Synthesis of new ruthenium complexes and their exploratory study as organic semiconductors

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Content

Figure S1: FTIR spectrum of ligand **1b**.

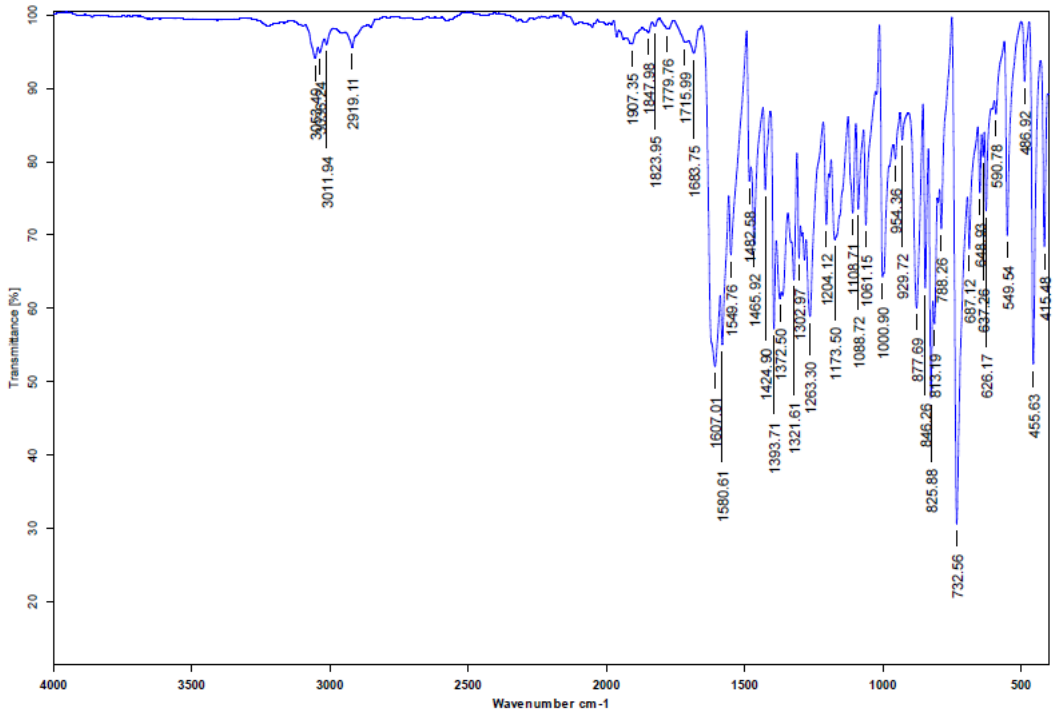


Figure S2: MS spectrum of ligand **1b**.

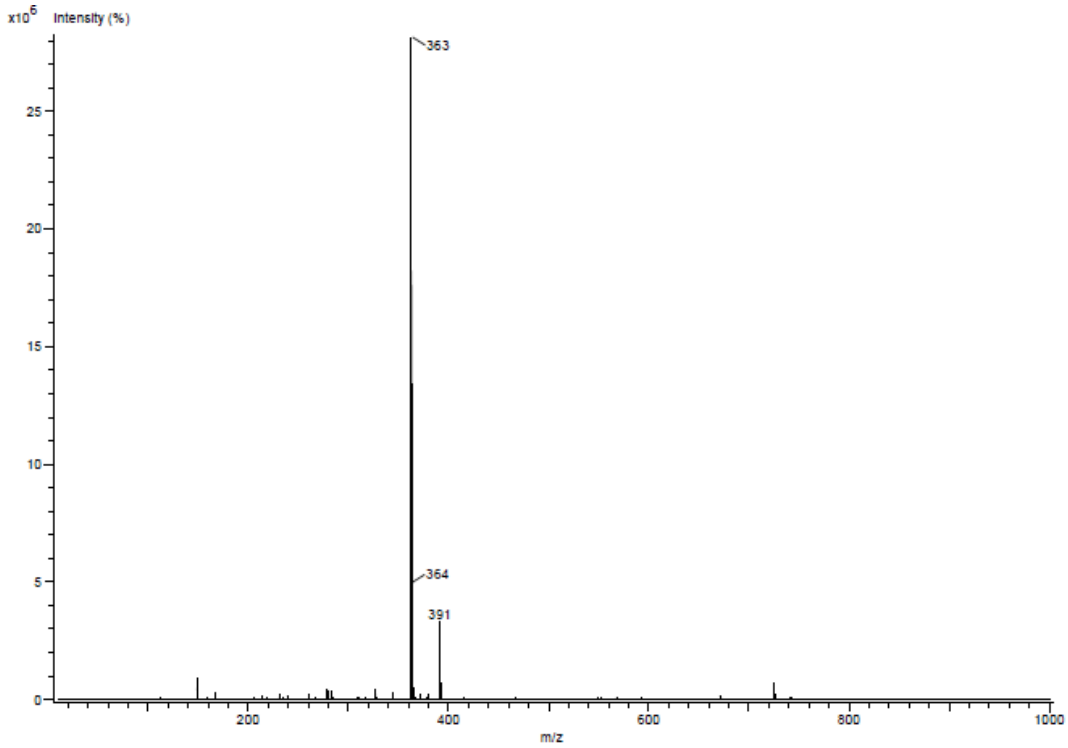
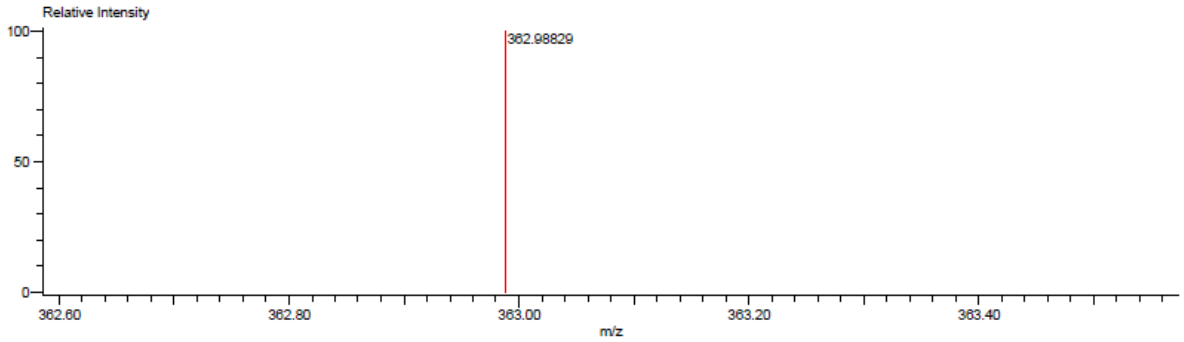


Figure S3: HRMS of ligand **1b**.



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
362.98829	4215.56	362.98820	0.10	0.27	$^{12}C_{15}{}^{1}H_{12}{}^{127}I_{1}{}^{16}O_{2}$	10.5

Figure S4: ^{1}H-NMR spectrum of ligand **1b** in $CDCl_3$ 400 MHz.

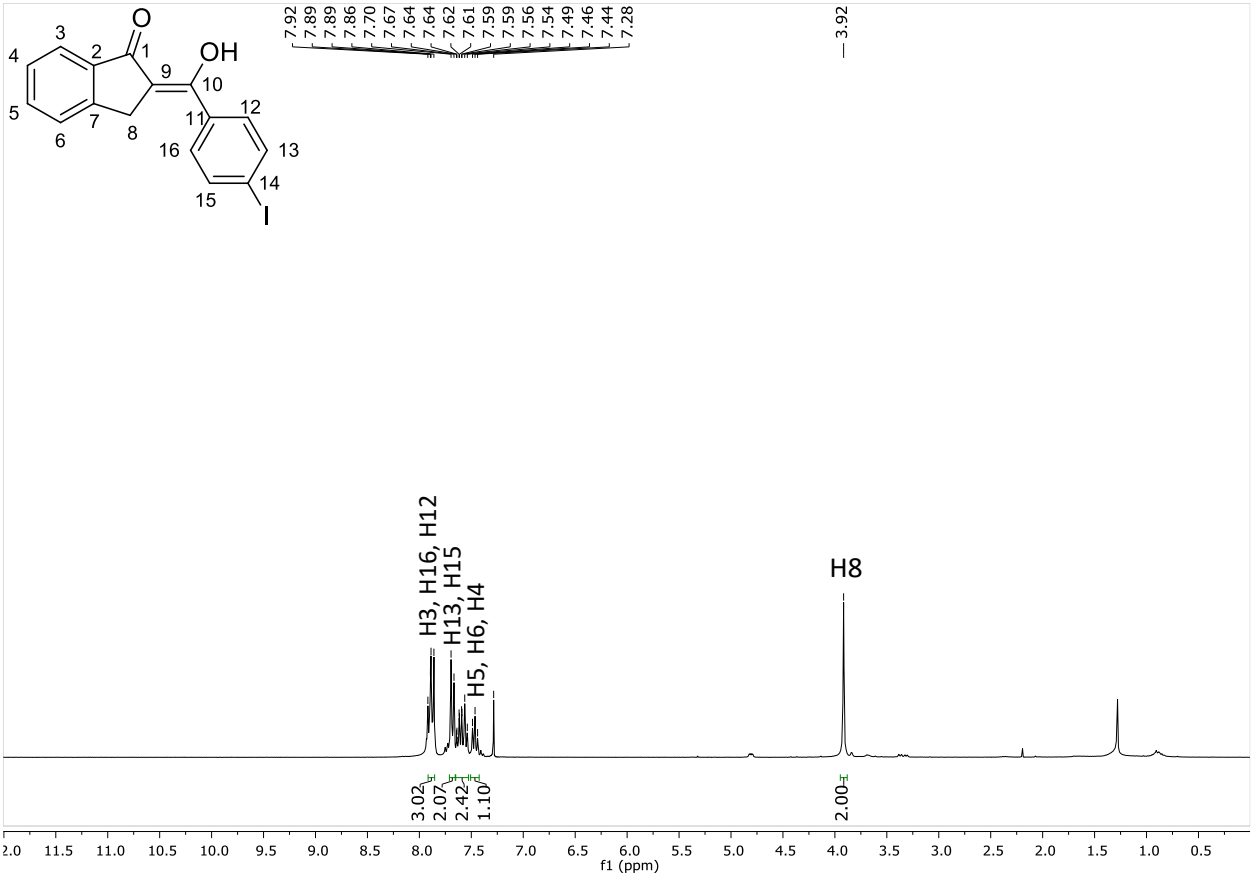


Figure S5: ^{13}C-NMR spectrum of **1b** in $CDCl_3$ 400 MHz:

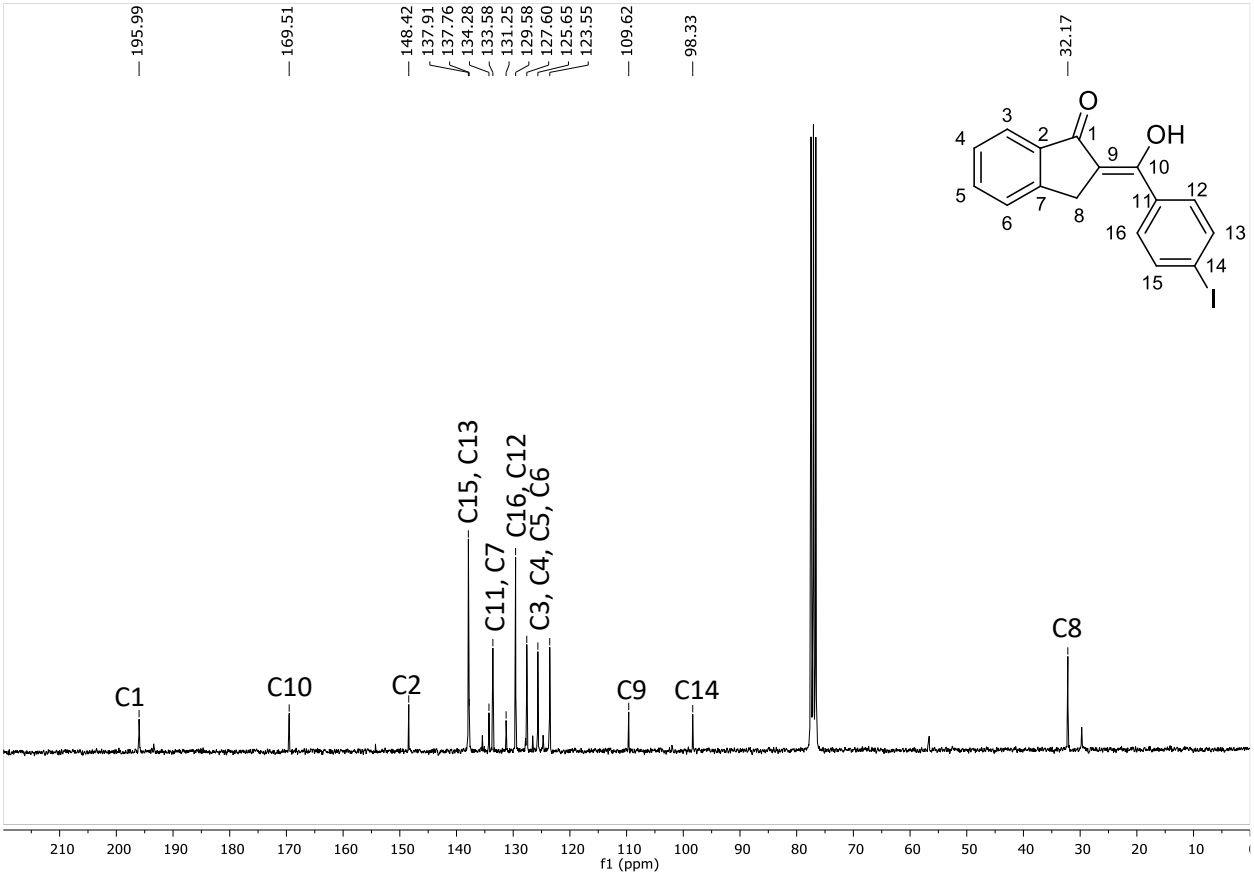


Figure S6: FTIR spectrum of complex **2a**.

