Supplementary material

Coordination chemistry of pyrazine derivatives analogues of *PZA*: design, synthesis, characterization and biological activity.

M. Ogryzek^{a,}, A. Chylewska^{a,*}, A. Królicka^b, R. Banasiuk^b, K. Turecka^c, D. Lesiak^d, D. Nidzworski^{d,e}, M. Makowski^{a,*}

^a Laboratory of Intermolecular Interactions, Faculty of Chemistry, University of Gdansk, W. Stwosza 63, 80-308 Gdansk, Poland

^b Laboratory of Biologically Active Compounds, Intercollegiate Faculty of Biotechnology, University of Gdansk and Medical University of Gdansk, Abrahama 58, 80-307 Gdansk, Poland ^c Faculty of Pharmacy with Subfaculty of Laboratory Medicine, Al. Hallera 107, 80-416 Gdansk, Poland

^d Laboratory of Molecular Virology, Intercollegiate Faculty of Biotechnology, University of Gdansk and Medical University of Gdansk, Kladki 24, 80-822 Gdansk, Poland

^e Institute of Biotechnology and Molecular Medicine, Trzy Lipy 3 St., 80-172 Gdańsk, Poland

Keywords: Ru(III) complexes; Pyrazine derivatives; Spectrophotometric titration; Cyclic voltammetry; Biological assay



Fig.S1. FT-IR spectrum of [RuCl(*PAOX*)₂(OH₂)]Cl₂.



Fig. S2. FT-IR spectrum of [RuCl(*PTCA*)₂(OH₂)]Cl₂.



Fig. S3. FT-IR spectrum of [RuCl(*DPP*)(OH₂)₃]Cl₂.



Fig. S4. FT-IR spectrum of [RuCl₂(*ABMAP*)₂]Cl.



Fig. S5. ¹H NMR spectrum of [RuCl(*PTCA*)₂(OH₂)]Cl₂ in DMSO-d₆ at 500 MHz.



Fig. S6. ¹H NMR spectrum of [RuCl(PAOX)₂(OH₂)]Cl₂ in DMSO-d₆ at 500 MHz.



Fig. S7. ¹H NMR spectrum of [RuCl₂(*ABMAP*)₂]Cl in DMSO-d₆ at 500 MHz.



Fig. S8. ¹H NMR spectrum of [RuCl(*DPP*)(OH₂)₃]Cl₂ in DMSO-d₆ at 500 MHz.



Fig. S9. ESI/MS of $[RuCl(PTCA)_2(OH_2)]Cl_2$ showing the m/z²⁺ for the experimental (red columns) and simulated (black columns) spectra.



Fig. S10. ESI/MS of $[RuCl(PAOX)_2(OH_2)]Cl_2$ showing the m/z²⁺ for the experimental (red columns) and simulated (black columns) spectra.



Fig. S11. ESI/MS of $[RuCl_2(ABMAP)_2]$ Cl showing the m/z²⁺ for the experimental (red columns) and simulated (black columns) spectra.



Fig. S12. ESI/MS of $[RuCl(DPP)(OH_2)_3]Cl_2$ showing the m/z²⁺ for the experimental (red columns) and simulated (black columns) spectra.



Fig. S13. Structure od Ru(III) complexes studied with pyrazine derivatives: **a)** pyrazine-2-amidoxime (*PAOX*); **b)** pyrazine-2-thiocarboxamide (*PTCA*); **c)** 2-amine-5-bromo-(3-methyl)-amine-pyrazine (*ABMAP*); **d)** 2,3-bis-(2-pyridyl)pyrazine (*DPP*).



Fig. S14. a) Spectrophotometric titration curves of pyrazine-2-thiocarboxamide $(1.00 \cdot 10^{-4} \text{ mol } L^{-1})$ using a mixture of *PTCA* at the same concentration and RuCl₃ $(1.81 \cdot 10^{-3} \text{ mol } L^{-1})$. **b)** The A-diagram plot for Ru(III) ion with pyrazine-2-thiocarboxamide complexation process, major stoichiometry 1:2. **c)** Dependence of absorbance at 228 nm for *PTCA* as a function of molar ratio $n_{\text{Ru(III)}/n_{PTCA}}$.



Fig. S15. **a)** Spectrophotometric titration curves of 2,3-bis(2-pyridyl)pyrazine ($5.15 \cdot 10^{-5}$ mol L⁻¹) using a mixture of *DPP* at the same concentration and RuCl₃ ($9.29 \cdot 10^{-4}$ mol L⁻¹). **b)** The A-diagram for Ru(III) ion with 2,3-bis(2-pyridyl)pyrazine for complexation process, major stoichiometry 1:2. **c)** Dependence of absorbance at 326 nm for *DPP* as a function of molar ratio $n_{Ru(III)}/n_{DPP}$.



Fig. S16. a) Spectrophotometric titration curves of pyrazine-2-amidoxime $(1.70 \cdot 10^{-4} \text{ mol } \text{L}^{-1})$ using a mixture of *PAOX* at the same concentration and RuCl₃ $(2.76 \cdot 10^{-3} \text{ mol } \text{L}^{-1})$. **b)** The A-diagram for Ru(III) ion with pyrazine-2-amidoxime for complexation process, major stoichiometry 1:2. **c)** Dependence of absorbance at 268 nm for *PAOX* as a function of molar ratio $n_{\text{Ru(III)}/n_{PAOX}}$.



Fig. S17. a) Spectrophotometric titration curves of 2-amine-5-bromo(3-methylamine)-pyrazine $(5.01 \cdot 10^{-5} \text{ mol } \text{L}^{-1})$ using a mixture of *ABMAP* at the same concentration and RuCl₃ $(1.00 \cdot 10^{-3} \text{ mol } \text{L}^{-1})$. **b)** The A-diagram plot for Ru(III) ion with 2-amine-5-bromo(3-methylamine)-pyrazine for complexation process, major stoichiometry 1:1. **c)** Dependence of absorbance at 284 nm for *ABMAP* as a function of molar ratio $n_{Ru(III)}/n_{ABMAP}$.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C(2)-C(1)	1.3964	C(7)-C(5)	1.3905	H(27)-C(17)	1.1000
N(3)-C(2)	1.4014	C(8)-C(4)	1.3370	H(28)-C(18)	1.1000
H(20)-C(2)	1.1000	Ru(29)-N(6)	1.5061	C(9)-C(7)	1.4122
N(6)-C(1)	1.3899	N(14)-C(8)	1.3509	N(13)-C(7)	1.3872
H(19)-C(1)	1.1000	C(18)-C(8)	1.3858	C(12)-N(13)	1.3899
C(4)-N(3)	1.3968	C(15)-N(14)	1.3509	O(32)-Ru(29)	1.8900
C(5)-N(6)	1.3871	C(16)-C(15)	1.3858	O(33)-Ru(29)	1.8900
C(17)-C(18)	1.3910	H(25)-C(15)	1.1000	O(34)-Ru(29)	1.8900
C(10)-C(9)	1.3967	H(26)-C(16)	1.1000	Cl(31)-Ru(29)	2.2400
H(22)-C(10)	1.1130	H(21)-C(9)	1.1130	C(11)-C(12)	1.3965
H(37)-O(32)	0.9420	H(23)-C(11)	1.1130	H(24)-C(12)	1.1130
H(40)-O(33)	0.9420	H(38)-O(32)	0.9420	H(39)-O(33)	0.9420
H(41)-O(34)	0.9420	H(42)-O(34)	0.9420	H(30)-C(11)	1.1035

