.263074	C -2.359769 -1.888123 -2.069138
C -6.033839 -1.215979 5.70265	C 1.988100 -5.289226 -0.197929	C 2.644552 -3.863019 1.037484	C -3.075435 -2.844791 -1.308869
H -6.675322 -1.481346 1.427575	H 1.686768 -6.034499 -0.953346	H 3.344526 -3.920697 1.887947	H -4.476648 -2.704361 -1.210105
C -5.116481 -0.156699 0.723526	C 2.457276 -4.035509 -0.645447	C 1.291981 -3.560170 1.302790	H -5.040009 -3.433675 -0.604603
C -3.546190 -0.141280 -2.795763	C 3.350870 -2.434993 2.751127	C -0.137222 -3.788909 -2.276478	C -5.173000 -1.675987 -1.869032
H -3.706444 -0.833445 -3.646143	H 3.357929 -2.900522 3.756340	H -0.497124 -2.762905 -2.499238	C -4.429643 -0.768197 -2.653866
H -2.465384 -0.139705 -2.540701	H 2.716528 -1.526340 2.799414	H -1.028488 -4.414935 -2.059003	H -4.956875 0.038979 -3.187963
H -3.779867 0.885178 -3.155330	H 4.388776 -2.110115 2.522613	H 0.343996 -4.190182 -3.190153	C -3.032852 -0.853602 -2.774552
C -7.110092 -3.110607 -0.737936	C 1.359683 -6.957478 1.615248	C 4.580856 -4.409623 -0.516033	C -2.398945 -0.026306 -0.649494
H -4.615846 -4.056913 -0.425038	O 0.272297 -6.882326 1.838471	H 5.069404 -4.854928 0.373998	H -2.861155 -4.253145 0.331429
H -7.636521 -3.255735 -1.779223	H 1.856246 -7.316631 2.540026	H 5.137757 -3.478106 -0.761122	H -1.317168 -3.857645 -0.486360
H -7.997372 -2.976582 -0.086264	H 1.478854 -7.734868 0.833526	H 4.716902 -5.104733 -1.369869	H -2.508254 -4.943418 -1.270275
C -5.049946 0.610362 2.022588	C 2.633688 -3.787521 -2.124437	C 0.822780 -3.415225 2.730857	H -6.672735 -1.535146 -1.753045
H -4.001274 0.804941 2.329154	H 2.266981 -2.786640 -2.432068	H 0.128758 -2.560232 2.860713	H -6.945236 -0.538917 -1.344300
H -5.549705 0.048515 2.836037	H 2.087960 -4.547739 -2.717375	H 1.682137 -3.260952 3.412479	H -7.110695 -2.308318 -1.092093
H -5.567762 1.592863 1.942922	H 3.707054 -3.861519 -2.414032	H 0.300001 -4.337401 3.070624	H -7.163017 -1.617332 -2.746473
C 0.791445 0.705007 0.268114	C 0.272353 1.148816 -0.046195	C -1.979672 0.934416 -0.071636	C -2.278861 0.147567 -3.616889
H 0.969203 0.820689 0.828009	H 0.813581 1.685138 0.758664	H -3.016725 0.689050 -0.367191	H -1.758079 0.874697 -2.959094
C 1.988324 0.913456 1.062028	C -0.784002 1.949600 -0.656205	C -1.615966 2.338600 -0.025899	H -2.969114 0.717042 -4.628569
C 3.280520 1.015966 0.424010	C -1.255922 3.133159 0.023940	C -2.892861 3.364470 -0.531971	H -1.518365 -0.334815 -4.266354
C 4.432637 1.250105 1.204862	C -2.256596 3.935507 -0.564658	C -2.110754 4.720226 -0.431928	C 1.802807 -0.740383 0.513376
H 5.421393 1.338045 0.734501	C -2.623318 4.837775 -0.056249	H -2.778058 5.517744 -0.786568	H 1.866301 -1.835428 0.693066
C 4.329603 1.360970 2.602170	C -2.805021 3.581677 -1.810201	C -0.863092 5.069208 0.114564	C 2.955758 -0.078565 1.107514
H 5.244024 1.538332 3.191558	H -3.587446 4.221051 -2.250485	H -0.587502 6.134752 0.174239	C 3.734360 -0.745275 2.128387
C 3.086181 1.232408 3.245646	H -2.368891 2.428037 -2.483758	C 0.026548 4.082384 0.576395	C 4.860826 -0.103057 2.689363
H 3.015424 1.298438 4.341983	H -2.801364 2.151894 -3.457586	H 1.013328 4.337685 0.988768	H 5.456219 -0.593571 3.471193
C 1.938732 1.001395 2.480933	H -1.379397 1.623912 -1.905750	H -0.359679 2.741988 0.510371	C 5.235266 1.178655 2.256234
H 0.955418 0.879386 2.958729	H -1.017768 0.720156 -2.491944	H 0.347146 1.986500 0.895194	H 6.116659 1.659671 2.709583
C 4.561876 0.759065 -1.645394	C -1.113859 4.524466 2.033800	H -4.599521 3.878427 -1.657563	C 4.501818 1.845056 1.256135
H 5.302383 0.237057 -0.997603	H -2.218783 4.645292 1.944808	H -4.038235 4.719402 -2.124963	H 4.809751 2.843714 0.911274
C 5.076649 2.156478 -2.002178	C -0.410438 5.793038 1.542092	C -5.511560 4.412258 -0.549103	C 3.379617 1.219437 0.706234