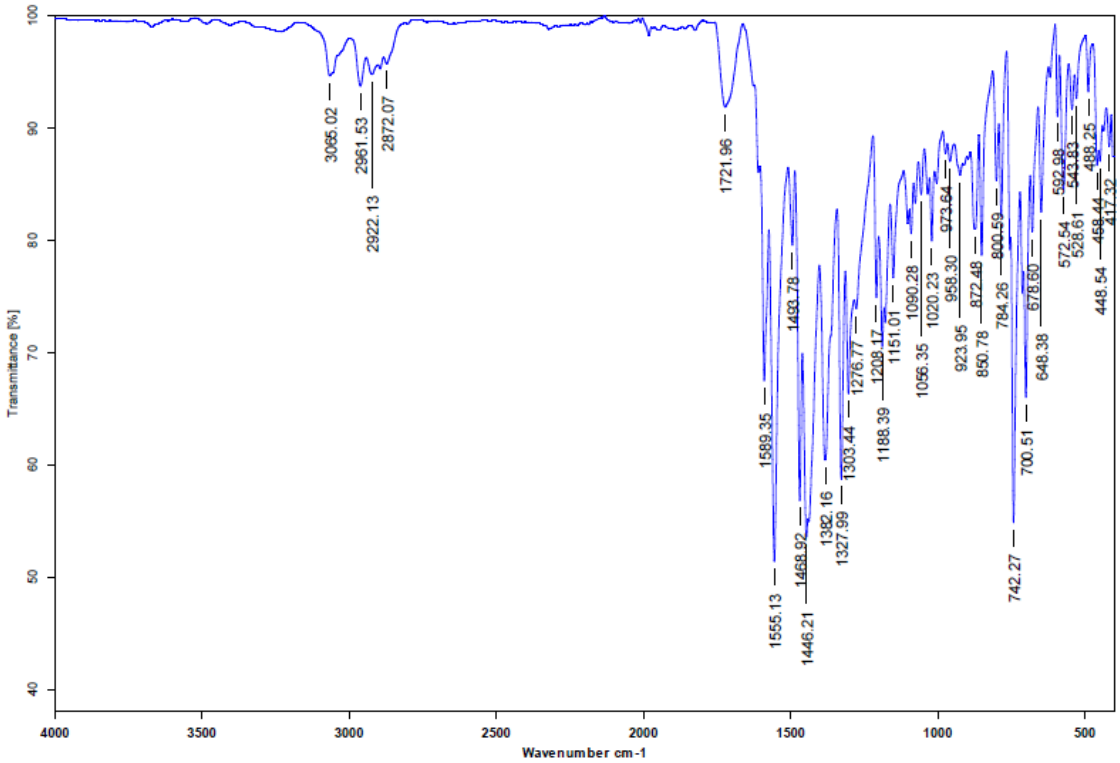


Figure S7: MS spectrum of complex **2a**.

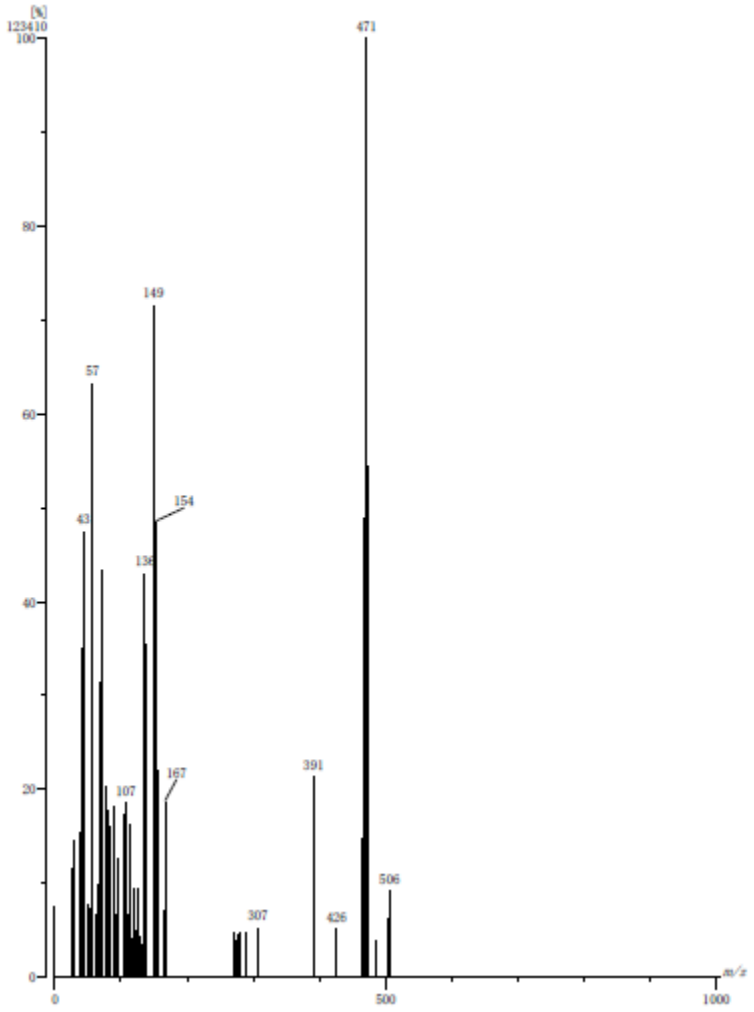


Figure S8: HRMS of complex **2a**.

Inlet : Direct Ion Mode : FAB+
RT : 6.71 min Scan# : (141,142)
Elements : C 26/0, H 29/0, Cl 1/0, O 2/0, Ru 1/0
Mass Tolerance : 1000ppm, 10mmu if m/z > 10
Unsaturation (U.S.) : 0.0 – 20.0

	Observed m/z	Int%							
	506.0600	100.00							
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	Cl	O	Ru
1	506.0587	+2.7 /	+1.3	14.5	26	25	1	2	1

Figure S9: ^{1}H-NMR spectrum of **2a** in $CDCl_3$ 400 MHz:

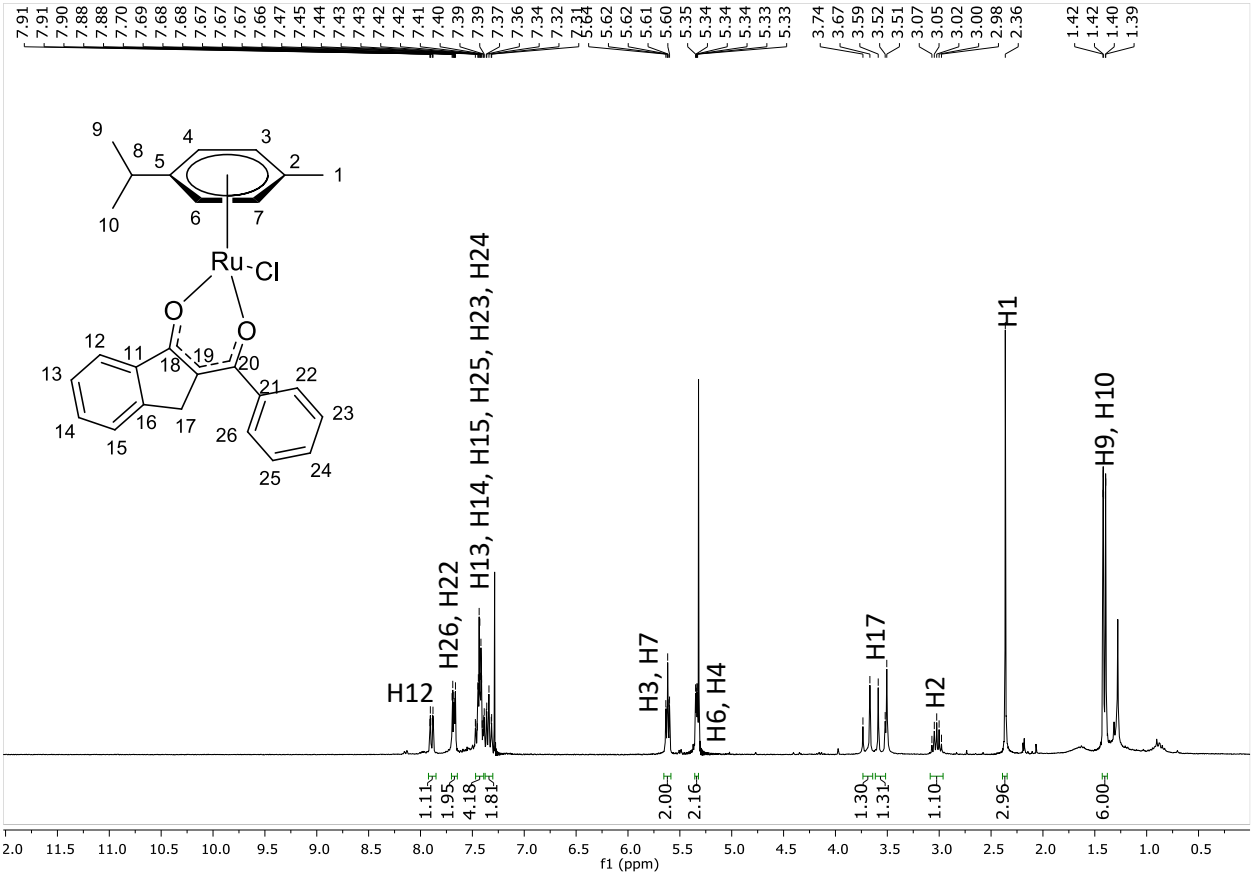


Figure S10: ^{13}C-NMR spectrum of **2a** in $CDCl_3$ 400 MHz:

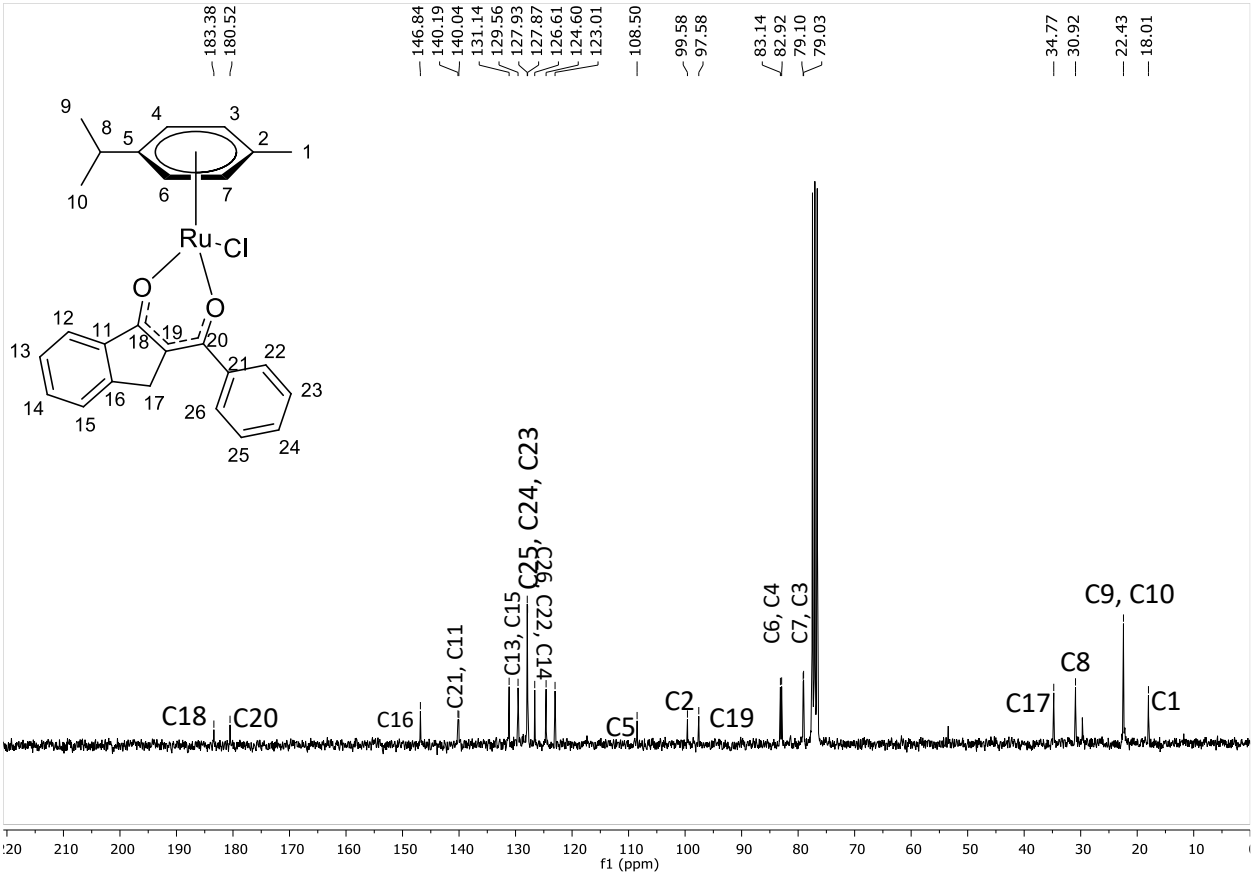


Figure S11: FTIR spectrum of complex **2b**.