Table S1. Selected bond lenghts (Å) of $[RuCl(DPP)(OH_2)_3]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4c.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C(2)-C(1)	1.3445	N(9)-C(7)	1.2744	N(13)-C(12)	1.2647
N(3)-C(2)	1.2652	N(8)-C(7)	1.2686	H(31)-C(12)	1.1026
H(25)-C(2)	1.1025	O(10)-N(9)	1.3230	C(14)-C(15)	1.3480
C(4)-N(3)	1.2665	N(16)-Ru(21)	1.9402	C(17)-C(15)	1.3463
C(5)-C(4)	1.3482	N(19)-Ru(21)	1.9448	N(18)-C(17)	1.2682
H(26)-C(4)	1.1013	O(22)-Ru(21)	1.9392	O(20)-N(19)	1.3221
N(6)-C(1)	1.2712	Cl(23)-Ru(21)	2.2477	H(32)-C(14)	1.1015
C(7)-C(5)	1.3482	C(11)-N(16)	1.2714	H(27)-N(8)	1.0481
Ru(21)-N(6)	1.9401	C(15)-N(16)	1.2748	H(28)-N(8)	1.0496
H(24)-C(1)	1.1065	C(12)-C(11)	1.3444	H(30)-C(11)	1.1035
H(29)-O(10)	0.9421	H(34)-N(18)	1.0499	H(36)-O(22)	1.0497
H(33)-N(18)	1.0481	H(35)-O(20)	0.9421	H(37)-O(22)	1.0595

Table S2. Selected bond lenghts (Å) of $[RuCl(PAOX)_2(OH_2)]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4d.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C(2)-C(1)	1.3432	H(12)-N(7)	1.0567	Br(29)-C(20)	1.8901
N(3)-C(2)	1.2648	H(32)-N(7)	1.0507	H(30)-C(14)	1.1022
Br(10)-C(2)	1.8928	H(33)-N(8)	1.0593	H(26)-N(13)	1.0569
C(4)-N(3)	1.2698	Cl(40)-Ru(37)	2.2510	H(38)-N(13)	1.0506
C(5)-C(4)	1.3540	Cl(41)-Ru(37)	2.2504	H(15)-C(9)	1.1147
N(8)-C(4)	1.2813	C(23)-N(21)	1.2827	H(16)-C(9)	1.1153
N(6)-C(1)	1.2644	C(28)-N(21)	1.5003	H(17)-C(9)	1.1148
N(7)-C(5)	1.2740	H(39)-N(21)	1.0595	H(34)-C(28)	1.1150
H(11)-C(1)	1.1024	N(22)-C(23)	1.2748	H(35)-C(28)	1.1153
C(9)-N(8)	1.4987	C(24)-N(13)	1.2737	H(36)-C(28)	1.1147
Ru(37)-N(8)	1.9492	N(25)-C(24)	1.2673	C(20)-N(22)	1.2688
N(13)-Ru(37)	1.9416	C(14)-N(25)	1.2647	N(21)-Ru(37)	1.9500

Table S3. Selected bond lenghts (Å) of $[RuCl_2(ABMAP)_2]Cl$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4a.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
C(2)-C(1)	1.3442	N(16)-Ru(10)	1.9422	H(26)-C(11)	1.1077
N(3)-C(2)	1.2642	N(9)-Ru(10)	1.9312	N(13)-C(12)	1.2646
H(23)-C(2)	1.1023	N(19)-Ru(10)	1.9295	H(27)-C(12)	1.1023
C(4)-N(3)	1.2657	O(21)-Ru(10)	1.9382	C(14)-C(15)	1.3506
C(5)-C(4)	1.3507	S(8)-C(7)	1.5771	C(17)-C(15)	1.3592
H(24)-C(4)	1.1029	Cl(20)-Ru(10)	2.2457	H(28)-C(14)	1.1029
N(6)-C(1)	1.2726	H(25)-N(9)	1.0078	S(18)-C(17)	1.5775
C(7)-C(5)	1.3577	C(11)-N(16)	1.2723	H(29)-N(19)	1.0080
Ru(10)-N(6)	1.9426	C(15)-N(16)	1.2787	H(30)-O(21)	1.0512
H(22)-C(1)	1.1077	C(12)-C(11)	1.3442	H(31)-O(21)	1.0560

Table S4. Selected bond lenghts (Å) of $[RuCl(PTCA)_2(OH_2)]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4b.

Angle	[Deg.]	Angle	[Deg.]
N(3)-C(2)-C(1)	120.5861	C(16)-C(15)-N(14)	123.7955
H(20)-C(2)-C(1)	119.7069	H(25)-C(15)-N(14)	118.1024
N(6)-C(1)-C(2)	118.6280	C(17)-C(18)-C(8)	118.2317
H(19)-C(1)-C(2)	120.6860	H(26)-C(16)-C(15)	120.8826
C(4)-N(3)-C(2)	120.2919	H(27)-C(17)-C(16)	120.3423
C(5)-N(6)-C(1)	121.8610	H(28)-C(18)-C(8)	120.8839
C(7)-C(5)-C(4)	131.2583	C(9)-C(7)-C(5)	131.2647
C(8)-C(4)-N(3)	120.4270	N(13)-C(7)-C(5)	109.2478
Ru(29)-N(6)-C(1)	127.3286	C(12)-N(13)-C(7)	121.8614
N(14)-C(8)-C(4)	118.0986	O(32)-Ru(29)-N(6)	108.5257
C(18)-C(8)-C(4)	118.0990	O(33)-Ru(29)-N(6)	89.9999
C(15)-N(14)-C(8)	116.6196	O(34)-Ru(29)-N(6)	103.4694
Cl(31)-Ru(29)-N(6)	89.9997	H(37)-O(32)-Ru(29)	119.9999
C(10)-C(9)-C(7)	119.1468	H(38)-O(32)-Ru(29)	119.9997
H(21)-C(9)-C(7)	106.9818	H(39)-O(33)-Ru(29)	120.0003
C(11)-C(12)-N(13)	118.6271	H(40)-O(33)-Ru(29)	119.9999
H(22)-C(10)-C(9)	106.6826	H(41)-O(34)-Ru(29)	119.9999
H(23)-C(11)-C(10)	106.6078	H(42)-O(34)-Ru(29)	120.0004
H(24)-C(12)-C(11)	107.1167		

Table S5. Selected bond angles (in degrees) of $[RuCl(DPP)(OH_2)_3]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4c.