H 4.360508 2.669901 -2.675740	H 0.688878 5.676920 1.631043	H -0.678517 3.578259 -0.086876	H 2.815072 1.717876 -0.092001
H 6.054447 2.085807 -2.522055	H -0.723027 6.669055 2.147334	H -6.236576 5.145029 -0.960021	C 3.974884 -2.724849 3.561340
H 5.211830 2.787692 -1.101641	H -0.646429 6.007130 0.480729	H -4.929673 4.915514 0.248880	H 4.292056 -2.011014 4.354492
C 4.294077 -0.105752 -2.875723	C -0.774008 4.181981 3.483669	C -5.356849 3.132173 -2.753876	C 5.194729 -3.448543 2.987426
H 3.958672 -1.119011 -2.579279	H -1.294878 3.256892 3.800864	H -4.659550 2.769440 -3.535156	H 4.882884 -4.200364 2.233023
H 5.217446 -0.206625 3.481692	H -1.080212 5.007721 4.157638	H -6.102438 3.800565 -3.230492	H 5.738500 -3.981033 3.794213
H 3.508662 0.353678 -3.510800	H 0.317312 4.021025 3.600234	H -5.887220 2.256179 -2.328240	H 5.904698 -2.747032 2.505834
C -0.206289 -2.234366 -2.369032	C -3.196431 -0.357489 3.018882	C 3.851617 -0.588400 -2.307694	C 2.935168 -3.676946 4.146260
H -1.161461 -1.874743 -2.782222	H -2.462036 -0.257527 3.818890	H 3.014812 -1.096430 -2.807025	H 2.069151 -3.117109 4.551977
C 0.787910 -2.831459 -3.174192	C -4.585974 -0.184903 3.179076	C 5.215541 -0.766746 -2.626724	H 3.381429 -4.268604 4.970497
H 0.645589 -2.891429 -4.263063	H -4.992933 0.079991 4.165111	H 5.494211 -1.451447 -3.440243	H 2.571362 -4.385193 3.373280
C 1.909971 -3.382559 -2.561290	C -5.419296 -0.372297 2.077771	C 6.186212 -0.068649 -1.908904	C -0.551064 -2.264592 1.851536
H 2.682628 -3.898515 -3.152088	H -6.510540 -0.260351 2.171398	H 7.255279 -0.191378 -2.142773	H 0.494015 -2.575992 1.720261
C 2.076514 -3.310573 -1.147863	C -4.889052 -0.721632 0.803270	C 5.826125 0.823234 -0.855587	C -1.384152 -2.903802 2.800204
C 1.060300 -2.602851 -0.395376	C -3.449766 -0.855547 0.690678	C 4.412551 0.966403 -0.575071	H -0.973940 -3.736128 3.390480
C 1.137416 -2.383592 1.041360	C -2.742031 -1.190204 -0.541383	C 2.325587 1.831526 0.458339	C -2.692115 -2.472320 2.975539
C 2.223144 -3.061877 1.685136	C -3.626763 -1.434435 -1.649162	C 4.836909 2.559929 1.191804	H -3.361001 -2.942844 3.715565
C 3.205521 -3.775034 0.971388	C -5.028478 -1.319388 -1.595807	C 6.214475 2.436022 0.939469	C -3.184734 -1.393411 2.187500
H 4.036032 -4.234638 1.526228	H -5.632867 -1.509416 -2.458449	C 6.917735 3.026037 1.545488	C -2.285691 -0.795278 1.229090
C 3.560898 -3.882145 -0.422402	C -5.660494 -0.960177 -0.365118	H 6.716828 1.586514 -0.060483	C -2.676153 0.298961 0.371373
Cl -1.465292 0.687030 2.720422	Cl 0.852255 -0.823454 -2.634338	Cl -0.612509 -0.186220 2.631066	C -3.998217 0.789508 0.547698
H -1.186074 -2.234422 -0.347570	H -1.638834 -0.831554 1.752241	H 2.513189 0.402809 -1.072840	C -4.888644

			H	-0.442906	2.511562	4.460513
			C	-0.231309	3.904851	2.808644
			H	-0.392719	4.813160	3.407542
			C	0.011242	4.030898	1.410998
			C	0.213384	2.817155	0.668197
			C	0.496984	2.875006	-0.724327
			C	0.533571	4.103178	-1.379188
			C	0.306880	5.310929	-0.673593
			H	0.333403	6.268355	-1.211662
			C	0.060487	5.274716	0.696000
			H	0.922273	1.771785	-2.306981

2b ⁺ H→2b ⁺				2b ⁺	2b ⁺ →3c	3c→4c ⁺					
-4735.1873824				-4735.2186817	-4735.2151938	-3799.8422569					
Ru	0.30054800	-0.18673900	-0.26965700	Ru	0.569132	-0.342380	-0.537991	Ru	0.679814	-0.081821	0.531205
Cl	-4.71336800	0.65717700	-1.17016700	Cl	-4.550268	-0.923173	-1.120801	Cl	-0.462253	4.439804	2.855137
Cl	-5.17445200	-1.34113400	3.87288400	Cl	-4.442690	-1.258632	4.311003	Cl	-1.426363	6.017520	-2.255679
Cl	-3.46353000	6.12586400	0.13389600	Cl	-5.222848	4.882733	0.719584	N	0.439901	-2.611301	-1.208014
Cl	-0.91172300	3.73013800	-4.03364600	Cl	-4.279621	2.475701	-0.047899	N	2.520552	-1.879879	-0.107577