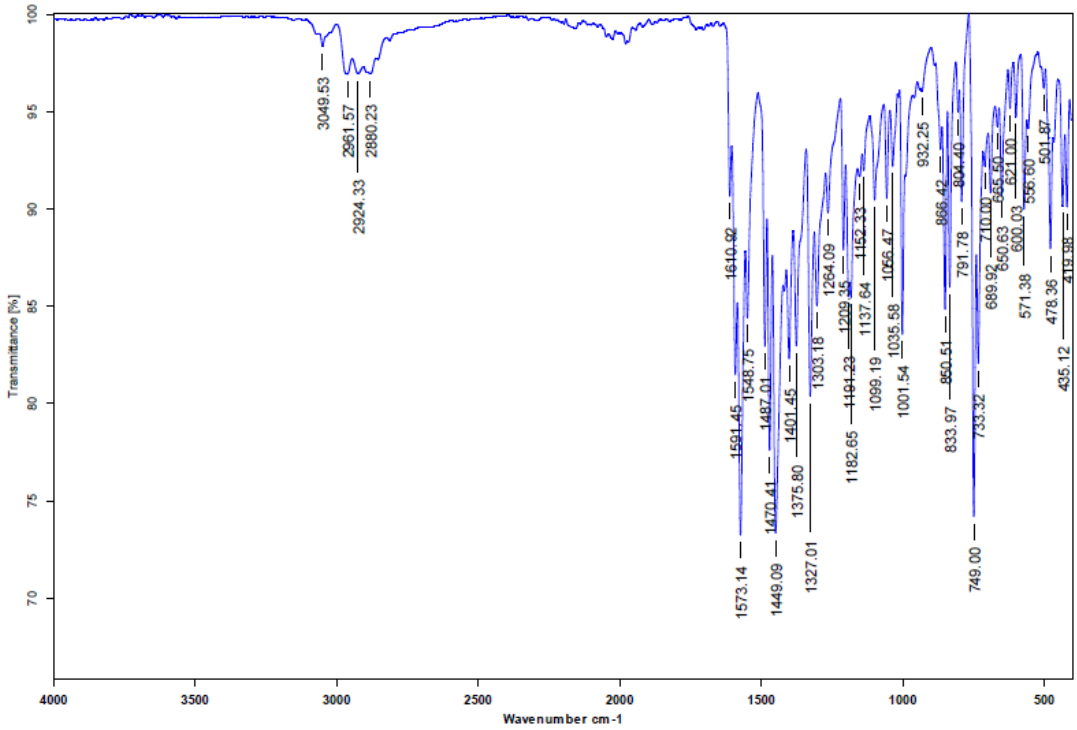


Figure S12: MS spectrum of complex **2b**.

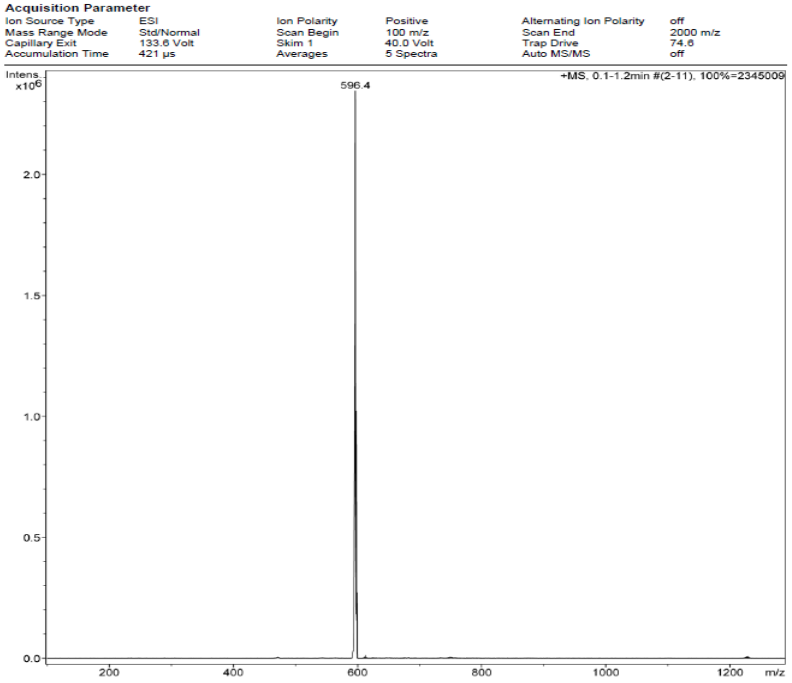


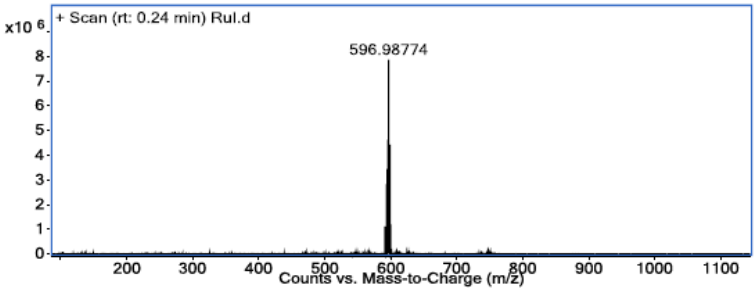
Figure S13: HRMS of complex **2b**.

Sample Group
Stream Name LC 1

Info.
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI (+)



Peak List

m/z	z	Abund
590.99089	1	1136845.02
592.98899	1	456021.35
593.9888		2844940.35
594.98802		3505012.05
595.98877		4640274.74
596.98774	1	8072395.01
597.17802		736918.85
597.99047	1	2234367.25
598.9884	1	4444355.6
599.99222	1	1228913.79

Figure S14: ^{1}H-NMR spectrum of complex **2b** in $CDCl_3$ 400 MHz:

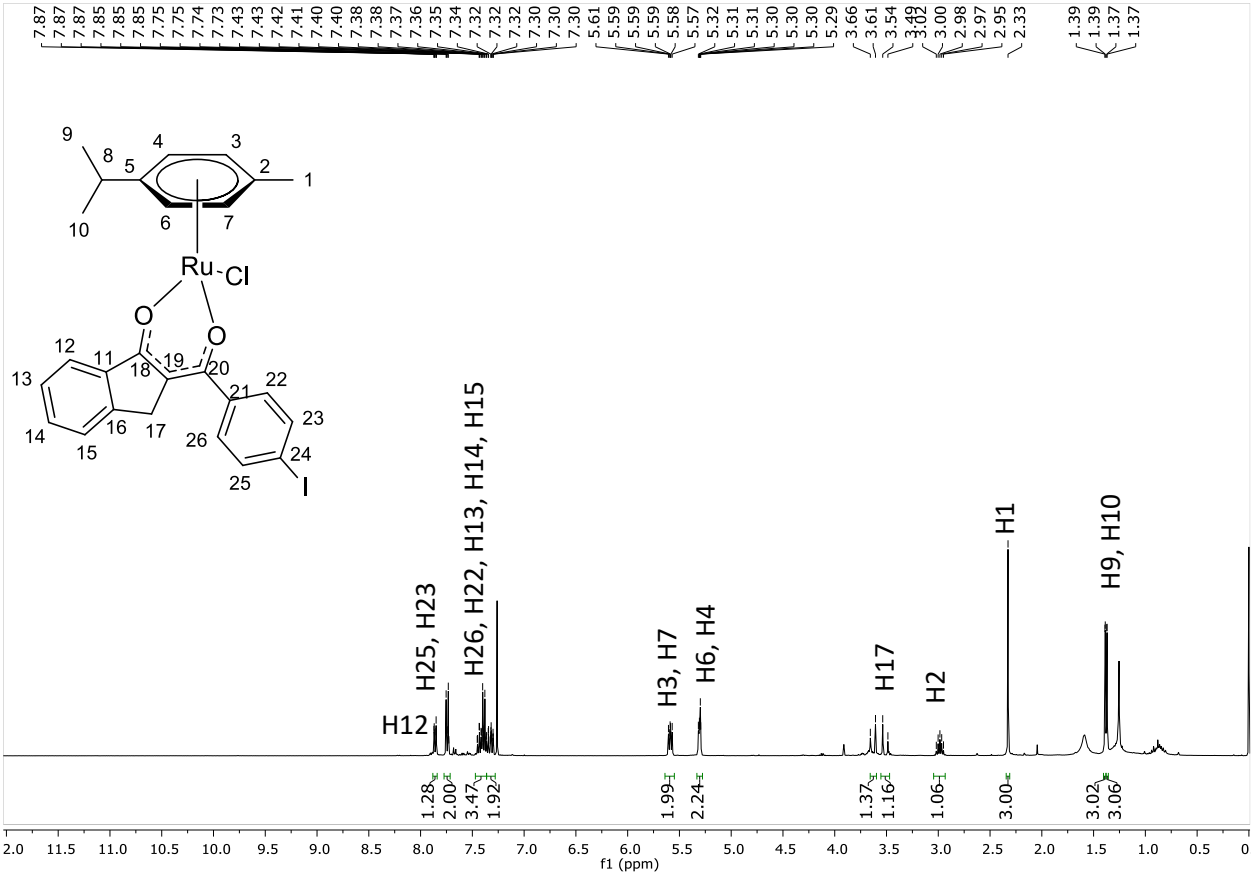


Figure S15: ^{13}C-NMR spectrum of complex **2b** in $CDCl_3$ 400 MHz:

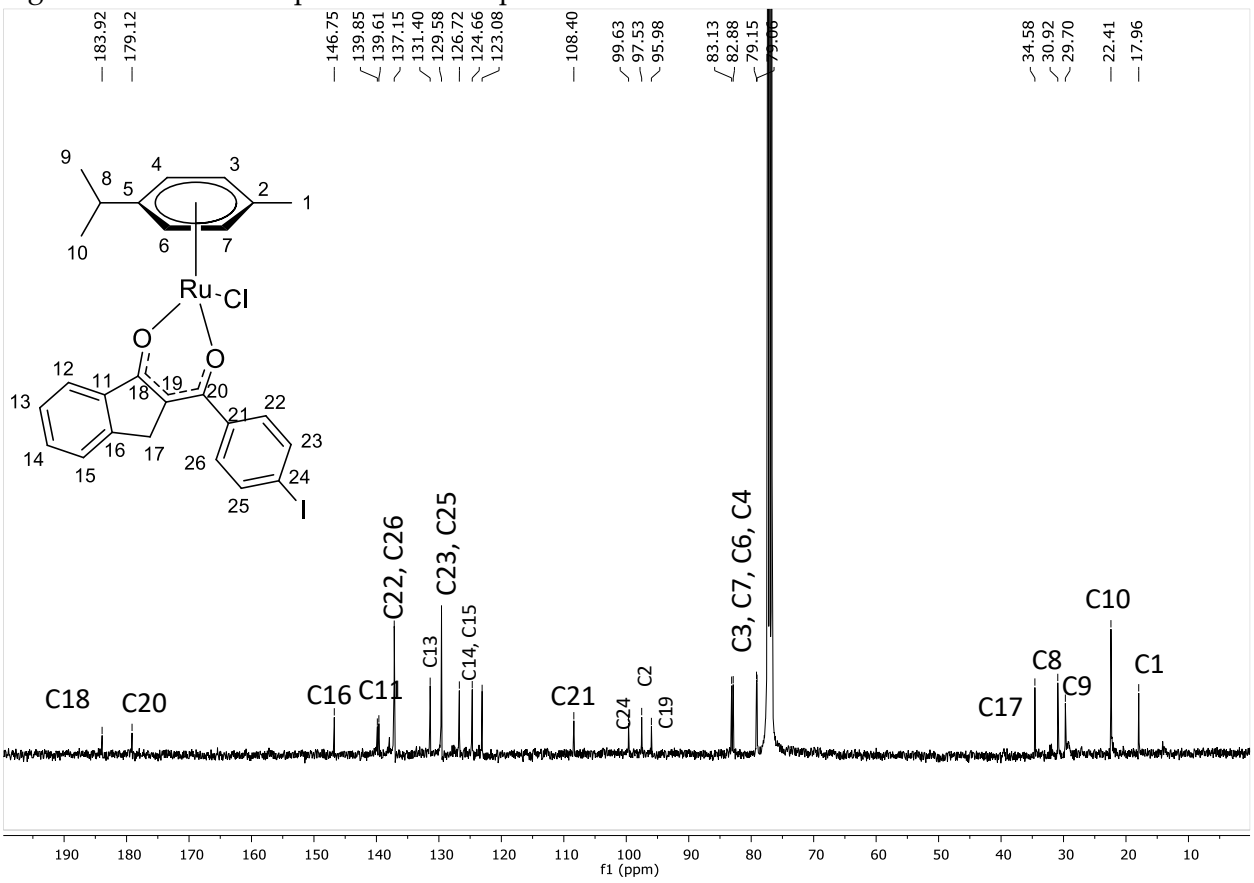


Figure S16: IR spectrum of complex **2c**.