Angle	[Deg.]	Angle	[Deg.]
N(3)-C(2)-C(1)	122.1158	C(11)-N(16)-Ru(21)	120.2191
H(25)-C(2)-C(1)	120.8925	C(15)-N(16)-C(11)	117.0381
C(4)-N(3)-C(2)	116.4129	C(12)-C(11)-N(16)	121.3299
C(5)-C(4)-N(3)	122.6950	H(30)-C(11)-C(12)	117.3928
H(26)-C(4)-N(3)	114.9263	N(13)-C(12)-C(11)	122.2155
N(6)-C(1)-C(2)	120.7375	H(31)-C(12)-C(11)	120.8558
C(7)-C(5)-C(4)	126.7921	C(14)-C(15)-N(16)	120.6255
Ru(21)-N(6)-C(1)	120.9908	C(17)-C(15)-C(14)	125.5614
H(24)-C(1)-C(2)	117.9977	N(18)-C(17)-C(15)	122.2790
N(9)-C(7)-C(5)	113.2311	O(20)-N(19)-C(17)	116.1785
N(8)-C(7)-C(5)	121.0709	H(32)-C(14)-N(13)	114.9634
O(10)-N(9)-C(7)	115.4612	H(27)-N(8)-C(7)	121.6432
N(16)-Ru(21)-N(6)	110.7465	H(28)-N(8)-C(7)	119.4669
N(19)-Ru(21)-N(6)	161.7345	H(29)-O(10)-N(9)	111.1263
O(22)-Ru(21)-N(6)	92.0746	H(33)-N(18)-C(17)	121.8395
Cl(23)-Ru(21)-N(6)	89.0088	H(34)-N(18)-C(17)	118.8826
H(35)-O(20)-N(19)	110.8119	H(37)-O(22)-Ru(21)	106.1700
H(36)-O(22)-Ru(21)	105.3142		

Table S6. Selected bond angles (in degrees) of $[RuCl(PAOX)_2(OH_2)]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4d.

Angle	[Deg.]	Angle	[Deg.]
N(3)-C(2)-C(1)	119.7568	C(28)-N(21)-C(23)	112.3373
Br(10)-C(2)-C(1)	120.2487	H(39)-N(21)-C(23)	107.7352
C(4)-N(3)-C(2)	119.5023	N(22)-C(23)-N(21)	126.2549
_C(5)-C(4)-N(3)	119.6111	C(24)-N(13)-Ru(37)	103.2801
N(8)-C(4)-N(3)	128.8825	N(25)-C(24)-N(13)	125.8472
N(6)-C(1)-C(2)	122.0601	C(14)-N(25)-C(24)	115.7610
N(7)-C(5)-C(4)	112.2941	C(20)-N(22)-C(23)	111.8045
_H(11)-C(1)-C(2)	121.7740	Br(29)-C(20)-C(14)	119.8779
<u>C(9)-N(8)-C(4)</u>	112.3896	H(30)-C(14)-C(20)	122.4016
_Ru(37)-N(8)-C(4)	102.9789	H(26)-N(13)-C(24)	108.4755
N(13)-Ru(37)-N(7)	90.1454	H(38)-N(13)-C(24)	115.0964
N(21)-Ru(37)-N(7)	160.9081	H(15)-C(9)-N(8)	110.7970
H(12)-N(7)-C(5)	109.3388	H(16)-C(9)-N(8)	113.7069
H(32)-N(7)-C(5)	114.9945	H(17)-C(9)-N(8)	110.4408
H(33)-N(8)-C(4)	108.4065	H(34)-C(28)-N(21)	110.4075
_Cl(40)-Ru(37)-N(7)	104.2654	H(35)-C(28)-N(21)	113.7423
_Cl(41)-Ru(37)-N(7)	84.6328	H(36)-C(28)-N(21)	110.8934
C(23)-N(21)-Ru(37)	104.1034		

Table S7. Selected bond angles (in degrees) of [RuCl₂(*ABMAP*)₂]Cl in gaseous phase from PM3 calculations. Atom labels as in Figure 4a.

Angle	Degree (°)	Angle	Degree (°)
N(3)-C(2)-C(1)	121.6435	H(25)-N(9)-C(7)	122.2726
H(23)-C(2)-C(1)	121.2212	C(11)-N(16)-Ru(10)	116.2602
C(4)-N(3)-C(2)	115.7469	C(15)-N(16)-Ru(10)	103.9610
C(5)-C(4)-N(3)	123.1702	C(12)-C(11)-N(16)	122.2288
H(24)-C(4)-N(3)	114.8885	H(26)-C(11)-C(12)	117.8395
N(6)-C(1)-C(2)	122.7640	N(13)-C(12)-C(11)	121.6544
C(7)-C(5)-C(4)	119.9335	H(27)-C(12)-C(11)	121.1570
Ru(10)-N(6)-C(1)	116.3274	C(14)-C(15)-N(16)	120.2453
H(22)-C(1)-C(2)	117.7442	C(17)-C(15)-C(14)	120.3962
N(16)-Ru(10)-N(6)	106.1515	H(28)-C(14)-N(13)	114.8301
N(9)-Ru(10)-N(6)	77.0872	S(18)-C(17)-C(15)	127.7193
N(19)-Ru(10)-N(6)	165.3079	H(29)-N(19)-Ru(10)	123.2818
O(21)-Ru(10)-N(6)	91.4324	H(30)-O(21)-Ru(10)	106.0504
S(8)-C(7)-C(5)	127.7973	H(31)-O(21)-Ru(10)	101.5025
Cl(20)-Ru(10)-N(6)	100.1856		

Table S8. Selected bond angles (in degrees) of $[RuCl(PTCA)_2(OH_2)]Cl_2$ in gaseous phase from PM3 calculations. Atom labels as in Figure 4b.

Table S9. Optimized structures of the favorable conformation of ruthenium(III) complexes with pyrazine derivatives: *PAOX*, *DPP*, *ABMAP* and *PTCA*, total energies (E in kcal/mol), and atom Cartesian (X,Y,Z) coordinates (Å). The data were obtained at the PM3 calculations.