N	1.97637700	-2.54887200	-1.34610300	N	2.844910	-2.360000	-0.846037	N	0.284933	1.220776	-1.061163
N	-0.20281200	-2.89438800	-1.53231000	N	0.852963	-3.301809	-0.671114	O	0.354122	1.835413	1.587415
N	-0.57294900	-0.90790100	1.40913800	N	-0.118830	-0.655622	1.427678	O	-3.858528	-0.104886	-0.123507
N	-0.35562500	1.96922700	0.72597600	N	-0.857872	2.144592	-0.205074	C	1.225800	-1.640470	-0.599904
N	-1.76914600	0.02190900	-0.79323800	O	-1.524450	-0.698686	-0.828862	C	1.239251	-3.612034	-1.952272
O	0.36530400	2.03687300	-1.80258400	O	-1.772361	1.636541	-2.878747	H	0.799493	-3.804753	-2.953089
O	3.53012800	1.33568500	2.50355400	O	3.477900	2.039056	2.015324	H	1.241752	-4.579730	-1.400656
C	0.73778500	-2.01643200	-1.04498100	C	1.502657	-2.087950	-0.654618	C	2.623509	-2.965341	-2.013573
C	1.87110500	-3.85029800	-2.04020800	C	3.135529	-3.808165	-0.902223	H	3.445734	-3.661295	-1.748820
H	2.14304500	-4.67729200	-1.34261400	H	3.684921	-4.123814	0.013837	H	2.857379	-2.542538	-3.018094
H	2.56339900	-3.89125600	-2.90378900	H	3.781713	-4.041169	-1.773501	C	-0.905090	-3.037465	-0.908654
C	0.40166100	-3.87817600	-2.45583200	C	1.742189	-4.433631	-0.999645	C	-1.912603	-2.868496	-1.895576
H	0.26020200	-3.53315500	-3.50412900	H	1.509292	-4.814417	-2.019751	C	-3.177729	-3.450048	-1.678081
H	-0.07545900	-4.87118700	-2.33888300	H	1.586842	-5.269850	-0.287881	H	-3.953925	-3.329446	-2.452785
C	3.29337200	-2.16664500	-0.90379100	C	4.001208	-1.501504	-0.845217	C	-3.469369	-4.194377	-0.520107
C	3.71750000	-2.50572600	0.41150300	C	4.708614	-1.287964	0.367128	C	-2.445003	-4.355941	0.430405
C	5.02454100	-2.16390200	0.81385000	C	5.904058	-0.541988	0.329467	H	-2.640841	-4.953679	1.339266
H	5.34197900	-2.41024100	1.84146100	H	6.448122	-0.366173	1.272878	C	-1.157813	-3.810866	0.260319
C	5.93893400	-1.54922600	-0.05974200	C	6.427088	-0.030231	-0.871329	C	-1.668256	-2.066033	-3.152173
C	5.52126500	-1.31641800	-1.38391200	C	5.735772	-0.317074	-2.065870	H	-1.696408	-0.975112	-2.938016
H	6.23109100	-0.87474000	-2.10321500	H	6.147864	0.038246	-2.035273	H	-2.445739	-2.273728	-0.913862
C	4.22439600	-1.62687900	-1.83646100	C	4.541709	-1.061789	-2.086449	H	-0.679046	-2.275428	-3.607535
C	2.85023300	-3.30530100	1.35464500	C	4.242310	-1.867644	1.684491	C	-4.834856	-4.804908	-0.297190
H	3.07845900	-3.06678500	2.41327100	H	4.369811	-1.134091	2.506615	H	-5.433841	-4.826270	-1.229690
H	3.03840200	-4.39495400	1.22817100	H	4.840206	-2.764316	1.960827	H	-5.412700	-4.227723	0.457481
H	1.77228100	-3.14209300	1.18053300	H	3.178508	-2.171951	1.657566	H	-4.758520	-5.843970	0.085533
C	7.32619000	-1.15636000	0.39551800	C	7.686441	0.806456	-0.887180	C	-0.087677	-4.071236	1.288029
H	7.59955600	-1.64454100	1.35251800	H	8.305045	0.636984	0.017158	H	0.849086	-4.448047	0.825971
H	7.39615700	-0.05681000	0.54717600	H	7.439597	1.890374	-0.922649	H	-0.426414	-4.822526	2.027638
H	8.09443500	-1.42431800	-0.35942800	C	8.310471	0.589402	-1.778414	H	0.193904	-3.14148	1.833565
C	3.88558200	-1.43757100	-3.29396400	C	3.888474	-1.409066	-3.400436	C	3.767245	-1.290807	-0.584662
H	3.99644500	-2.39706200	-3.84940200	H	3.784085	-2.508461	-3.527970	C	4.354353	-0.230393	-1.319208
H	4.57939200	-0.71599400	-3.76913200	H	4.487326	-1.028453	-4.250688	C	5.625300	0.234798	-0.928292
H	2.84506300	-1.08091000	-3.44364200	H	2.866704	-0.980434	-3.465970	H	6.076665	1.069545	-1.098045
C	-1.60078800	-3.05881600	-1.20866300	C	-0.542180	-3.620659	-0.496837	C	6.326438	-0.323786	0.155301
C	-1.92516000	-3.82852300	-0.50460300	C	-0.977661	-4.076552	0.773768	C	5.735108	-1.406279	0.834523
C	-3.27839000	-4.08214600	0.23413300	C	-2.319778	-4.485505	0.917624	H	6.277506	-1.880042	1.669903
H	-3.52645400	-4.66756000	1.13559600	H	-2.670179	-4.816640	1.909560	C	4.473413	-1.918083	0.478609