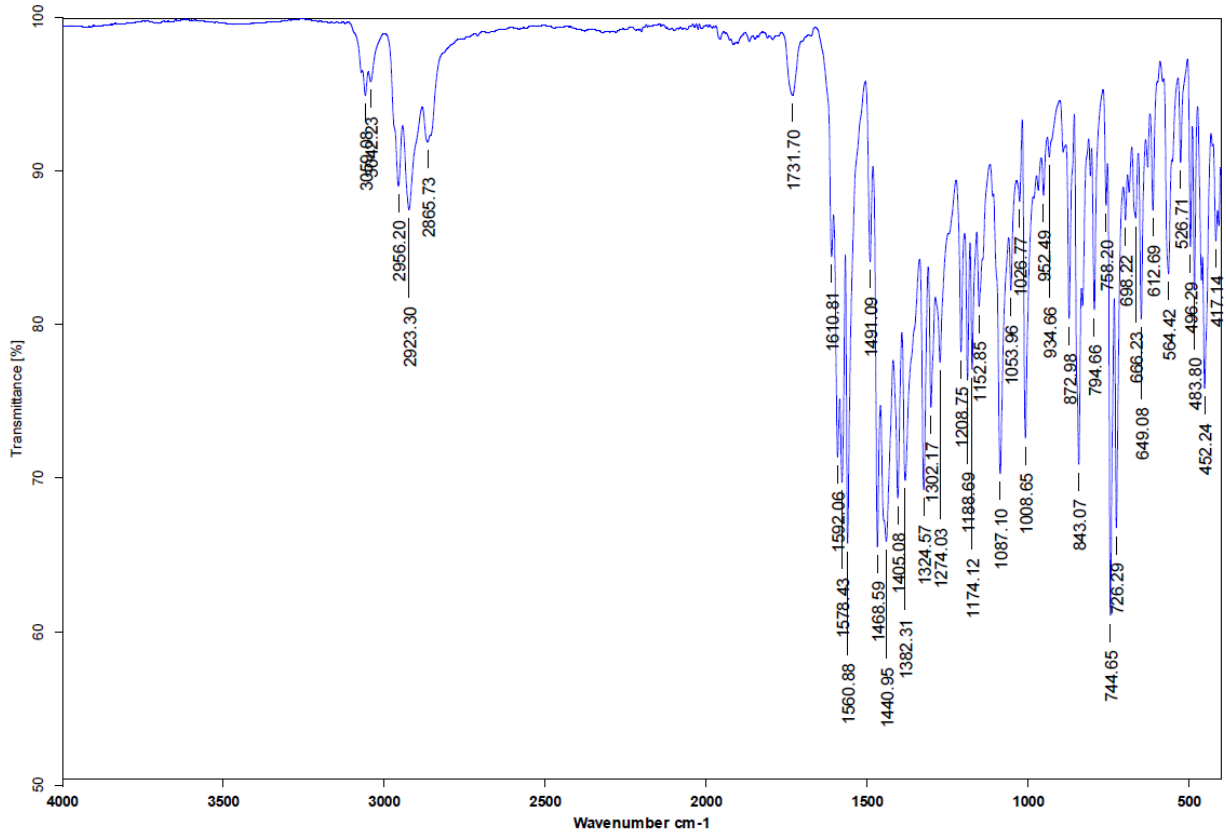


Figure S17: MS spectrum of complex **2c**.

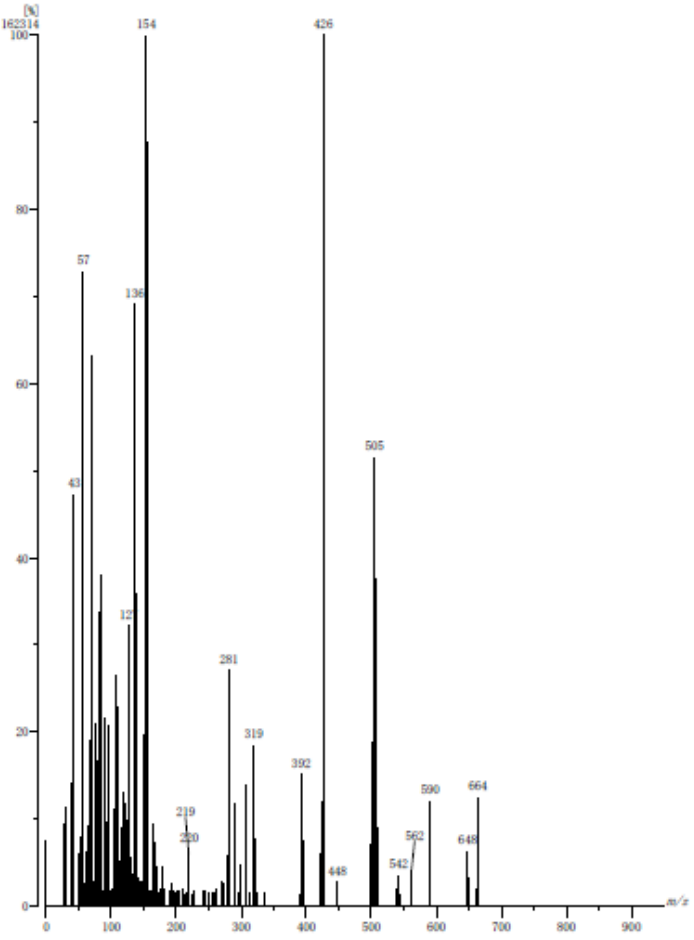


Figure S18: HRMS of complex **2c**.

Inlet : Direct Ion Mode : FAB+
RT : 1.58 min Scan# : (34,38)
Elements : C 26/0, H 30/0, Cl 2/0, O 2/0, Ru 1/0
Mass Tolerance : 1000ppm, 10mmu if m/z > 10
Unsaturation (U.S.) : 0.0 - 30.0

	Observed m/z	Int%							
	540.0201	4.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	Cl	O	Ru
1	540.0197	+0.8 / +0.4	14.5	26	24	2	2	1

Figure S19: ^{1}H-NMR spectrum of **2c** in $CDCl_3$ 400 MHz:

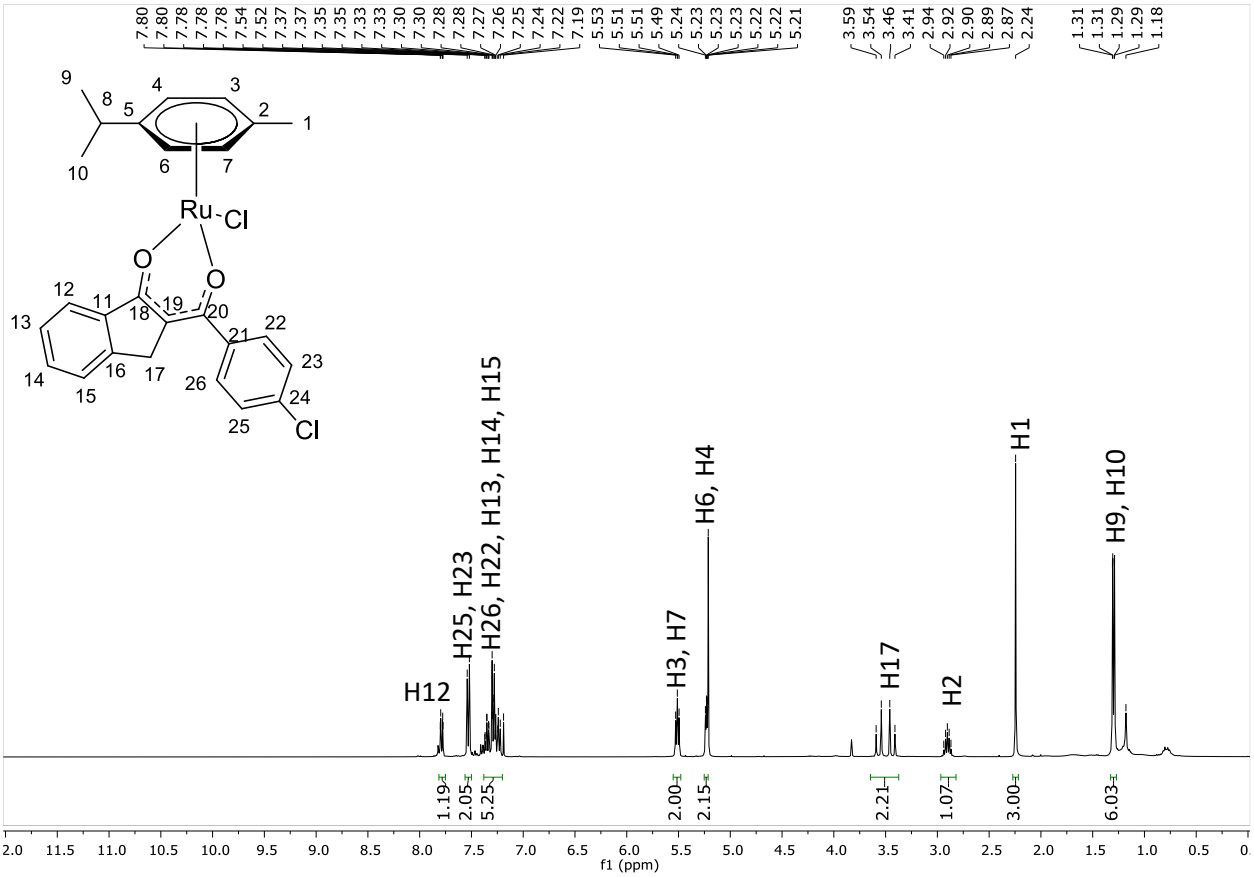


Figure S20: ^{13}C-NMR spectrum of **2c** in $CDCl_3$ 400 MHz:

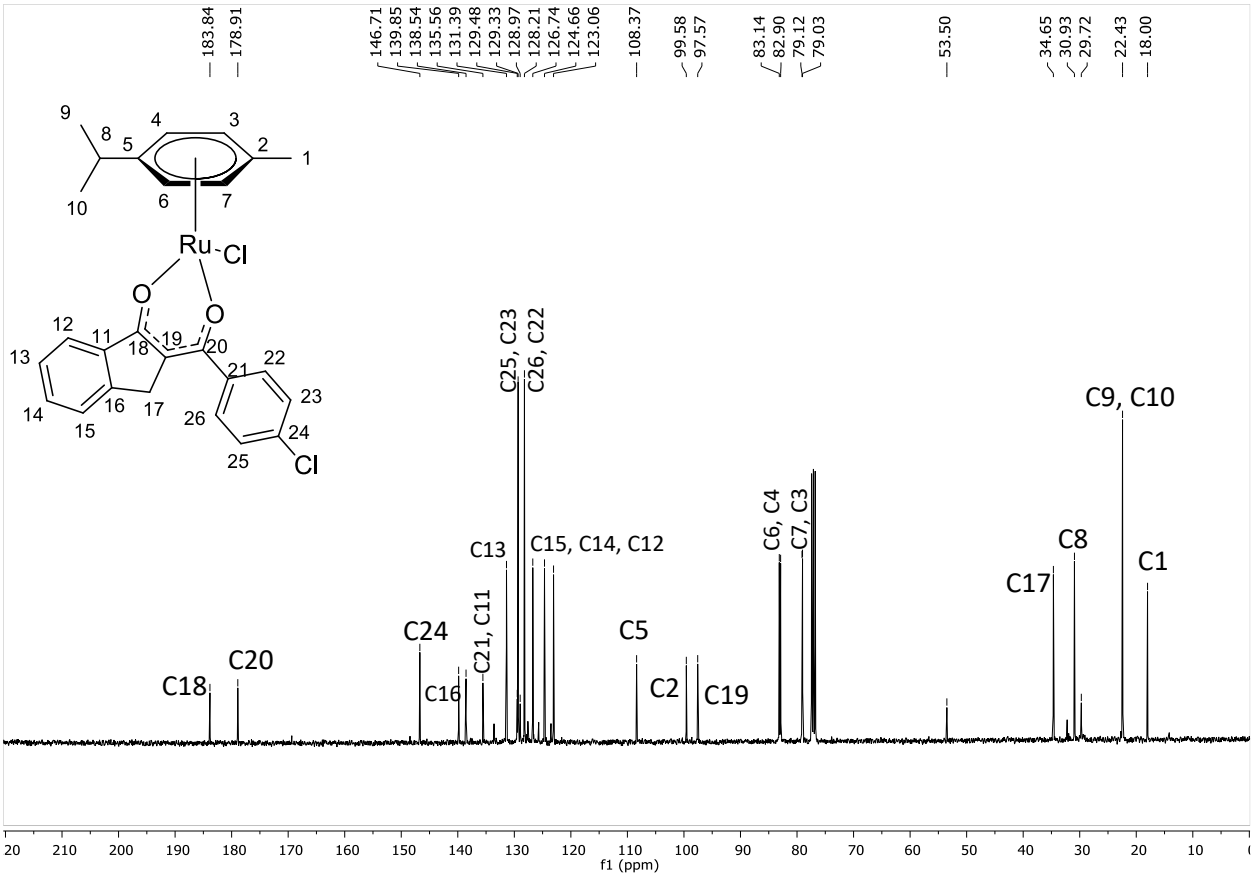


Figure S21: HSQC 2D spectrum of complex **2c**.

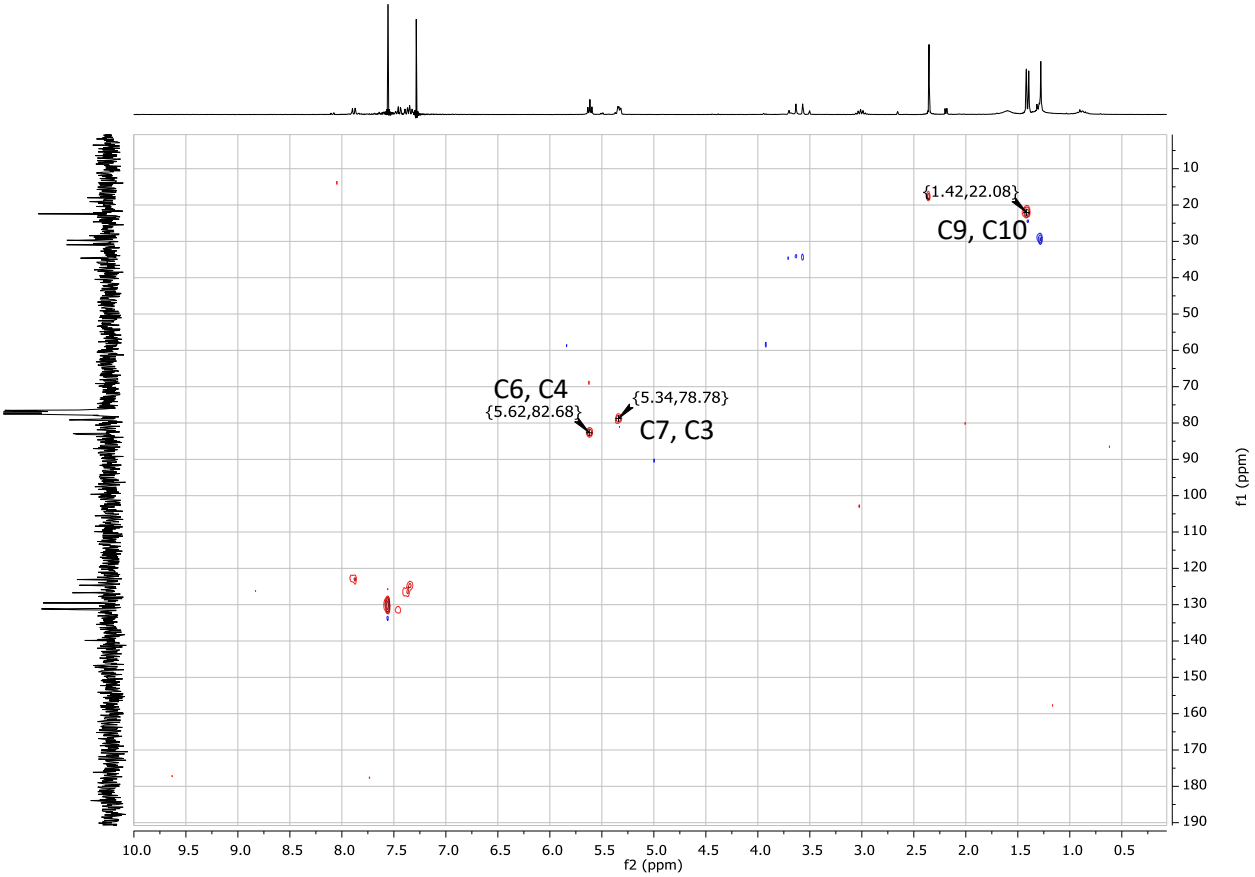


Figure S22: FTIR spectrum of complex **2d**.