Complex	Total energy and atom coordinates					
	E = 262					
	Atoms	Χ	Y	Ζ		
	C(1)	2.641049	-1.681573	-0.840185		
	C(2)	3.631160	-1.755560	-1.747350		
	N(3)	3.968254	-0.612462	-2.511264		
	C(4)	3.339951	0.503806	-2.356231		
	C(5)	2.255031	0.585205	-1.365930		
	N(6)	1.950426	-0.457307	-0.669318		
	C(7)	1.447639	1.779223	-1.080414		
	N(8)	0.555291	1.590150	-0.162870		
	N(9)	1.647822	3.007996	-1.753569		
	O(10)	-0.277791	2.488224	0.277099		
	C(11)	-1.165968	0.662371	2.913894		
	C(12)	-2.347357	0.901145	3.510834		
	N(13)	-3.550001	0.658378	2.805902		
	C(14)	-3.535212	0.211726	1.595851		
	C(15)	-2.243342	-0.048380	0.942219		
	N(16)	-1.146967	0.170881	1.585939		
	C(17)	-2.069577	-0.553380	-0.425138		
	N(18)	-0.830307	-0.702163	-0.763814		
	N(19)	-3.166949	-0.850147	-1.268416		
$[RuCl(PAOX)_2(OH_2)]Cl_2$	O(20)	-0.413646	-1.146512	-1.914282		
see Fig. S5a	Ru(21)	0.489097	-0.211516	0.597606		
	Cl(22)	2.072353	0.362661	2.107750		
	O(23)	0.540522	-1.992125	1.336475		
	H(24)	2.385446	-2.524401	-0.270139		
	H(25)	4.153992	-2.655191	-1.891296		
	H(26)	3.611459	1.335057	-2.935928		
	H(27)	1.051328	3.786622	-1.589521		
	H(28)	2.380167	3.106192	-2.419420		
	H(29)	-0.307513	3.368907	-0.044050		
	H(30)	-0.272239	0.841513	3.432636		
	H(31)	-2.380965	1.265833	4.495499		
	H(32)	-4.442110	0.040136	1.097163		
	H(33)	-3.027991	-1.203454	-2.187405		
	H(34)	-4.099336	-0.698929	-0.957171		
	H(35)	-0.988134	-1.397975	-2.611712		
	H(36)	0.245249	-1.903905	2.266064		
	H(47)	-0.179730	-2.487644	0.896394		
	E = 203					
	Atoms	X	Y	Z		
	C(1)	-0.878892	-1.390374	-2.277264		
	C(2)	-1.987850	-2.178895	-1.734610		
	N(3)	-2.197560	-2.179982	-0.463625		
	C(4)	-1.366290	-1.461940	0.435556		