C	-4.31591900	-3.62476500	-0.60240100	C	-3.216272	-4.484185	-0.166069	C	3.650815	0.443536	-2.472094
C	-3.95759400	-2.92257800	-1.76564600	C	-2.733979	-0.473400	-1.425314	H	3.051732	1.303410	-2.103217
H	-4.75014900	-2.56960200	-2.44587800	H	-3.417649	-4.074221	-2.290188	H	2.958986	-0.237456	-3.004913
C	-2.61608100	-2.63821400	-2.10436000	C	-1.409812	-3.641563	-1.622007	H	4.380759	0.838615	-3.206778
C	-0.85314100	-4.42487300	0.82851800	C	-0.033039	-4.185959	1.950004	C	7.662413	0.233463	0.591175
H	-1.30038600	-5.08604600	1.59637300	H	-0.578909	-4.088691	2.909279	H	7.523822	0.103930	1.354257
H	-0.26772800	-3.64802300	1.36008600	H	0.758794	-3.413144	1.924128	H	8.216262	0.685911	-0.256579
H	-0.12629800	-5.02922600	0.24515600	H	0.473248	-5.177657	1.968752	H	8.304036	-0.547184	1.048385
H	-5.76254300	-3.88538900	-0.24813500	C	-4.663189	-4.887062	0.002825	C	3.903919	-3.102318	1.219686
H	-6.44669500	-3.57323600	-1.06196500	H	-5.329923	-4.015940	-1.761019	H	3.017001	-2.790961	1.813498
H	-6.05193300	-3.32862800	0.66959200	H	-4.869636	-5.271467	1.021381	H	4.654221	-3.531873	1.911974
H	-5.94401700	-4.96146900	-0.04043300	H	-4.956088	-5.670605	-0.727882	H	3.576646	-3.912047	0.532554
C	-2.31451600	-1.93914100	-3.40481600	C	-0.957061	-3.193697	-2.988391	C	-1.172850	-0.412187	0.949712
H	-3.14699100	-1.26308000	-3.68211500	H	-0.924330	-2.084792	-3.044123	H	-1.647205	-0.517855	-0.502532
H	-2.20595600	-2.67947400	-4.22997800	H	-1.649400	-3.558020	-3.772314	C	-2.160205	-0.280648	1.552483
H	-1.38375900	-1.33943000	-3.35964200	H	0.063946	-3.549419	-3.235872	C	-3.558276	-0.129923	1.202670
C	2.00079200	0.10755100	0.53554600	C	2.120379	0.560332	0.807296	C	-4.526994	0.020385	2.218529
H	2.21080900	-0.31647400	1.54472800	H	2.629314	0.171670	0.995420	H	-5.590518	0.128723	1.966398
C	3.01381300	1.09990700	0.19123200	C	2.635727	1.897181	-0.216508	C	-4.141601	0.038826	3.569078
C	3.82403000	1.70116200	1.22105700	C	3.382103	2.626293	0.783591	H	-4.916517	0.158596	4.343857
C	4.81851900	2.64345400	0.88189900	C	3.920674	3.895744	0.485943	C	-2.788548	-0.082276	3.931620
H	5.44198000	3.10878900	1.65783700	H	4.489930	4.456610	1.239793	H	-2.488984	-0.503484	4.990350
C	5.01346600	3.00778900	-0.46218500	C	3.723764	4.468003	-0.783198	C	-1.819996	-0.228039	2.934833
H	5.79094600	3.74983200	-0.70696600	H	4.149174	5.462681	-0.993925	H	-0.755494	-3.168081	3.197797
C	4.23263100	2.43733900	-1.48304400	C	2.985525	3.787881	-1.766494	C	-5.183323	0.252985	-0.587613
H	4.39292200	2.72199900	-2.53415700	H	2.826485	4.239974	-2.757608	H	-5.592141	1.031977	0.096289
C	3.24906600	1.49888700	-1.15205800	C	2.444058	2.530822	-1.474679	C	-6.107880	-0.967702	-0.599947
H	2.63963000	1.03212400	-1.94117500	H	1.864266	1.982979	-2.231844	H	-5.708882	-1.743497	-1.284354
C	4.29193900	1.84495500	3.62199800	C	4.131212	2.714961	3.115521	H	-7.121277	-0.679799	-0.948476
H	4.50249400	2.92484600	3.44544400	H	3.864842	3.796094	3.069474	C	-6.207257	-1.419634	0.406850
C	5.60808900	1.07666900	3.77608100	C	5.652358	2.552067	3.308836	C	-4.993883	0.865765	-1.974532
H	5.40580600	0.00636900	3.98759400	H	5.931138	1.481850	3.127838	H	-4.323000	1.746271	-1.928293
H	6.20429600	1.49106000	4.61523200	H	6.142180	3.107046	3.865566	H	-5.970263	1.189887	-2.388708
H	6.22339300	1.13451100	2.85629700	H	6.059288	2.932943	2.081354	H	-4.550181	0.123750	-2.669991
C	3.38389000	1.72022900	4.84432500	C	3.538619	2.121252	4.392824	C	0.282807	0.921506	-2.368122
H	2.44771500	2.29488400	4.69869300	H	2.438182	2.248992	4.415278	H	0.575579	-0.105183	-2.624469
H	3.89678300	2.10979600	5.74701100	H	3.967418	2.621793	5.284603	C	-0.080523	1.851534	-3.371009
H	3.11799400	0.65837100	5.02675000	H	3.766088	1.037207	4.463626	H	-0.049335	1.539735	-4.425531