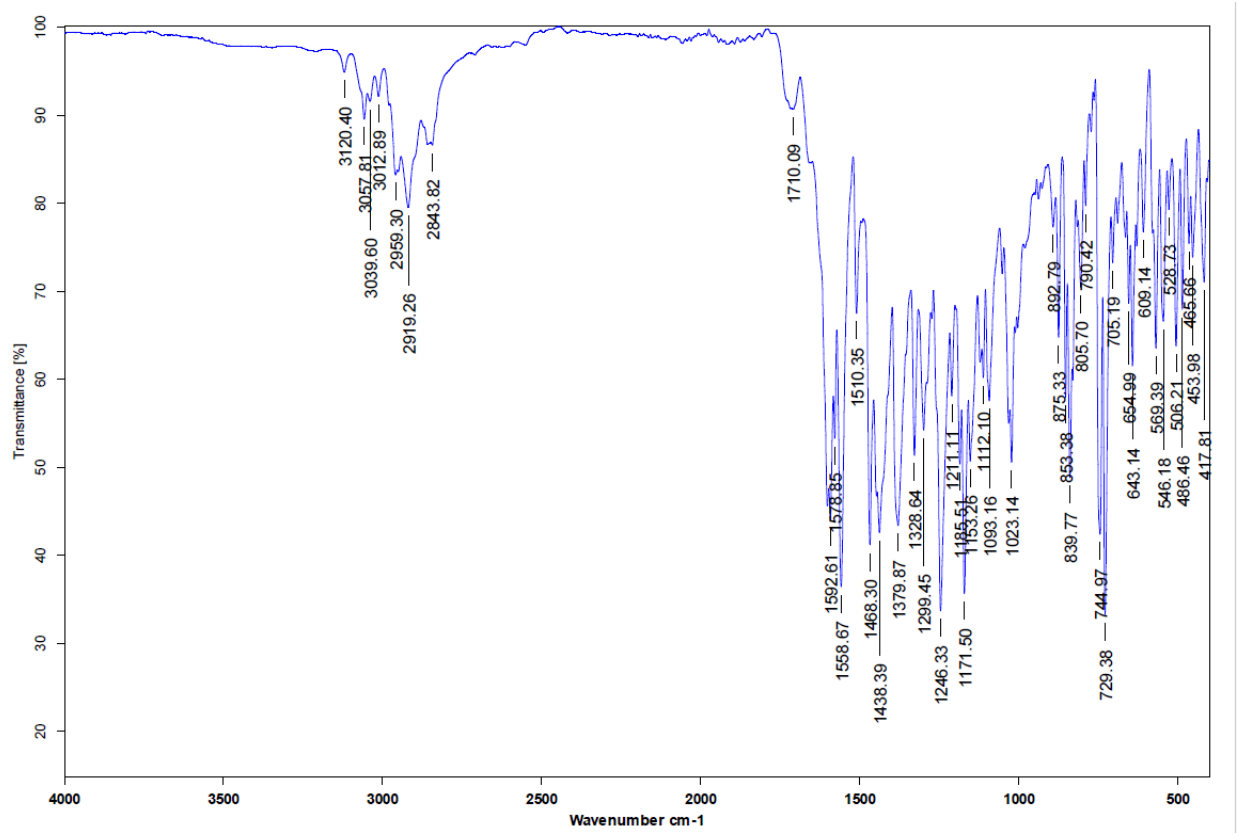


Figure S23: MS spectrum of complex **2d**.

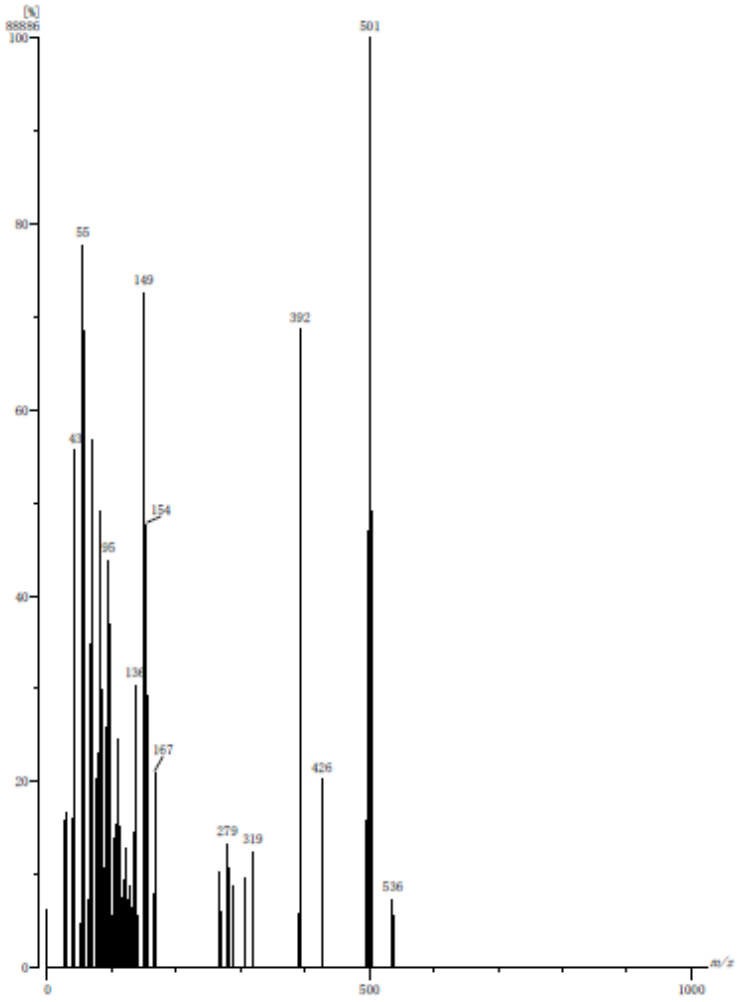


Figure S24: HRMS of complex **2d**.

Inlet : Direct Ion Mode : FAB+
RT : 0.19 min Scan# : (5,9)
Elements : C 27/0, H 30/0, Cl 1/0, O 3/0, Ru 1/0
Mass Tolerance : 1000ppm, 5mmu if m/z > 5
Unsaturation (U.S.) : 0.0 – 30.0

	Observed m/z	Int%						
	536.0672	1.49						
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	Cl	O	Ru
1	536.0692	-3.8 / -2.0	14.5	27	27	1	3	1

Figure S25: ^{1}H-NMR spectrum of complex **2d** in $CDCl_3$ 400 MHz:

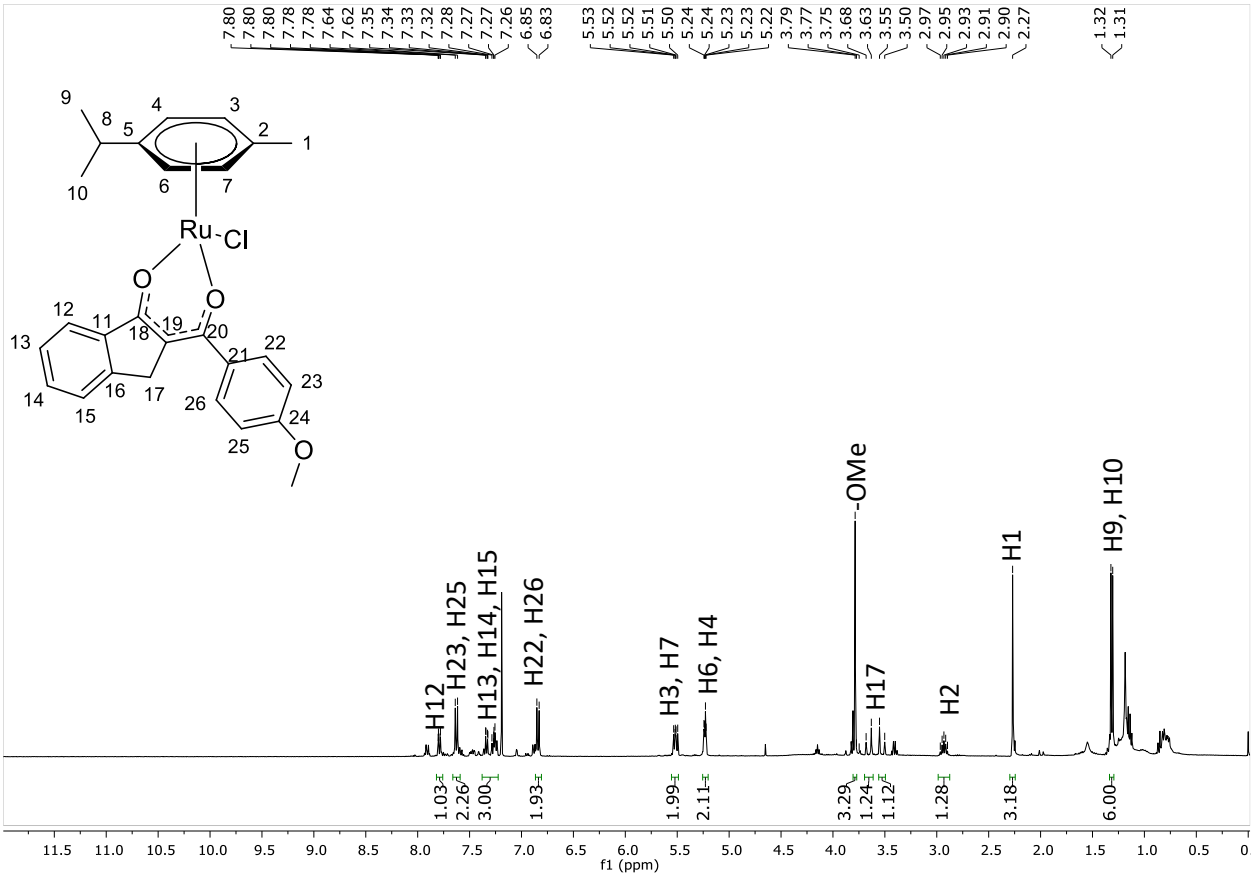


Figure S26: ^{13}C-NMR spectrum of **2d** in $CDCl_3$ 400 MHz:

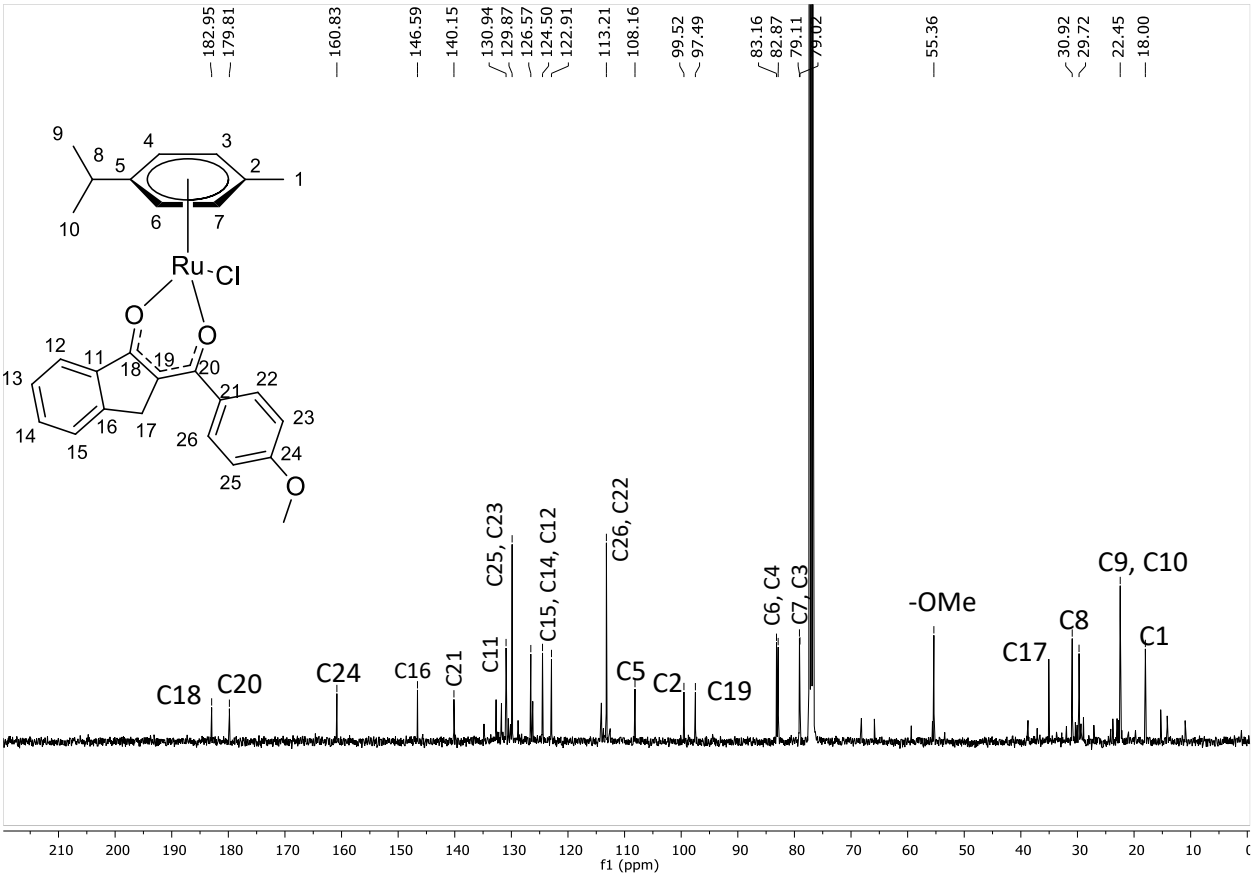


Figure S27: FTIR spectrum of complex **2e**.