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		C(5)	0 202282	0 702252	0.061147
$ \begin{bmatrix} N(0) & -0.110990 & -0.739700 & -1.4302481 \\ C(7) & 0.749478 & -0.049597 & 0.656941 \\ C(8) & -1.760662 & -1.493077 & 1.847679 \\ C(9) & 0.975354 & -0.074659 & 2.115404 \\ C(10) & 1.990780 & 0.629914 & 2.641751 \\ C(11) & 2.867858 & 1.393965 & 1.752823 \\ C(12) & 2.653052 & 1.350934 & 0.426965 \\ N(13) & 1.573986 & 0.596219 & -0.108977 \\ N(14) & -2.142593 & -0.403712 & 2.428838 \\ C(15) & -2.561256 & -0.377779 & 3.781385 \\ C(16) & -2.589098 & -1.512470 & 4.502680 \\ C(17) & -2.185503 & -2.774267 & 3.869622 \\ C(18) & -1.786618 & -2.767137 & 2.586153 \\ C(16) & -2.581098 & -1.512470 & 4.502680 \\ C(17) & -2.185503 & -2.774267 & 3.869622 \\ C(18) & -1.786618 & -2.767137 & 2.586153 \\ H(20) & -2.621000 & -2.718344 & -2.375581 \\ H(21) & 0.386219 & -0.660390 & 2.752256 \\ H(22) & 2.171014 & -0.61606 & 3.676613 \\ H(23) & 3.666566 & 1.951848 & 2.146197 \\ H(24) & 3.291994 & 1.886054 & -0.209841 \\ H(25) & -2.884325 & 0.533315 & 4.219175 \\ H(26) & -2.897490 & -1.498425 & 5.506849 \\ H(27) & -2.210154 & -3.672077 & 4.414868 \\ H(28) & -1.493756 & -3.661134 & 2.117889 \\ Ru(29) & 1.311513 & 0.454771 & -2.047598 \\ C(131) & 2.735921 & -1.302222 & -2.033068 \\ O(32) & 2.722697 & 1.693577 & -2.495282 \\ O(33) & 0.104381 & 1.962247 & -2.048797 \\ O(34) & 0.947073 & 0.221666 & -3.929769 \\ H(37) & 2.309123 & 2.401313 & -3.030661 \\ H(38) & 3.31134 & 1.22227 & -2.033068 \\ O(32) & 0.777228 & 1.600379 & -2.273531 \\ H(40) & 0.024087 & 2.248433 & -1.116431 \\ H(41) & 1.786432 & -0.074436 & -4.337370 \\ H(42) & 0.798087 & 1.118598 & -4.293157 \\ E = 185 \\ \hline E = 185 \\ \hline C(1) & 1.177651 & -2.568560 & -1.125722 \\ C(2) & 1.016449 & -3.736468 & -1.773587 \\ N(3) & -0.186685 & -3.990720 & -2.475665 \\ C(4) & -1.135900 & -3.118769 & -2.506557 \\ C(5) & -0.959130 & -1.842990 & -1.798353 \\ N(6) & 0.137942 & -1.607028 & -1.125722 \\ C(2) & 1.016449 & -3.736468 & -1.773587 \\ N(3) & -0.186685 & -3.990720 & -2.475665 \\ C(4) & -1.136900 & -3.118769 & -2.506557 \\ C(5) & -0.959130 & -1.842990 & -1.798353 \\ N(6) & 0.137942 & -1.607028 & -1.125722 \\ C(2) & 1.016449 & -3.736468$		$\mathbf{U}(\mathbf{S})$	-0.302382	-0./92555	-0.00114/
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		N(0)	-0.110090	-0.739700	-1.403481
$ \begin{bmatrix} C(8) & -1.00062 & -1.49307 & 1.847679 \\ C(9) & 0.975354 & -0.074659 & 2.115404 \\ C(10) & 1.990780 & 0.629914 & 2.641751 \\ C(11) & 2.867858 & 1.393965 & 1.752823 \\ C(12) & 2.653052 & 1.350934 & 0.426965 \\ N(13) & 1.573986 & 0.596219 & -0.108977 \\ N(14) & -2.142593 & -0.403712 & 2.428838 \\ C(15) & -2.561256 & -0.377779 & 3.781385 \\ C(16) & -2.58098 & -1.512470 & 4.502680 \\ C(17) & -2.185503 & -2.774267 & 3.869622 \\ C(18) & -1.786618 & -2.767137 & 2.586153 \\ E(16) & -2.621000 & -2.718344 & -2.375581 \\ H(20) & -2.621000 & -2.718344 & -2.375581 \\ H(21) & 0.386219 & -0.660390 & 2.752256 \\ H(22) & 2.171014 & 0.611606 & 3.676613 \\ H(22) & 2.171014 & 0.611606 & 3.676613 \\ H(23) & 3.666566 & 1.951848 & 2.146197 \\ H(24) & 3.291994 & 1.886054 & -0.209841 \\ H(25) & -2.884325 & 0.533315 & 4.219175 \\ H(26) & -2.897490 & -1.498425 & 5.506849 \\ H(27) & -2.210154 & -3.672077 & 4.414868 \\ H(28) & -1.493756 & -3.661134 & 2.117889 \\ Ru(29) & 1.311513 & 0.454771 & -2.047598 \\ C(13) & 1.2735921 & -1.302222 & -2.033068 \\ O(32) & 2.722697 & 1.693577 & -2.495282 \\ O(33) & 0.104381 & 1.962417 & -2.047598 \\ C(31) & 2.309123 & 2.401313 & -3.030661 \\ H(38) & 3.311334 & 1.222873 & -3.119955 \\ H(39) & -0.777228 & 1.600379 & -2.273531 \\ H(40) & 0.024087 & 2.248433 & -1.116431 \\ H(41) & 1.786432 & -0.074436 & -4.337370 \\ H(42) & 0.798087 & 1.118598 & -4.293157 \\ E = 185 \\ \hline T E = 185 \\ \hline T M T T T T T T T T T T T T T T T T T$		C(7)	0.749478	-0.049507	0.050941
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		C(8)	-1./60662	-1.4930//	1.84/6/9
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		C(9)	0.975354	-0.0/4659	2.115404
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		C(10)	1.990780	0.629914	2.641751
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		C(11)	2.867858	1.393965	1.752823
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		C(12)	2.653052	1.350934	0.426965
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		N(13)	1.573986	0.596219	-0.108977
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $		N(14)	-2.142593	-0.403712	2.428838
$ \begin{bmatrix} \text{C}(16) & -2.589098 & -1.512470 & 4.502680 \\ \text{C}(17) & -2.185503 & -2.774267 & 3.869622 \\ \text{C}(18) & -1.786618 & -2.767137 & 2.586153 \\ \text{H}(19) & -0.739496 & -1.335102 & -3.314801 \\ \text{see Fig. S5d} & \text{H}(20) & -2.621000 & -2.718344 & -2.375581 \\ \text{H}(21) & 0.386219 & -0.660390 & 2.752256 \\ \text{H}(22) & 2.171014 & 0.611606 & 3.676613 \\ \text{H}(23) & 3.666566 & 1.951848 & 2.146197 \\ \text{H}(24) & 3.291994 & 1.886054 & -0.209841 \\ \text{H}(25) & -2.848325 & 0.533315 & 4.219175 \\ \text{H}(26) & -2.897490 & -1.498425 & 5.506849 \\ \text{H}(27) & -2.210154 & -3.672077 & 4.414868 \\ \text{H}(28) & -1.493756 & -3.661134 & 2.117889 \\ \text{R}u(29) & 1.311513 & 0.454771 & -2.047598 \\ \text{C}I(31) & 2.735921 & -1.302222 & -2.033068 \\ \text{O}(32) & 2.722697 & 1.693577 & -2.495282 \\ \text{O}(33) & 0.104381 & 1.962417 & -2.048797 \\ \text{O}(34) & 0.947073 & 0.221666 & -3.929769 \\ \text{H}(37) & 2.309123 & 2.401313 & -3.030661 \\ \text{H}(38) & 3.311334 & 1.222873 & -3.119955 \\ \text{H}(39) & -0.77228 & 1.600379 & -2.273531 \\ \text{H}(40) & 0.024087 & 2.248433 & -1.116431 \\ \text{H}(41) & 1.786432 & -0.074436 & -4.337370 \\ \text{H}(42) & 