C	0.03891800	-1.39461100	2.50735200	C	0.613993	-0.655203	2.555835	C	-0.478271	3.132328	-3.010627
H	1.13092900	-1.47584400	2.46240700	H	1.696462	-0.512171	2.438418	H	-0.775445	3.878673	-3.761925
C	-0.67046300	-1.76925000	3.67257600	C	0.038794	-0.798594	3.840311	C	-0.505604	3.490154	-1.632829
H	-0.10413300	-2.15897300	4.53173400	H	0.697289	-0.787521	4.721736	C	-0.103191	2	

H	-1.37089700	3.09506400	3.76669700	H	-0.774331	3.567110	2.887287	H	1.322002	-3.461337	3.073513	
C	-1.93648300	4.01172300	1.87926400	C	-2.433394	3.768322	1.499564	C	2.939651	-3.703766	1.645255	
H	-2.57763500	4.79182400	2.31674800	H	-3.063834	4.386475	2.156183	H	3.603402	-4.268443	2.317450	
C	-1.77320300	3.96619000	0.46731500	C	-2.916667	3.439959	0.203098	C	3.380904	-3.431538	0.319832	
C	-0.91345100	2.93910800	-0.06608900	C	-2.070974	2.618645	-0.648708	C	2.484918	-2.679234	-0.535578	
C	-0.59261100	2.89261000	-1.46502300	C	-2.496847	2.319118	-1.998222	C	2.858657	-2.374625	-1.897792	
C	-1.24710200	3.78991500	-2.32205400	C	-3.747087	2.817211	-2.421072	C	4.105614	-2.838581	-2.355231	
C	-2.14856100	4.76577800	-1.82254600	C	-4.582014	3.591349	-1.585116	C	4.986592	-3.571871	-1.524182	
H	-2.63242700	5.45810600	-2.52543500	H	-5.547269	3.947923	-1.969895	H	5.950808	-3.906539	-1.931056	
C	-2.39013700	4.86673900	-0.45798400	C	-4.173260	3.899642	-0.295421	C	4.634372	-3.861604	-0.212097	
H	0.29992900	1.48373000	-2.68102200	H	-0.962144	1.202931	-2.495821	H	1.265437	-1.342794	-2.258058	
Cl	0.69053500	-0.13879800	-3.43872200	Cl	0.750654	-0.011155	-2.901118	Cl	-0.700345	-0.167692	-2.834377	

4c ⁺ →5b	2b	5b	4c ⁺
-3799.8326341	-4274.4098975	-2403.6708311	-3799.8496541
Ru -1.275090 -0.184288 0.751958	Ru 0.087051 -0.052250 -0.166373	Ru 0.625211 -0.753351 -0.448582	Ru 0.719838 -0.004917 0.575342
Cl 4.767770 -2.176085 2.887190	Cl -4.691726 1.937373 0.218974	N 0.428630 2.238676 -0.091365	Cl -1.339837 4.220487 2.993596
Cl 5.564529 -4.037299 -2.149089	Cl -5.399635 -2.234913 3.646579	N 2.473862 1.412807 0.124201	Cl -2.327299 5.753488 -2.116248
N -1.695231 1.222193 -1.956785	Cl -0.058809 6.712063 1.659862	O -3.505642 -1.368586 1.036066	N 0.854506 -2.476073 -1.216977
N -3.273454 -0.237475 -1.390281	Cl 0.697689 4.087550 -3.054069	C 1.148691 1.063479 -0.067826	N 2.828890 -1.504622 -0.967445
N 1.028257 -1.921529 -0.630969	N 1.188995 -1.858565 -2.417656	C 1.267036 3.422187 0.188293	N 0.134179 1.287398 -0.957685
O 2.043365 -1.621817 2.001134	N -1.009226 -1.812273 -2.452576	H 1.059101 3.814127 1.211027	O -0.026010 1.844017 1.746024
O 2.729456 1.955888 0.577838	N -0.916805 -1.434015 1.064272	H 1.044671 4.235273 -0.532858	O -3.755133 -0.383629 -0.221582
C -2.116071 0.374537 -0.949856	N 0.089389 1.505771 1.311686	C 2.691448 2.868043 0.048571	C 1.505366 -1.421905 -0.583847
C -2.661610 1.265608 -3.080354	O -1.970427 0.668319 -0.234078	H 3.153531 3.143743 -0.926723	C 1.779651 -3.361123 -1.958987
H -2.139660 1.216162 -4.057911	O 0.554016 1.603354 -1.326599	H 3.373284 3.205664 0.856082	H 1.389292 -3.576539 -2.975778
H -3.228617 2.224245 -3.050855	O 3.400336 -1.692820 2.461494	C -0.992888 2.433041 -0.145029	H 1.877772 -4.336040 -1.429970
C -3.551707 0.047946 -2.810270	C 0.085463 -1.334654 -1.777573	C -1.739167 2.412529 1.060586	C 3.082325 -2.561732 -1.967122
H -4.630514 0.246710 -2.972043	C 0.848994 -2.784151 -3.519863	C -3.116887 2.705714 0.996861	H 3.968926 -3.163975 -1.681303
H -3.274377 -0.828333 -3.441919	H 1.131138 -3.826441 -3.249230	H -3.703693 2.695529 1.930961	H 3.300940 -2.102080 -2.958560
C -0.794630 2.343503 -1.861393	H 1.409115 -2.515530 -4.439574	C -3.759514 3.011928 -0.218495	C -0.437927 -3.063466 -0.963880