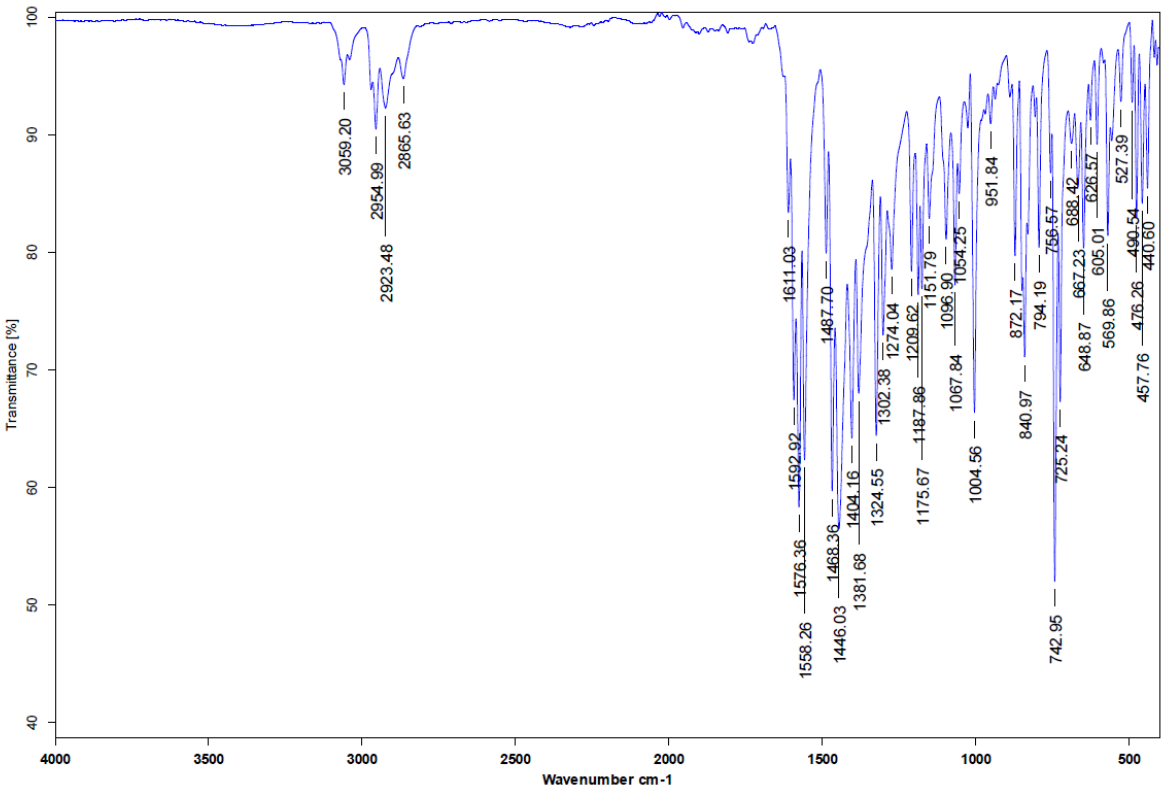


Figure S28: MS spectrum of complex **2d**.

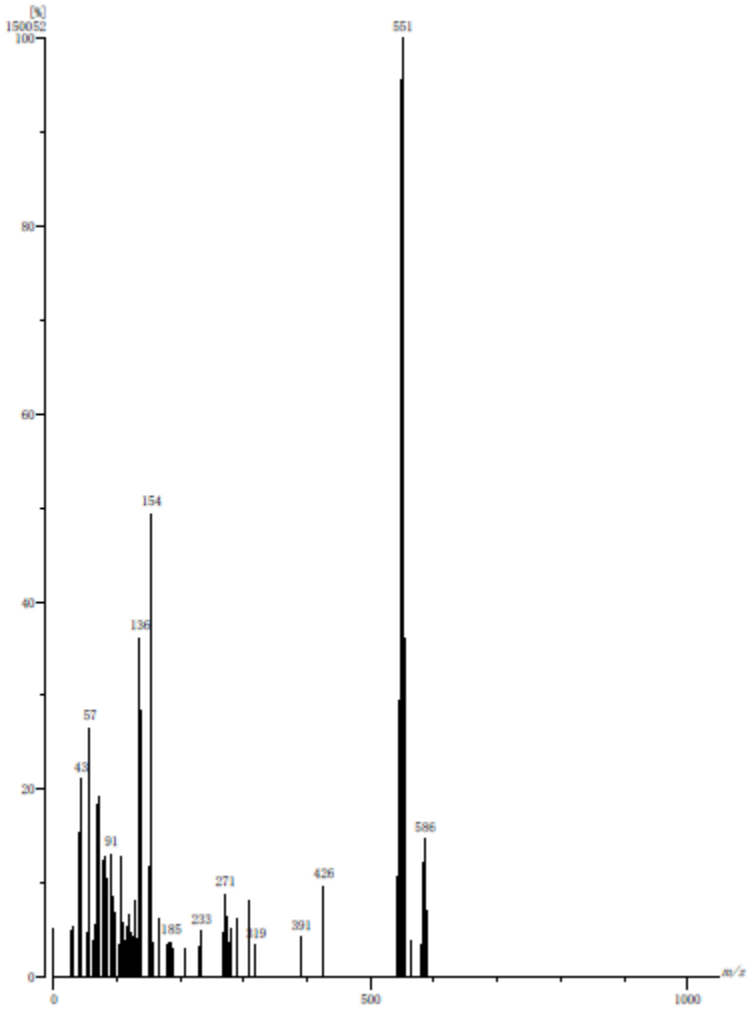


Figure S29: HRMS of complex **2e**.

Inlet : Direct Ion Mode : FAB+
RT : 1.29 min Scan# : (27,28)
Elements : C 26/0, H 26/0, Br 1/0, Cl 1/0, O 2/0, Ru 1/0
Mass Tolerance : 1000ppm, 10mmu if m/z > 10
Unsaturation (U.S.) : 0.0 - 30.0

	Observed m/z	Int%								
	583.9691	2.90								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	Br	Cl	O	Ru	
1	583.9692	-0.1 / -0.1	14.5	26	24	1	1	2	1	

Figure S30: [1]HNMR spectrum of complex **2e**.

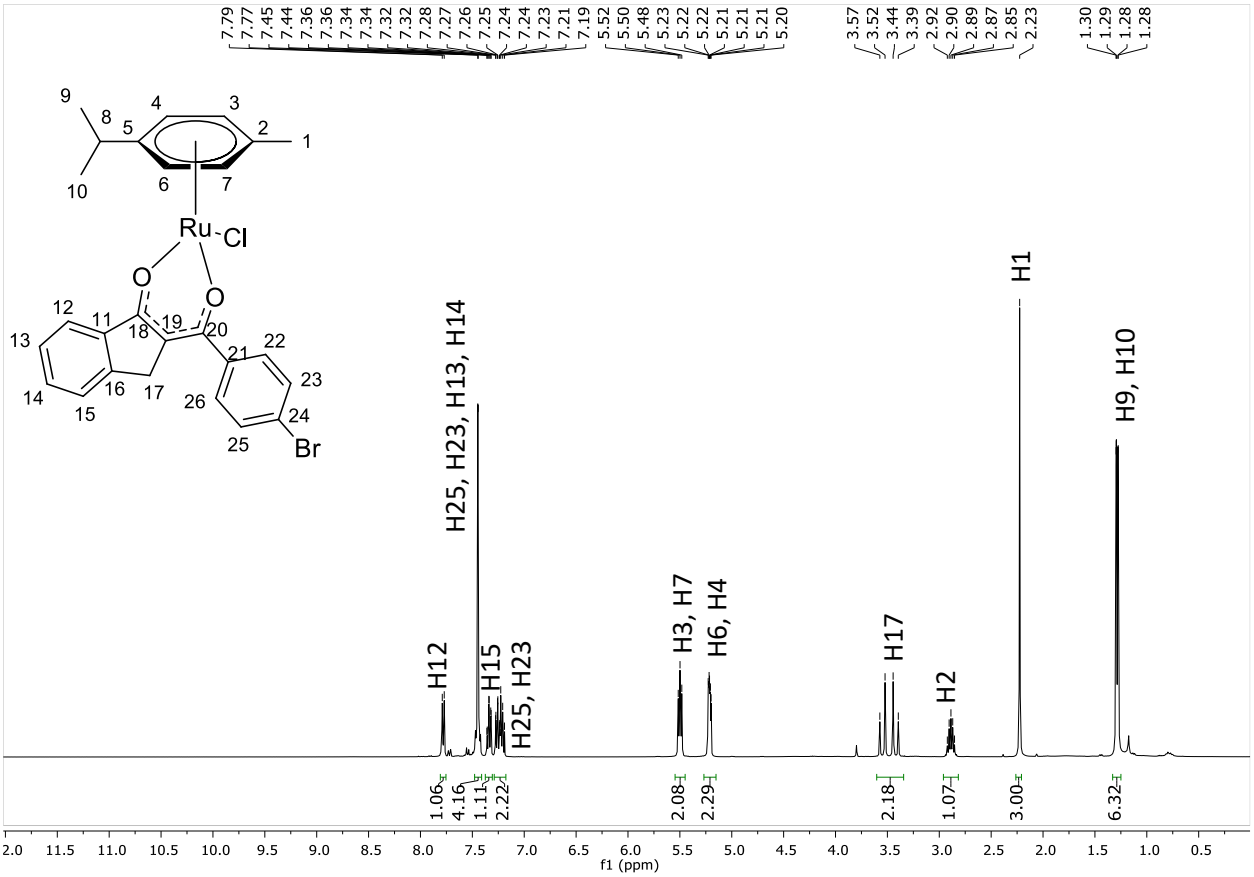


Figure S31: ^{13}CNMR spectrum of complex **2e**.