0.798087 & 1.118598 & -4.293157 \\ \hline \text{E} = 185 \\ \hline \text{Xoms} X Y Z \\ \hline \text{C}(1) & 1.177651 & -2.568560 & -1.125722 \\ \text{C}(2) & 1.016449 & -3.736468 & -1.773587 \\ \text{N}(3) & -0.186685 & -3.990720 & -2.475665 \\ \text{C}(4) & -1.136900 & -3.118769 & -2.506557 \\ \text{C}(5) & -0.959130 & -1.842990 & -1.798353 \\ \text{N}(6) & 0.137942 & -1.607028 & -1.156038 \\ \text{C}(7) & -1.949194 & -0.767198 & -1.747683 \\ \text{S}(8) & -3.504220 & -0.857705 & -2.400437 \\ \text{N}(9) & -1.499697 & 0.343540 & -1.015371 \\ \text{R}u(10) & 0.269187 & 0.112825 & -0.230858 \\ \text{C}(11) & 0.285915 & 3.003588 & 0.455171 \\ \text{C}(12) & 0.034398 & 4.046440 & 1.267118 \\ \text{R}u(10) & 0.269187 & 0.112825 & -0.230858 \\ \text{C}(11) & 0.285915 & 3.003588 & 0.455171 \\ \text{C}(12) & 0.034398 & 4.046440 & 1.267118 \\ \text{R}u(10) & 0.269187 & 0.112825 & -0.230858 \\ \text{C}(11) & 0.285915 & 3.003588 & 0.455171 \\ \text{C}(12) & 0.034398 & 4.046440 & 1.267118 \\ \text{R}u(10) & 0.269187 & 0.112825 & -0.230858 \\ \text{C}(11) & 0.285915 & 3.003588 & 0.455$		C(15)	-2.561256	-0.377779	3.781385
$ \begin{bmatrix} \text{RuCl}(DPP)(\text{OH}_{2})_3 \text{Cl}_2 \\ \text{C(17)} & -2.185503 & -2.774267 & 3.869622 \\ \text{C(18)} & -1.786618 & -2.767137 & 2.586153 \\ \text{H(19)} & -0.739496 & -1.335102 & -3.314801 \\ \text{H(20)} & -2.621000 & -2.718344 & -2.375581 \\ \text{H(21)} & 0.386219 & -0.660390 & 2.752256 \\ \text{H(22)} & 2.171014 & 0.611606 & 3.676613 \\ \text{H(23)} & 3.666566 & 1.951848 & 2.146197 \\ \text{H(24)} & 3.291994 & 1.886054 & -0.209841 \\ \text{H(25)} & -2.84325 & 0.533315 & 4.219175 \\ \text{H(26)} & -2.897490 & -1.498425 & 5.506849 \\ \text{H(27)} & -2.210154 & -3.672077 & 4.414868 \\ \text{H(28)} & -1.493756 & -3.661134 & 2.117889 \\ \text{Ru(29)} & 1.311513 & 0.454771 & -2.047598 \\ \text{Cl(31)} & 2.735291 & -1.302222 & -2.033068 \\ \text{O(32)} & 2.722697 & 1.693577 & -2.495282 \\ \text{O(33)} & 0.104381 & 1.962417 & -2.048797 \\ \text{O(34)} & 0.947073 & 0.221666 & -3.929769 \\ \text{H(37)} & 2.309123 & 2.401313 & -3.030661 \\ \text{H(38)} & 3.311334 & 1.222873 & -3.119955 \\ \text{H(39)} & -0.777228 & 1.600379 & -2.273531 \\ \text{H(40)} & 0.024087 & 2.248433 & -1.116431 \\ \text{H(41)} & 1.786432 & -0.074436 & 4.337370 \\ \text{H(42)} & 0.798087 & 1.18598 & 4.293157 \\ \hline \text{E} = 185 \\ \hline \text{C(1)} & 1.177651 & -2.568560 & -1.125722 \\ \text{C(2)} & 1.016449 & -3.736468 & -1.77387 \\ \text{N(3)} & -0.186685 & -3.990720 & -2.475665 \\ \text{C(4)} & -1.136900 & -3.118769 & -2.506557 \\ \text{C(5)} & -0.959130 & -1.842990 & -1.798353 \\ \text{N(6)} & 0.137942 & -1.607028 & -1.156038 \\ \text{C(7)} & -1.949194 & -0.767198 & -1.747683 \\ \text{S(8)} & -3.504220 & -0.857705 & -2.404037 \\ \text{N(9)} & -1.499697 & 0.343540 & -1.015371 \\ \text{Ru(10)} & 0.269187 & 0.112825 & -0.230858 \\ \text{C(11)} & 0.285915 & 3.003588 & 0.455171 \\ \text{C(12)} & 0.034398 & 4.046440 & 1.267118 \\ \text{IRuCl(PTC4)_0}(\text{OH}_3)\text{IC} \\ \text{N(3)} & -0.565638 & 3.826006 & 2.529901 \\ \hline \end{tabular}$		C(16)	-2.589098	-1.512470	4.502680
$ \begin{bmatrix} \text{RuCl}(DPP)(\text{OH}_{2})_3]\text{Cl}_2 \\ \text{see Fig. S5d} \\ H(19) & -0.739496 & -1.335102 & -3.314801 \\ H(20) & -2.621000 & -2.718344 & -2.375581 \\ H(21) & 0.386219 & -0.660390 & 2.752256 \\ H(22) & 2.171014 & 0.611606 & 3.676613 \\ H(23) & 3.666566 & 1.951848 & 2.146197 \\ H(24) & 3.291994 & 1.886054 & -0.209841 \\ H(25) & -2.848325 & 0.533315 & 4.219175 \\ H(26) & -2.897490 & -1.498425 & 5.506849 \\ H(27) & -2.210154 & -3.672077 & 4.414868 \\ H(28) & -1.493756 & -3.661134 & 2.117889 \\ Ru(29) & 1.311513 & 0.454771 & -2.047598 \\ Cl(31) & 2.735921 & -1.302222 & -2.033068 \\ O(32) & 2.722697 & 1.693577 & -2.495282 \\ O(33) & 0.104381 & 1.962417 & -2.048797 \\ O(34) & 0.947073 & 0.221666 & -3.929769 \\ H(37) & 2.309123 & 2.401313 & -3.030661 \\ H(38) & 3.311334 & 1.222873 & -3.119955 \\ H(39) & -0.777228 & 1.600379 & -2.273531 \\ H(40) & 0.024087 & 2.248433 & -1.116431 \\ H(41) & 1.786432 & -0.074436 & -4.337370 \\ H(42) & 0.798087 & 1.118598 & -4.293157 \\ \hline \\ $		C(17)	-2.185503	-2.774267	3.869622
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		C(18)	-1.786618	-2.767137	2.586153
see Fig. S5d H(20) -2.621000 -2.718344 -2.375581 H(21) 0.386219 -0.660390 2.752256 H(22) 2.171014 0.611606 3.676613 H(23) 3.666566 1.951848 2.146197 H(24) 3.291994 1.886054 -0.209841 H(25) -2.848325 0.533315 4.219175 H(26) -2.897490 -1.498425 5.506849 H(27) -2.210154 -3.672077 4.414868 H(28) -1.493756 -3.661134 2.117889 Ru(29) 1.311513 0.454771 -2.047598 Cl(31) 2.735921 -1.302222 -2.033068 O(32) 2.722697 1.693577 -2.495282 O(33) 0.104381 1.962417 -2.048797 O(34) 0.947073 0.221666 -3.929769 H(37) 2.309123 2.401313 -3.030661 H(38) 3.311334 1.222873 -3.119955 H(39) -0.777228 1.600379 -2.273531 H(40) 0.024087 2.248433 -1.116431 H(41) 1.786432 -0.074436 4.337370 H(42) 0.798087 1.118598 -4.293157 E = 185 E = 185 E = 185 C(1) 1.177651 -2.568560 -1.125722 C(2) 1.016449 -3.736468 -1.773587 N(3) -0.186685 -3.990720 -2.475665 C(4) -1.136900 -3.118769 -2.506557 C(5) -0.959130 -1.842990 -1.798353 N(6) 0.137942 -1.607028 -1.156038 C(7) -1.949194 -0.767198 -1.747683 S(8) -3.504220 -0.857705 -2.404037 N(9) -1.499697 0.343540 -1.015371 Ru(10) 0.269187 0.112825 -0.230858 C(11) 0.285915 3.003588 0.455171 C(12) 0.034398 4.046440 1.267118 Ru(10) 0.269187 0.112825 -0.230858 C(11) 0.285915 3.003588 0.455171 C(12) 0.034398 4.046440 1.267118 Ruc10/ <i>PTC4</i> b ₂ (OH ₂)[C1] N(13) -0.5565638 3.826006 2.529901	[RuCl(<i>DPP</i>)(OH ₂) ₃]Cl ₂	H(19)	-0.739496	-1.335102	-3.314801