C 0.388575 2.340445 -2.643359	C -0.664956 -2.599306 -3.657503	C -2.985168 3.017290 -1.396903	C -1.440339 -2.973763 -1.966006
C 1.176746 3.509070 -2.676830	H -0.951350 -2.032031 -4.571577	H -3.469495 3.250837 -2.360229	C -2.637919 -3.696813 -1.792297
H 2.089418 3.511041 -3.296485	H -1.224247 -3.556986 -3.671520	C -1.604367 2.740120 -1.388374	H -3.411318 -3.634805 -2.576733
C 0.825115 4.669743 -1.963514	C 2.587164 -1.621767 -2.187521	C -1.087250 2.042266 2.373385	C -2.866196 -4.504551 -0.663311
C -0.354867 4.637789 -1.193786	C 3.356028 -2.584642 -1.484270	H -1.819963 2.071343 3.203202	C -1.841117 -5.453539 1.299086
H -0.658177 5.537900 -0.632942	C 4.741782 -2.365681 -3.183953	H -0.255812 2.729930 2.638473	H -1.983961 -5.243741 1.079594
C -1.187280 3.504230 -1.136709	H 5.340168 -3.100870 -0.779701	H -0.654279 1.019693 2.331221	C -0.617477 -3.911485 0.166936
C 0.821430 1.119471 -3.420188	C 5.379950 -1.243765 -1.902369	C -5.239806 3.319888 -0.270003	C -1.265630 -2.112203 -2.194754
H 1.129585 0.300217 -2.737615	C 4.595517 -0.338975 -2.647824	H -5.683069 3.377096 0.744714	H -1.463149 -1.042936 -2.960851
H 1.682557 1.352152 -4.076869	H 5.081316 0.528860 -3.124974	H -5.793503 2.541111 -0.837825	H -1.973362 -2.411444 -3.939194
H 0.100700 0.710173 -4.058405	C 3.209899 -0.509034 -2.819633	H -5.435361 4.286347 -0.781214	H -0.238657 -2.162626 -3.609668
C 1.671459 5.921690 -2.023295	C 2.733539 -3.833555 -0.899985	C -0.801746 2.761556 -2.667123	C -4.162957 -5.261338 -0.482735
H 2.501580 5.819290 -2.743807	H 3.193350 -4.084461 0.077134	H 0.007320 3.523189 -2.631531	H -4.776237 -5.253790 -1.405942
H 2.108205 6.161259 -1.030060	H 2.891466 -4.711894 -1.564792	H -1.446786 3.000642 -3.535115	H -4.775462 -4.815570 0.331058
H 1.067205 6.802998 -2.326582	H 1.642103 -3.721868 -0.748920	H -0.309949 1.782753 -2.852795	C -3.980355 -6.319624 -0.201115
C -2.464679 3.547590 -0.335978	C 6.858857 -1.000209 -1.703969	C 3.592064 0.530616 0.338705	C 0.466601 -4.103979 1.195229
H -3.340208 3.213795 -0.931952	H 7.385918 -1.915842 -1.367958	C 3.892161 0.135306 1.671650	H 1.427241 -4.412930 0.730330
H -2.671495 4.575784 0.019340	H 7.028300 -0.215978 -0.934017	C 5.003932 -0.698938 1.886659	H 0.180359 -4.885432 1.925662
H -4.221608 2.876239 0.548637	H 7.343784 -0.646085 -2.637353	H 5.232600 -0.101875 2.917239	H 0.682143 -3.164428 1.751144
C -4.171725 -1.096702 -0.653150	C 2.417173 0.455756 -3.666424	C 5.829234 -1.132783 0.829523	C 3.997242 -0.759572 -0.553192
C -3.928797 -2.489880 -0.542619	H 1.808165 -0.075841 -4.428466	C 5.540752 -0.669626 -0.467607	C 4.436218 0.357452 -1.306322
C -4.871501 -3.282485 0.143617	H 3.089667 1.156259 -4.198968	H 6.196092 -0.965227 -1.304313	C 5.647151 0.977794 -0.943236
H -4.467695 -4.363784 0.239454	H 1.711781 1.052863 -3.049852	C 4.445142 0.175977 -0.740171	H 5.980847 1.858561 -1.517437
C -6.045812 -2.742340 0.697417	C -2.405331 -1.496019 -2.292873	C 3.049094 0.599511 2.835204	C 6.431876 0.517550 1.028906
C -6.276772 -1.361951 0.533623	C -3.258836 -2.453445 -1.691823	H 3.549707 0.377944 3.798209	C 5.990782 -0.624000 0.825170
H -7.196911 -0.915770 0.946938	C -4.642573 -2.183460 -1.651237	H 2.068034 0.078718 2.830921	H 6.602390 -1.022061 1.652432
C -5.365371 -0.523076 -0.132216	H -5.311302 -2.916088 -1.69103	H 2.848717 1.690872 2.793748	C 4.793601 -1.288351 0.498306
C -2.695225 -3.138840 -1.121083	C -5.187537 -1.009491 -2.202509	C 6.982436 -2.077251 1.083644	C 3.627479 0.932219 -2.442462
H -1.816282 -2.979253 -0.458778	C -4.309372 -0.095004 -2.819481	H 7.753367 -2.008308 0.289856	H 2.868191 1.636486 -2.041149
H -2.442252 -2.731770 -2.121139	H -4.716250 0.831000 -3.258408	H 6.629887 -3.132015 1.109357	H 3.089120 0.154966 -3.021327