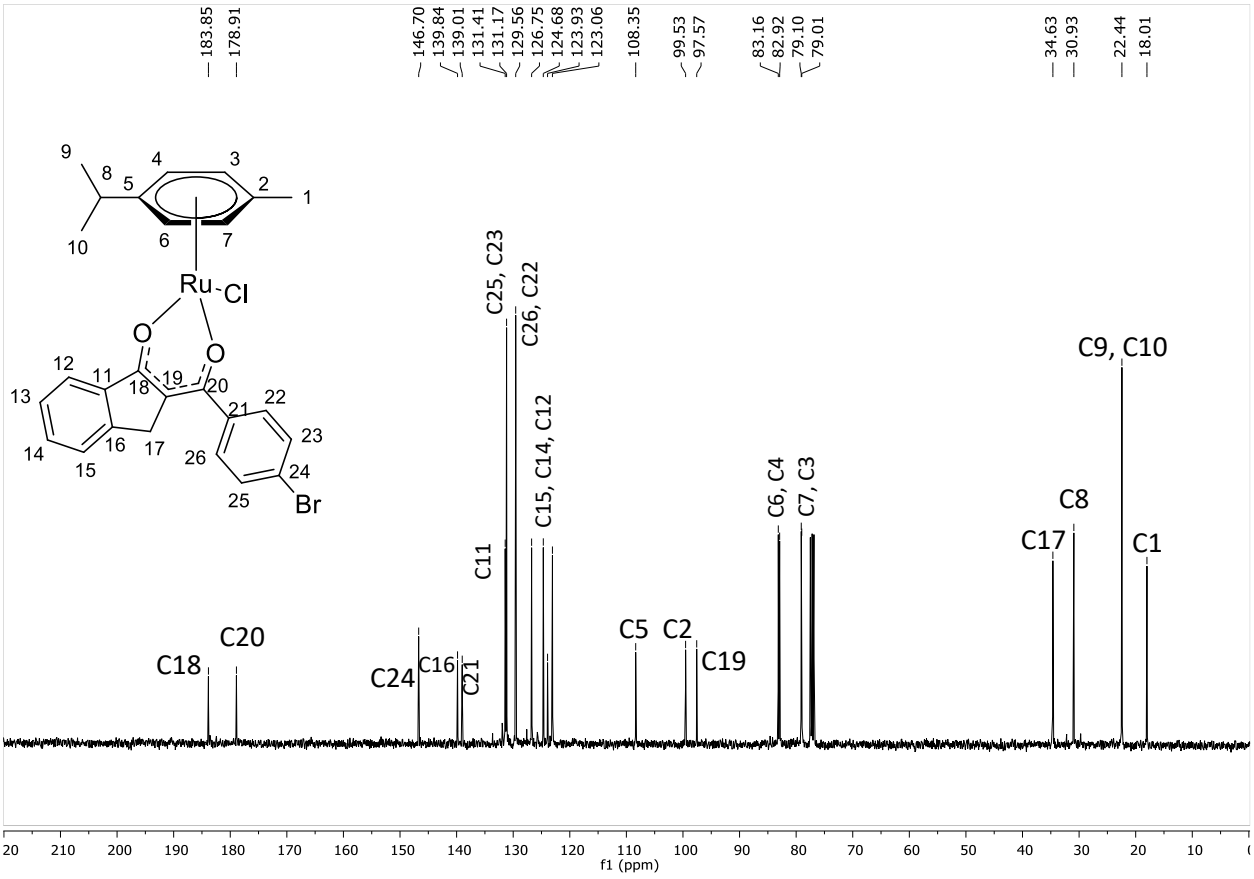
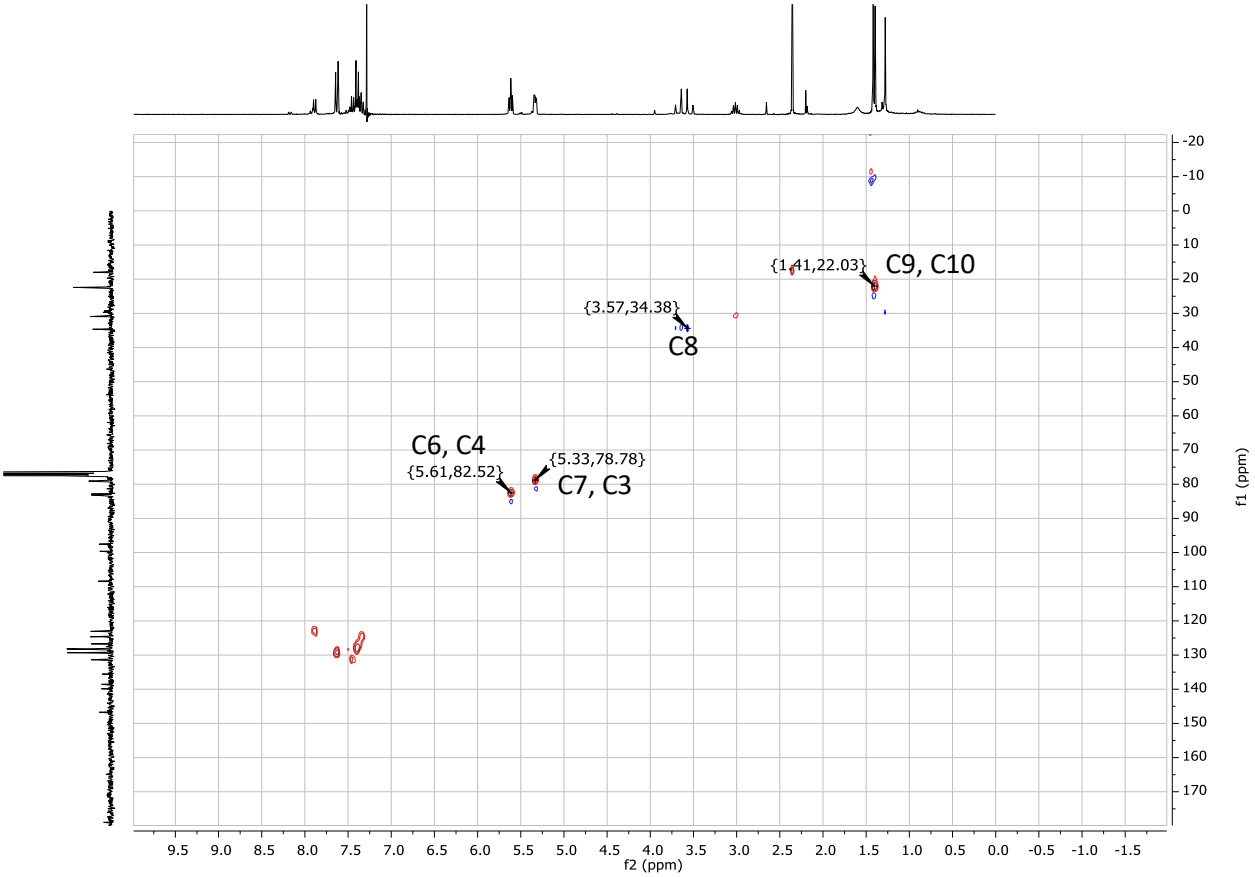


Figure S32: HSQC 2D spectrum of complex 2e in $CDCl_3$.



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Content

Figure IR1: FTIR spectrum of complex **2a** (KBr).

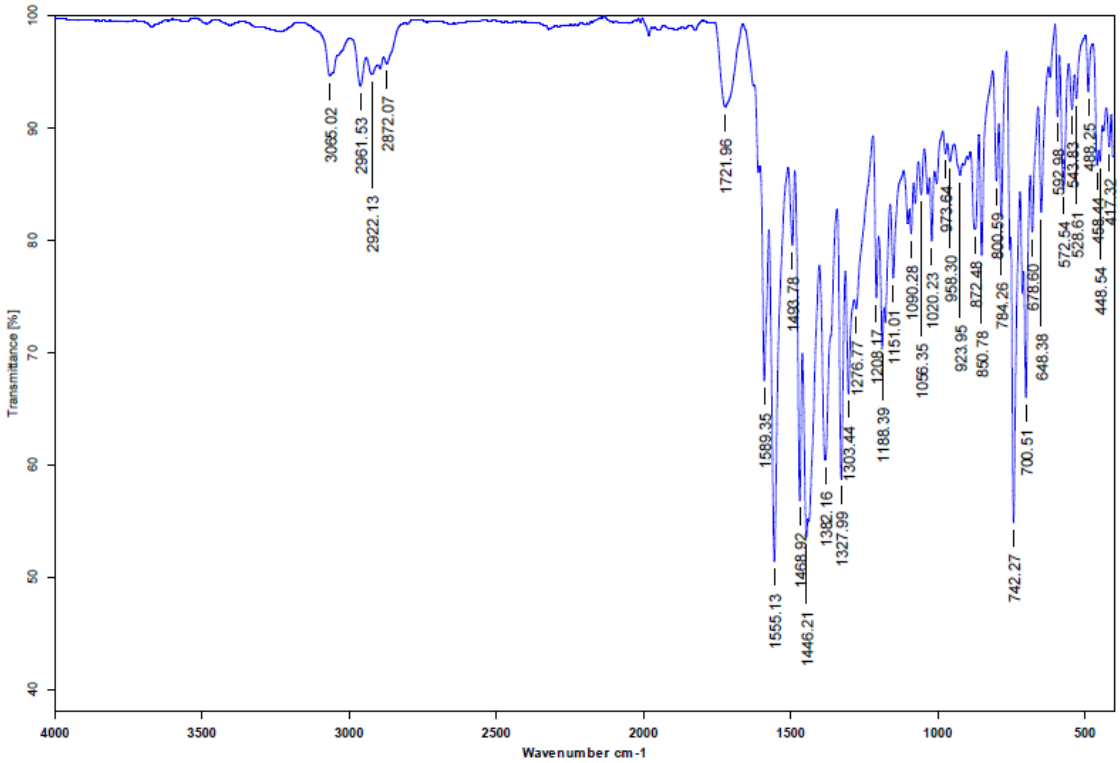

Figure IR2: FTIR spectrum of complex **2a** (hybrid film).

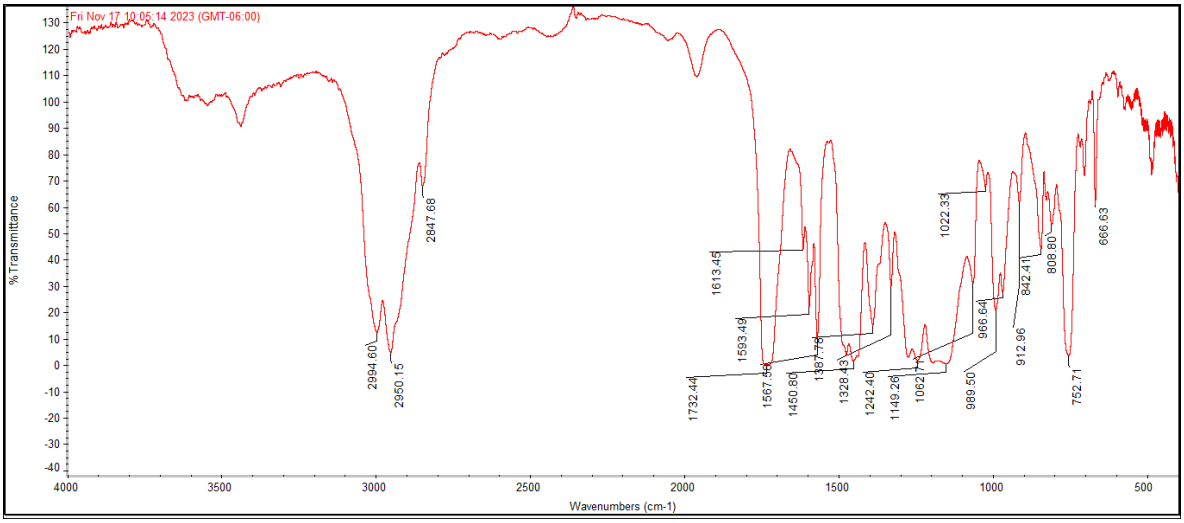

Figure IR3: FTIR spectrum of complex **2b** (KBr).

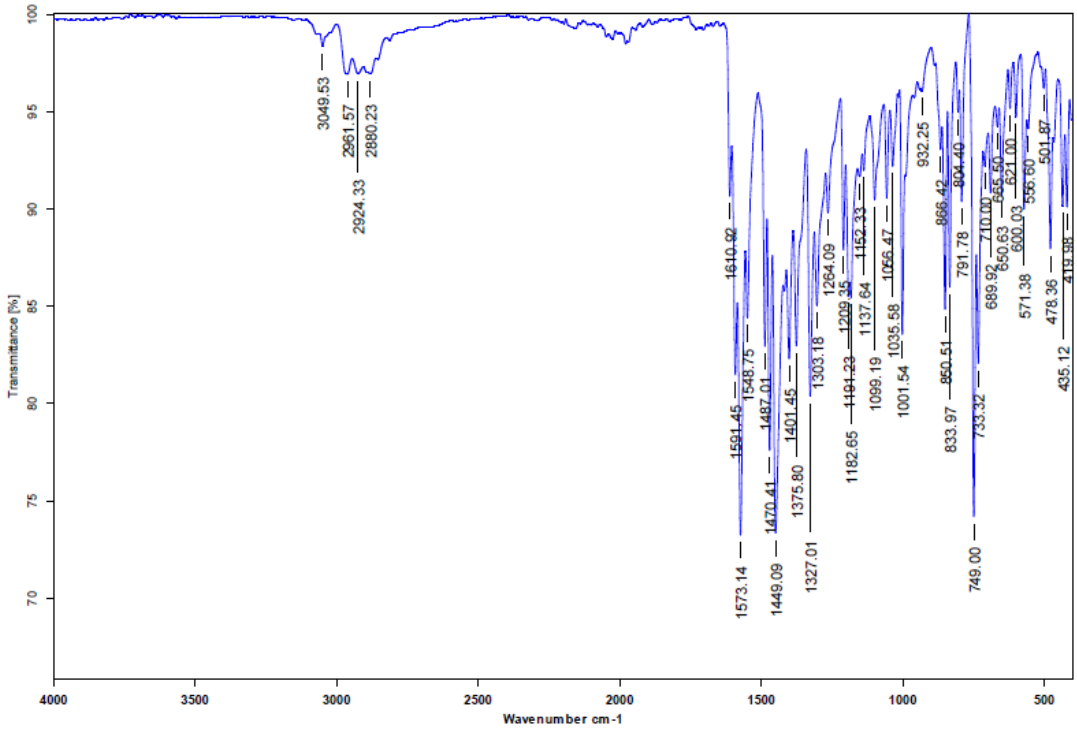

Figure IR4: FTIR spectrum of complex **2b** (hybrid film).

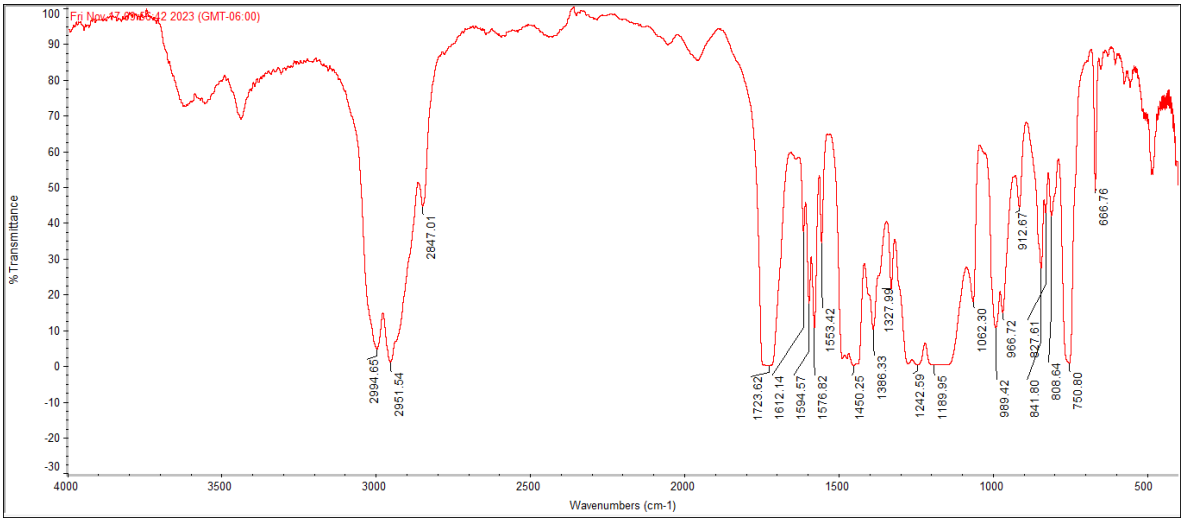

Figure IR5: IR spectrum of complex **2c** (KBr).