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	see Fig. S5d	H(20)	-2.621000	-2.718344	-2.375581
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(21)	0 386219	-0 660390	2 752256
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H(22)	2 171014	0.611606	3 676613
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H(23)	3 666566	1 951848	2 146197
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(24)	3 291994	1 886054	-0 209841
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(25)	-2 848325	0 533315	4 219175
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(26)	-2.848323	-1 /08/25	5 506849
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H(20) H(27)	-2.077470	-1.470423	1 11 1969
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H(27) H(29)	-2.210134	-3.072077	4.414000
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		$\Pi(20)$ $\Pi(20)$	-1.495/30 1 211512	-3.001134	2.11/009
$\begin{array}{c ccccc} Cl(31) & 2.735921 & -1.302222 & -2.033068 \\ O(32) & 2.722697 & 1.693577 & -2.495282 \\ O(33) & 0.104381 & 1.962417 & -2.048797 \\ O(34) & 0.947073 & 0.221666 & -3.929769 \\ H(37) & 2.309123 & 2.401313 & -3.030661 \\ H(38) & 3.311334 & 1.222873 & -3.119955 \\ H(39) & -0.777228 & 1.600379 & -2.273531 \\ H(40) & 0.024087 & 2.248433 & -1.116431 \\ H(41) & 1.786432 & -0.074436 & -4.337370 \\ H(42) & 0.798087 & 1.118598 & -4.293157 \\ \hline E = 185 \\ \hline \\ \hline \\ \hline \\ C(1) & 1.177651 & -2.568560 & -1.125722 \\ C(2) & 1.016449 & -3.736468 & -1.773587 \\ N(3) & -0.186685 & -3.990720 & -2.475665 \\ C(4) & -1.136900 & -3.118769 & -2.506557 \\ C(5) & -0.959130 & -1.842990 & -1.798353 \\ N(6) & 0.137942 & -1.607028 & -1.156038 \\ C(7) & -1.949194 & -0.767198 & -1.747683 \\ S(8) & -3.504220 & -0.857705 & -2.404037 \\ N(9) & -1.499697 & 0.343540 & -1.015371 \\ Ru(10) & 0.269187 & 0.112825 & -0.230858 \\ C(11) & 0.285915 & 3.003588 & 0.455171 \\ C(12) & 0.034398 & 4.046440 & 1.267118 \\ \hline \\ RuCl(PTCA)_2(OH_5)IC1_2 & N(13) & -0.565638 & 3.826006 & 2.529901 \\ \hline \end{array}$		Ku(29)	1.311313	0.454771	-2.04/398
$\begin{array}{c ccccc} O(32) & 2.722697 & 1.693577 & -2.495282 \\ O(33) & 0.104381 & 1.962417 & -2.048797 \\ O(34) & 0.947073 & 0.221666 & -3.929769 \\ H(37) & 2.309123 & 2.401313 & -3.030661 \\ H(38) & 3.311334 & 1.222873 & -3.119955 \\ H(39) & -0.777228 & 1.600379 & -2.273531 \\ H(40) & 0.024087 & 2.248433 & -1.116431 \\ H(41) & 1.786432 & -0.074436 & -4.337370 \\ H(42) & 0.798087 & 1.118598 & -4.293157 \\ \hline E = 185 & & & & & & & & & & & & & & & & & & &$		CI(31)	2.735921	-1.302222	-2.033068
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		O(32)	2./2269/	1.6935//	-2.495282
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		O(33)	0.104381	1.962417	-2.048/9/
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		O(34)	0.947073	0.221666	-3.929769
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(37)	2.309123	2.401313	-3.030661
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(38)	3.311334	1.222873	-3.119955
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(39)	-0.777228	1.600379	-2.273531
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		H(40)	0.024087	2.248433	-1.116431
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		H(41)	1.786432	-0.074436	-4.337370
$E = 185$ $Atoms X Y Z$ $C(1) 1.177651 -2.568560 -1.125722$ $C(2) 1.016449 -3.736468 -1.773587$ $N(3) -0.186685 -3.990720 -2.475665$ $C(4) -1.136900 -3.118769 -2.506557$ $C(5) -0.959130 -1.842990 -1.798353$ $N(6) 0.137942 -1.607028 -1.156038$ $C(7) -1.949194 -0.767198 -1.747683$ $S(8) -3.504220 -0.857705 -2.404037$ $N(9) -1.499697 0.343540 -1.015371$ $Ru(10) 0.269187 0.112825 -0.230858$ $C(11) 0.285915 3.003588 0.455171$ $C(12) 0.034398 4.046440 1.267118$ $IRuCl(PTC4)_2(OH_2)ICh_2 N(13) -0.565638 3.826006 2.529901$		H(42)	0.798087	1.118598	-4.293157
AtomsXYZ $C(1)$ 1.177651 -2.568560 -1.125722 $C(2)$ 1.016449 -3.736468 -1.773587 $N(3)$ -0.186685 -3.990720 -2.475665 $C(4)$ -1.136900 -3.118769 -2.506557 $C(5)$ -0.959130 -1.842990 -1.798353 $N(6)$ 0.137942 -1.607028 -1.156038 $C(7)$ -1.949194 -0.767198 -1.747683 $S(8)$ -3.504220 -0.857705 -2.404037 $N(9)$ -1.499697 0.343540 -1.015371 $Ru(10)$ 0.269187 0.112825 -0.230858 $C(11)$ 0.285915 3.003588 0.455171 $C(12)$ 0.034398 4.046440 1.267118 [RuCl(<i>PTCA</i>) ₂ (OH ₂)]Ch $N(13)$ -0.565638 3.826006 2.529901		E = 185			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		Atoms	X	Y	Z
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C(1)	1.177651	-2.568560	-1.125722
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C(2)	1.016449	-3.736468	-1.773587
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		N(3)	-0.186685	-3.990720	-2.475665
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C(4)	-1.136900	-3.118769	-2.506557
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C(5)	-0.959130	-1.842990	-1.798353
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		N(6)	0.137942	-1.607028	-1.156038
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		C(7)	-1.949194	-0.767198	-1.747683
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		S(8)	-3.504220	-0.857705	-2.404037
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		N(9)	-1.499697	0.343540	-1.015371
$\begin{array}{cccc} C(11) & 0.285915 & 3.003588 & 0.455171 \\ C(12) & 0.034398 & 4.046440 & 1.267118 \\ [RuCl(PTCA)2(OH2)]Cl2 N(13) -0.565638 & 3.826006 & 2.529901 \\ \end{array}$		Ru(10)	0.269187	0.112825	-0.230858
$\begin{array}{c} C(12) & 0.034398 & 4.046440 & 1.267118 \\ [RuCl(PTCA)2(OH2)]Cl2 N(13) -0.565638 & 3.826006 & 2.529901 \\ \end{array}$		C(11)	0.285915	3.003588	0.455171
$[RuCl(PTCA)_2(OH_2)]Cl_2 N(13) -0.565638 -3.826006 -2.529901$		$\dot{C(12)}$	0.034398	4.046440	1.267118
				-	