H -2.836082 -4.232667 -1.224841	C -2.921686 -0.312339 -2.882808	H 7.470175 -1.875958 2.059609	H 4.272480 1.496890 -3.144916
C -7.017737 -3.608473 1.465906	C -2.722440 -3.749889 -1.127164	C 4.247539 0.724579 -2.133851	C 7.697758 1.236260 0.537802
H -6.774734 -3.603021 2.551391	H -3.478914 -4.244617 -0.487132	H 3.182220 0.715092 -2.439407	H 7.490551 1.960224 1.356548
H -6.982396 -4.664327 1.129158	H -1.807913 -3.592534 -0.520927	H 4.816841 0.129378 -2.874810	H 8.135537 1.810262 -3.303974
H -8.060858 -3.245679 1.364001	H -2.457212 -4.472001 -1.932080	H 4.618944 1.771667 -2.205334	H 8.467490 0.531727 0.914708
C -5.647175 0.955727 -0.246212	C -6.665594 -0.706813 -2.109450	C -1.216058 -0.702049 -0.336234	C 4.388445 -2.528258 1.257453
H -4.902869 1.525833 0.349770	H -6.843393 0.125346 -1.393861	H -1.761602 0.109832 0.179611	H 3.467050 -2.337984 1.849826
H -6.657040 1.195646 0.139980	H -7.246364 -1.583993 -1.760771	C -2.016699 -1.855740 -0.744891	H 5.192151 -2.842971 1.951559
H -5.591632 1.324329 -1.292515	H -7.079753 -0.384638 -3.088055	C -3.222452 -2.173878 -0.023909	H 4.174837 -3.384045 0.580940
C 0.147158 0.996668 0.787672	C -2.014513 0.698062 -3.540574	C -4.002019 -3.283867 -0.412170	C -1.078125 -0.621660 0.471073
C 0.852748 0.784774 -0.050412	H -1.336129 1.170650 -2.799630	H -4.926354 -3.536156 0.125759	H -1.523594 -0.679317 -0.543886
C 0.668084 1.922643 1.780972	H -2.603544 1.500081 -4.025872	C -3.599560 -4.090556 -1.491497	C -2.115970 -0.702454 1.489057
C 0.263631 2.400144 1.653032	H -1.368355 0.237059 -4.318308	H -4.222992 -4.953709 -1.775455	C -3.507112 -0.602307 1.099025
C 2.560472 3.269192 2.363100	C 1.795782 -0.644187 0.431508	C -2.423685 -3.801620 -2.203834	C -4.522621 -0.688568 2.075956
H 3.592507 3.635658 2.546857	H 1.928943 -1.731127 0.622838	H -2.117782 -4.426973 -3.056391	H -5.581643 -0.618124 1.792764
C 1.781146 3.671871 3.726240	C 2.940080 0.095960 0.958683	C -1.647066 -2.697693 -1.828741	C -4.189793 -0.856010 3.430601
H 2.222389 4.347117 4.477285	C 3.785254 -0.474155 1.977899	H -0.744267 -2.435109 -2.403368	H -4.999962 -0.916070 4.175721
C 0.459227 3.214910 3.871886	C 4.908090 0.238123 2.449819	C -4.679095 -1.589425 1.852584	C -2.845582 -0.934584 3.835910
H -0.146424 3.222716 4.737959	H 5.551549 -0.181516 3.235609	H -4.819286 -2.687541 1.979501	H -2.589204 -1.054005 4.899757
C -0.077391 2.348438 2.915087	C 5.214543 1.505594 1.922052	C -5.917280 -0.977258 1.190662	C -1.832676 -0.846796 2.876433
H -1.101561 1.962324 3.024933	H 6.093816 2.046954 2.307318	H -5.785780 0.118311 1.075545	H -0.772906 -0.895538 3.170878
C 4.413436 2.247828 4.430962	C 4.414597 2.076129 0.917257	H -6.819197 -1.158186 1.811335	C -5.096418 -0.131436 -0.704192
H 4.161010 2.210517 1.440481	H 4.664126 3.062266 0.496598	H -6.100200 -1.408868 0.186218	H -5.631105 0.484521 0.055055
C 4.348279 3.630021 -0.195492	C 3.292807 1.376097 0.455323	C -4.364138 -0.977673 3.216220	C -5.850319 -1.444234 -0.935813
H 3.890151 3.662905 -1.204945	H 2.670158 1.787352 -0.350224	H -3.459494 -1.443199 3.655005	H -5.328808 -2.054970 -1.700021
H 5.431636 3.849043 -0.294147	C 4.163078 -2.362465 3.491633	H -5.213476 -1.130067 3.912813	H -6.880408 -1.239696 -1.294156
H 3.889573 4.433407 0.414364	H 4.489836 -1.602753 4.238567	H -4.182145 0.112394 3.118908	H -5.923171 -2.047487 -0.009262
C 4.721830 1.121587 -0.421247	C 5.387334 -3.065303 2.896150	Cl 1.111336 -1.928172 1.502141	C -4.939132 0.693013 -1.980997
H 4.552017 0.138223 0.058961	H 5.070083 -3.853562 2.182255	Cl 1.023386 -0.570634 -2.751332	H -4.387595 1.632278 -1.778598
H 5.813923 1.263640 -0.551551	H 5.986583 -3.545622 3.697081		H -5.934385 0.952812 -2.395558
H 4.250556 1.109080 -1.425557	H 6.043884 -2.355706 2.354628		H -4.381820 0.119288 -2.750008