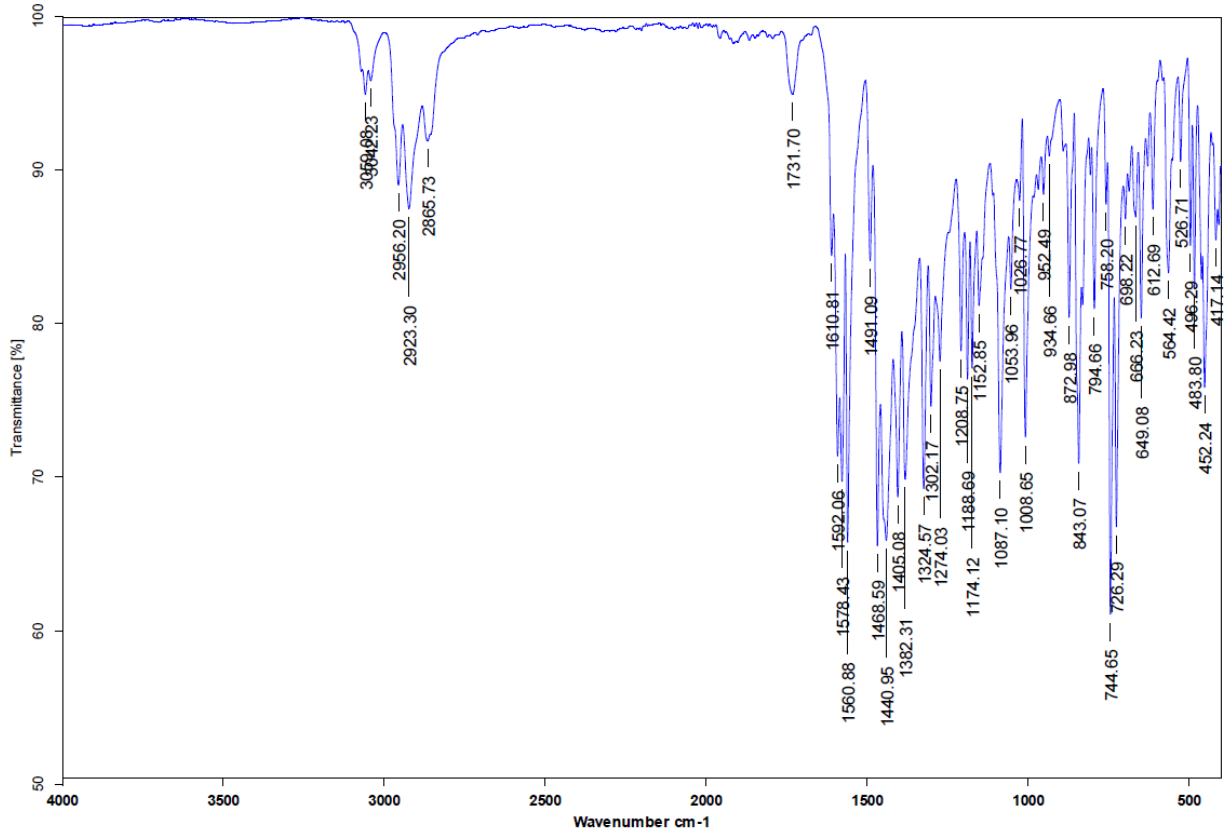

Figure IR6: FTIR spectrum of complex **2c** (hybrid film).

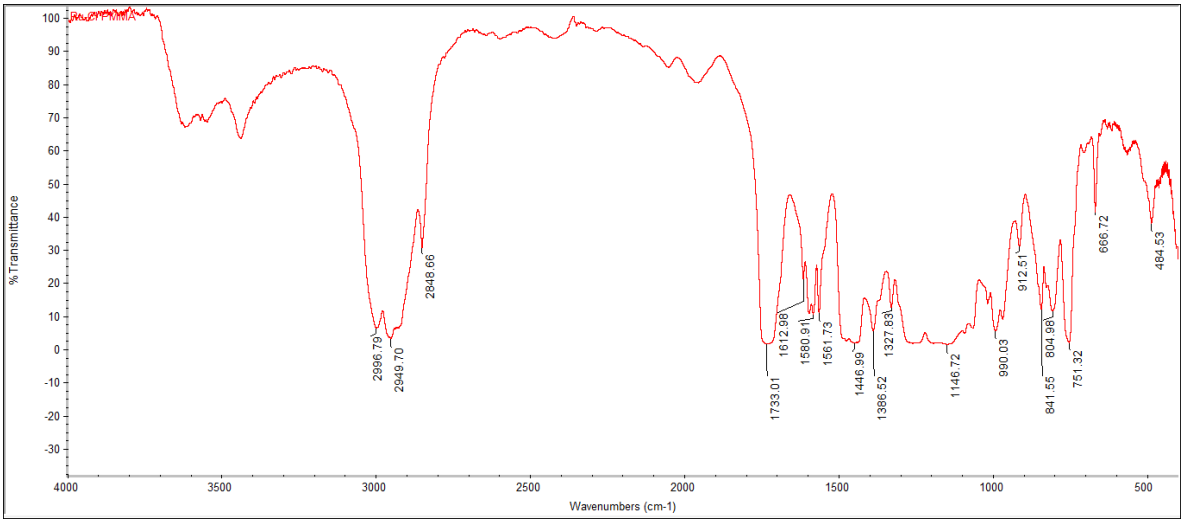

Figure IR7: FTIR spectrum of complex **2d** (KBr).

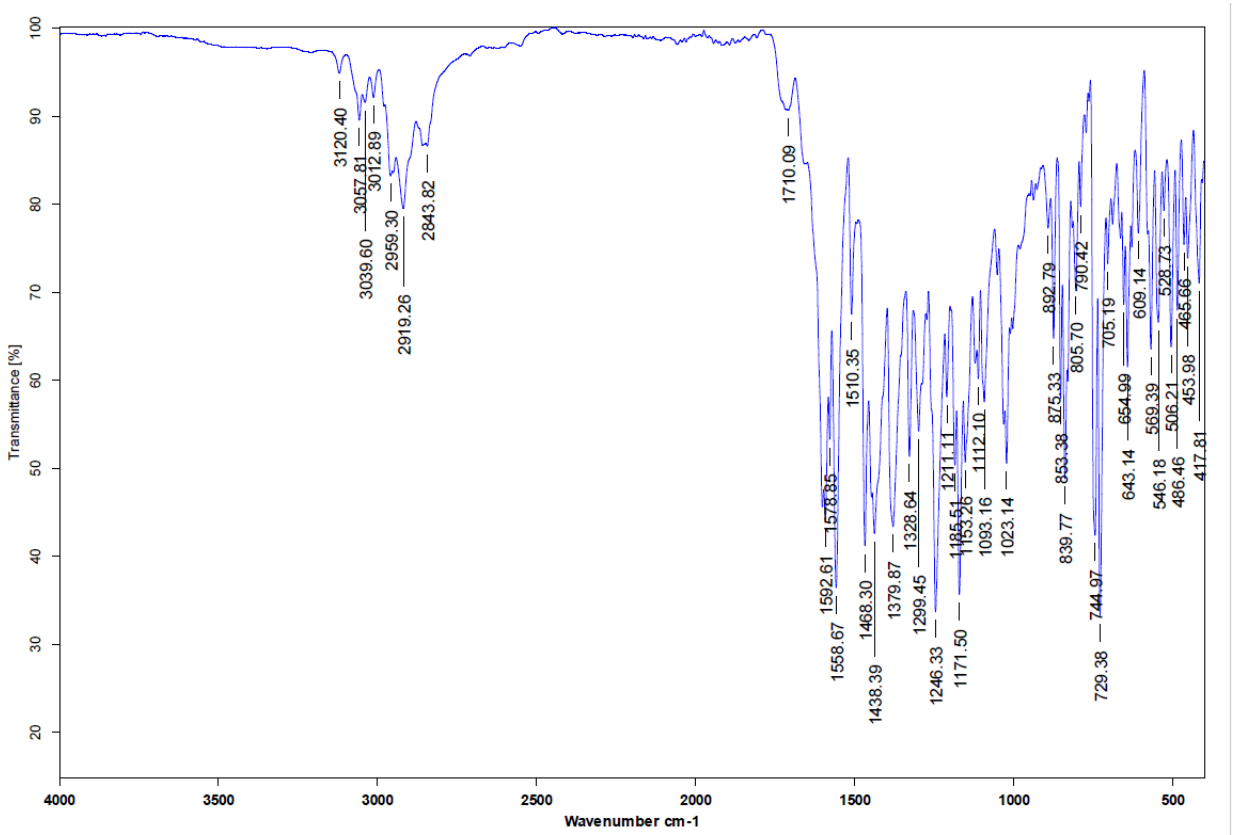

Figure IR8: FTIR spectrum of complex **2d** (hybrid film).

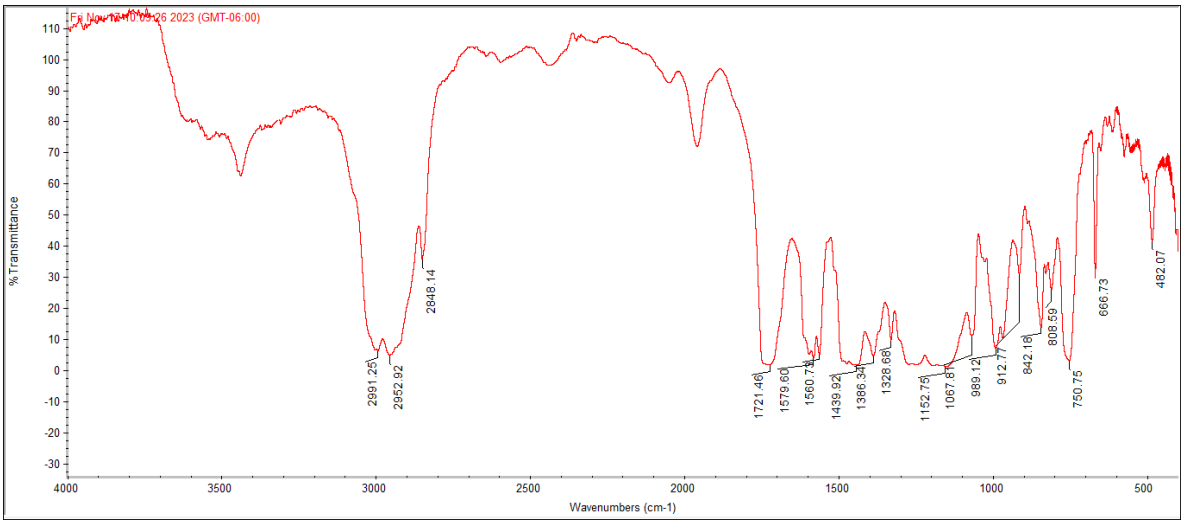

Figure IR9: FTIR spectrum of complex **2e** (KBr).

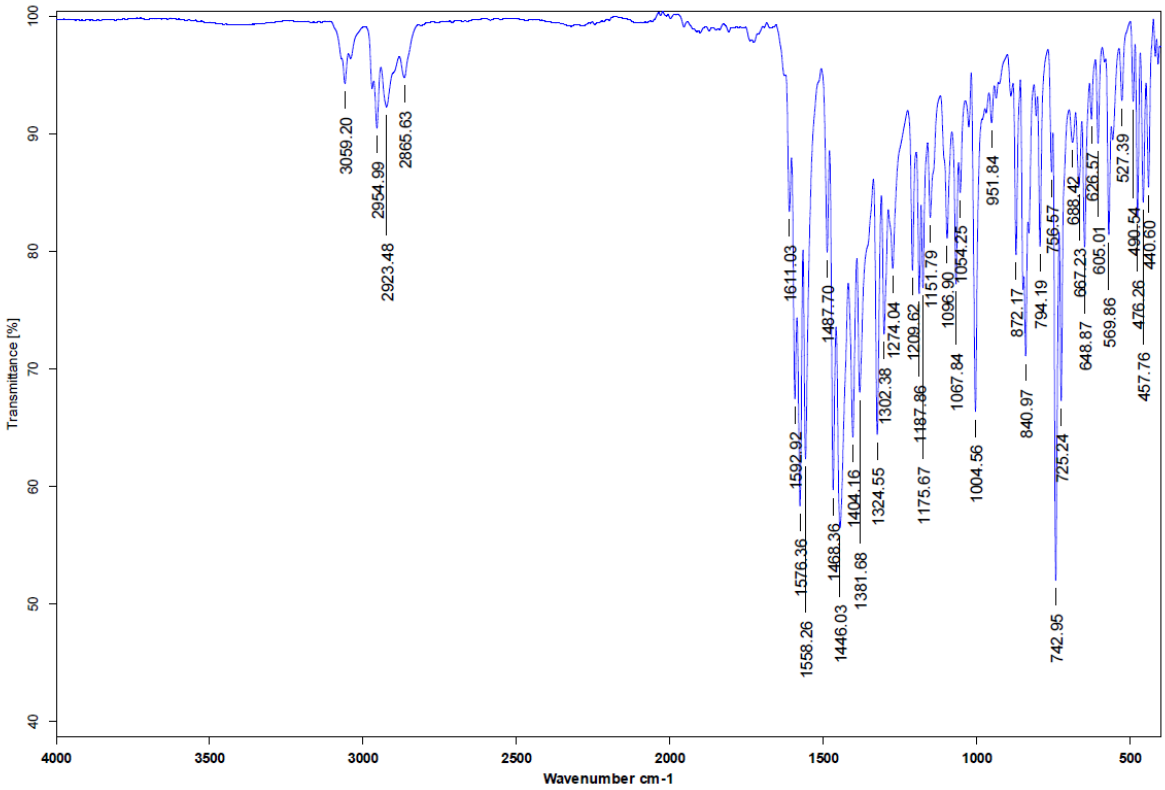

Figure IR10: FTIR spectrum of complex **2e** (hybrid film).