see Fig. S5D	C(14)	-0.879007	2.636756	2.918402
C	C(15)	-0.603903	1.498236	2.030097
	N(16)	-0.053244	1.693860	0.876804
	C(17)	-0.907028	0.102488	2.342481
	S(18)	-1.605451	-0.436596	3.784025
	N(19)	-0.535013	-0.770898	1.309558
	Cl(20)	1.192883	0.963983	-2.110563
	O(21)	2.060595	-0.073612	0.455783
	H(22)	2.067030	-2.375265	-0.603257
	H(23)	1.778097	-4.459980	-1.761079
	H(25)	-2.020875	-3.327195	-3.033255
	H(26)	0.729014	3.164930	-0.481741
	H(27)	0.280591	5.023007	0.968256
	H(28)	-1.323524	2.494845	3.858890
	H(29)	-2.090962	1.106941	-0.779499
	H(30)	2 389389	0.838908	0 592065
	H(31)	1 964300	-0.436812	1 359692
	H(34)	-0 534870	-1 759057	1 416922
	E = 163	0.001070	1.709007	1.110)22
	Atoms	X	Y	Z
	$\frac{1}{C(1)}$	-4 624497	2 255132	-0.510529
	C(2)	-4 380343	1 790804	-1 884141
	N(3)	-3 306349	1 128015	-2 151691
	C(4)	-2.359830	0.838003	-1 137901
	C(5)	-2 584097	1 267744	0 114934
	N(6)	-3 761037	1 995701	0.411555
	N(7)	1 600567	0.005200	1 11/200
		- (()()())() /	(1 77)/77	1 1 1 4 / 11 9
	N(7) N(8)	-1.144381	0.993299	-1 411508
	N(7) N(8) C(9)	-1.144381 -1.441780	0.121032	-1.411508 -1 945848
	N(7) N(8) C(9) Br(10)	-1.144381 -1.441780 -5.611803	0.393239 0.121032 -1.227223 2.156513	-1.411508 -1.945848 -3.243052
	N(7) N(8) C(9) Br(10) H(11)	-1.144381 -1.441780 -5.611803 -5.493245	0.393239 0.121032 -1.227223 2.156513 2.797860	-1.411508 -1.945848 -3.243052 -0.278646
	N(7) N(8) C(9) Br(10) H(11) H(12)	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677	-1.411508 -1.945848 -3.243052 -0.278646 1.553192
	N(7) N(8) C(9) Br(10) H(11) H(12) N(13)	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452
	$ \begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \end{array} $	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266
		-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711
	$ \begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \end{array} $	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2 135876	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1 293396
	$ \begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \end{array} $	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826
[RuCl ₂ (<i>ABMAP</i>) ₂]C]	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299	$\begin{array}{c} -1.411209\\ -1.411508\\ -1.945848\\ -3.243052\\ -0.278646\\ 1.553192\\ 1.954452\\ 2.935266\\ -2.037711\\ -1.293396\\ -2.936826\\ 1.673750\\ -0.382357\\ 0.653018\end{array}$
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423 3.008382
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423 3.008382 2.732509
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423 3.008382 2.732509 -1.529580
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \\ Br(29) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818 5.951235	0.393299 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441 -2.966918	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423 3.008382 2.732509 -1.529580 1.539354
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \\ Br(29) \\ H(30) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818 5.951235 4.687450	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441 -2.966918 -1.348263	$\begin{array}{c} -1.411209\\ -1.411508\\ -1.945848\\ -3.243052\\ -0.278646\\ 1.553192\\ 1.954452\\ 2.935266\\ -2.037711\\ -1.293396\\ -2.936826\\ 1.673750\\ -0.382357\\ 0.653018\\ 0.731418\\ 1.887423\\ 3.008382\\ 2.732509\\ -1.529580\\ 1.539354\\ 3.774221\end{array}$
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \\ Br(29) \\ H(30) \\ H(32) \end{array}$	-1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818 5.951235 4.687450 -2.003960	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441 -2.966918 -1.348263 0.390859	-1.411508 -1.945848 -3.243052 -0.278646 1.553192 1.954452 2.935266 -2.037711 -1.293396 -2.936826 1.673750 -0.382357 0.653018 0.731418 1.887423 3.008382 2.732509 -1.529580 1.539354 3.774221 1.828243
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \\ Br(29) \\ H(30) \\ H(32) \\ H(23) \end{array}$	-1.600367 -1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818 5.951235 4.687450 -2.003960 0.626961	0.393239 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441 -2.966918 -1.348263 0.390859 0.635752	$\begin{array}{c} -1.114209\\ -1.411508\\ -1.945848\\ -3.243052\\ -0.278646\\ 1.553192\\ 1.954452\\ 2.935266\\ -2.037711\\ -1.293396\\ -2.936826\\ 1.673750\\ -0.382357\\ 0.653018\\ 0.731418\\ 1.887423\\ 3.008382\\ 2.732509\\ -1.529580\\ 1.539354\\ 3.774221\\ 1.828243\\ 2.133061\end{array}$
[RuCl ₂ (<i>ABMAP</i>) ₂]Cl see Fig. S5c	$\begin{array}{c} N(7) \\ N(8) \\ C(9) \\ Br(10) \\ H(11) \\ H(12) \\ N(13) \\ C(14) \\ H(15) \\ H(16) \\ H(17) \\ C(20) \\ N(21) \\ N(22) \\ C(23) \\ C(24) \\ N(25) \\ H(26) \\ C(28) \\ Br(29) \\ H(30) \\ H(32) \\ H(33) \\ H(24) \end{array}$	-1.000367 -1.144381 -1.441780 -5.611803 -5.493245 -1.310921 0.924399 4.062837 -0.523792 -2.135876 -1.893799 4.401950 1.549318 3.623557 2.445982 2.135642 2.988131 0.357892 2.240818 5.951235 4.687450 -2.003960 -0.636961 2.990326	0.393299 0.121032 -1.227223 2.156513 2.797860 1.868677 0.346507 -1.253871 -1.805980 -1.757748 -1.144194 -1.928574 -0.873366 -1.801299 -1.017300 -0.407622 -0.544462 0.009996 -0.242441 -2.966918 -1.348263 0.390859 0.635752 0.926288	$\begin{array}{c} -1.114209\\ -1.411508\\ -1.945848\\ -3.243052\\ -0.278646\\ 1.553192\\ 1.954452\\ 2.935266\\ -2.037711\\ -1.293396\\ -2.936826\\ 1.673750\\ -0.382357\\ 0.653018\\ 0.731418\\ 1.887423\\ 3.008382\\ 2.732509\\ -1.529580\\ 1.539354\\ 3.774221\\ 1.828243\\ -2.133061\\ 1.934326\end{array}$

 H(35)	2 741739	0 675998	-1 221400
H(36)	1.526380	-0.012741	-2.318939
Ru(37)	-0.051772	0.117746	0.246112
H(38)	1.147348	1.327619	2.114368
H(39)	1.259019	-1.809290	-0.670109
Cl(40)	-0.820361	-1.849996	1.082133
Cl(41)	0.651649	2.198719	-0.333521