C 0.570738 -2.122527 -1.862859	C 3.197150 -3.330253 4.173272		C 0.230170 1.043382 -2.273645
H -0.445647 -1.751561 -2.070411	H 2.322854 -2.788795 4.585733		H 0.700252 0.089968 -2.547782
C 1.312065 -2.765004 -2.890544	H 3.705223 -3.861585 5.003485		C -0.239730 1.933996 -3.265815
H 0.860528 -2.917624 -3.882490	H 2.829331 -4.088569 3.451153		H -0.111879 1.668089 -4.325520
C 2.608071 -3.171391 -2.617827	C -0.404435 -2.530667 1.653457		C -0.861259 3.117004 -2.889561
H 3.324683 -3.656771 -3.381276	H 0.641932 -2.770949 1.419734		H -1.249611 3.829676 -3.631250
C 3.156252 -2.953375 -1.322422	C -1.145194 -3.329701 2.556458		C -1.004006 3.411176 -1.504206
C 2.297793 -2.338732 -0.324544	H -0.663744 -4.212927 3.002448		C -0.474765 2.470393 -0.547098
C 2.783877 -2.135580 1.023350	C -2.452390 -2.987562 2.874015		C -0.573339 2.722563 0.858376
C 4.128266 -2.468746 1.289723	H -3.050541 -3.580132 3.582106		C -1.218359 3.890201 1.296060
C 4.976367 -3.042551 0.313301	C -3.037781 -1.836869 2.269407		C -1.764108 4.817785 0.367508
H 6.010209 -3.297697 0.584010	C -2.228727 -1.084719 1.337743		H -2.264327 5.721773 0.740675
C 4.965628 -3.294353 -0.965236	C -2.727124 0.080010 0.630864		C -1.650476 4.583775 -0.996770
Cl -2.947118 0.796831 2.025356	C -4.048602 0.493658 0.972185		Cl 1.491143 -1.048768 2.584194
H 1.053769 -1.706424 1.837041	C -4.843622 -0.216943 1.890242		H 1.032589 2.037536 1.768882
Cl -0.937711 -1.981835 2.283710	H -5.859244 0.140771 2.111677		Cl 2.615252 1.802311 0.993231
	C -4.359165 -1.368252 2.518226		
	C -0.092038 1.404113 2.632087		
	H -0.137667 0.384268 3.044386		
	C -0.221164 2.545286 3.464130		

	H	-0.373554	2.408950	4.545110		
	C	-0.163030	3.814472	2.902728		
	H	-0.268767	4.720548	3.518041		
	C	0.033724	3.955997	1.497688		
	C	0.163693	2.746606	0.728336		
	C	0.380828	2.743976	-0.697746		
	C	0.437436	4.012836	-1.324308		
	C	0.299039	5.213617	-0.592537		
	H	0.348415	6.173402	-1.125784		
	C	0.104861	5.192126	0.789248		

ⁱ Instead of a normal ^{13}C measurement an APT measurement was performed

ⁱⁱ Gaussian 09, Revision A.1, M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G.A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H.P. Hratchian, A.F. Izmaylov, J. Bloino, G. Zheng, J.L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J.A. Montgomery, Jr., J.E. Peralta, F. Ogliaro, M. Bearpark, J.J. Heyd, E. Brothers, K.N. Kudin, V.N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J.C. Burant, S.S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J.M. Millam, M. Klene, J.E. Knox, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, R.L. Martin, K. Morokuma, V.G. Zakrzewski, G.A. Voth, P. Salvador, J.J. Dannenberg, S. Dapprich, A.D. Daniels, Ö. Farkas, J.B. Foresman, J.V. Ortiz, J. Cioslowski, and D.J. Fox, Gaussian, Inc., Wallingford CT, 2009.

ⁱⁱⁱ (a) A. Becke, *Phys. Rev. A* 1988, **38**, 3098-3100; (b) J.P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822-8824; (c) J.P. Perdew, *Phys. Rev. B*, 1986, **34**, 7406-7406.

^{iv} (a) U. Haeusermann, M. Dolg, H. Stoll and H. Preuss, *Mol. Phys.*, 1993, **78**, 1211-1224; (b) W. Kuechle, M. Dolg, H. Stoll and H. Preuss, *J. Chem. Phys.*, 1994, **100**, 7535-7542; (c) T. Leininger, A. Nicklass, H. Stoll, M. Dolg and P. Schwerdtfeger, *J. Chem. Phys.*, 1996, **105**, 1052-1059.

^v A. Schaefer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571-2577.

^{vi} D. Rappoport and F. Furche, *J. Chem. Phys.*, 2010, **133**, 134105.

^{vii} Y. Zhao and D.G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.

^{viii} (a) V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995-2001; (b) J. Tomasi and M. Persico, *Chem. Rev.*, 1994, **94**, 2027-2094.