

Electronic Supplementary Information

Half-Sandwich Complexes of Ir(III), Rh(III) and Ru(II) with the MaxPhos Ligand: Metal Centred Chirality and Cyclometallation

Juan Téllez,^a Albert Gallen,^b Joaquina Ferrer,^{a*} Fernando J. Lahoz,^a Pilar García-Orduña,^a Antoni Riera,^{c,d} Xavier Verdager,^{c,d} Daniel Carmona,^{a*} and Arnald Grabulosa^{b*}

^a Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC - Universidad de Zaragoza, Departamento de Química Inorgánica, Pedro Cerbuna 12, Zaragoza 50009, Spain, E-mail: dcarmona@unizar.es.

^b Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Universitat de Barcelona, Martí i Franquès 1-11, Barcelona 08028, Spain, E-mail: arnald.grabulosa@qi.ub.es.

^c Institute for Research in Biomedicine (IRB-Barcelona), The Barcelona Institute of Science and Technology, Baldiri i Reixac 10, Barcelona 08028, Spain.

^d Departament de Química Inorgànica i Orgànica, Secció de Química Orgànica, Universitat de Barcelona, Martí i Franquès 1-11, 08028, Barcelona, Spain.

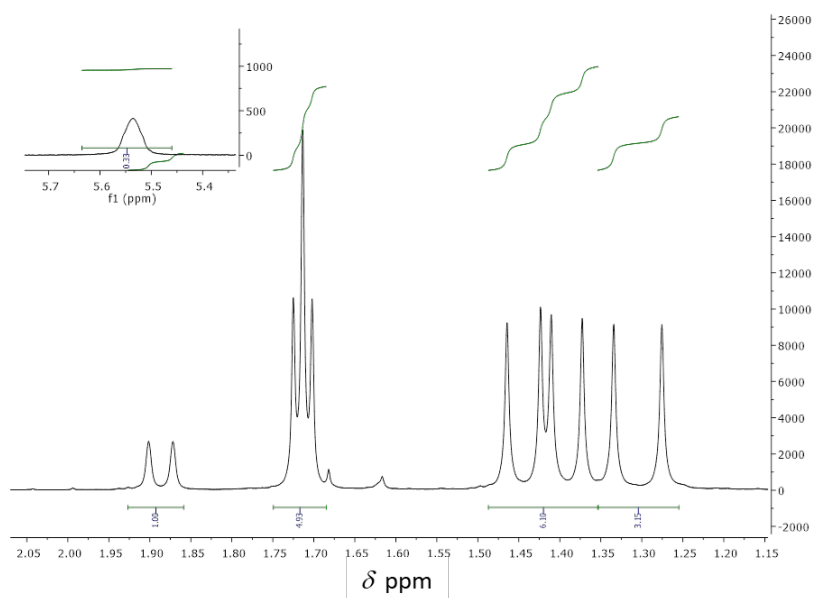
Table of contents

1. Selected NMR spectra	S2
2. Selected IR spectra	S15
3. Mass spectra of complex 6	S18
4. Selected CD spectra	S20

1. Selected NMR spectra

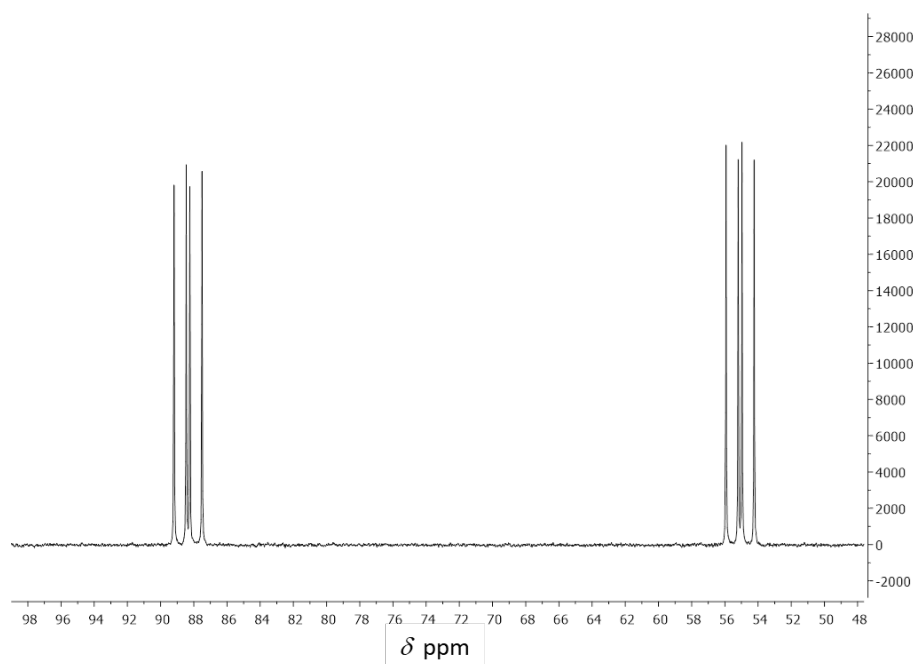
Complex 1

^1H -NMR (300.13 MHz, CDCl_3 , 298 K)



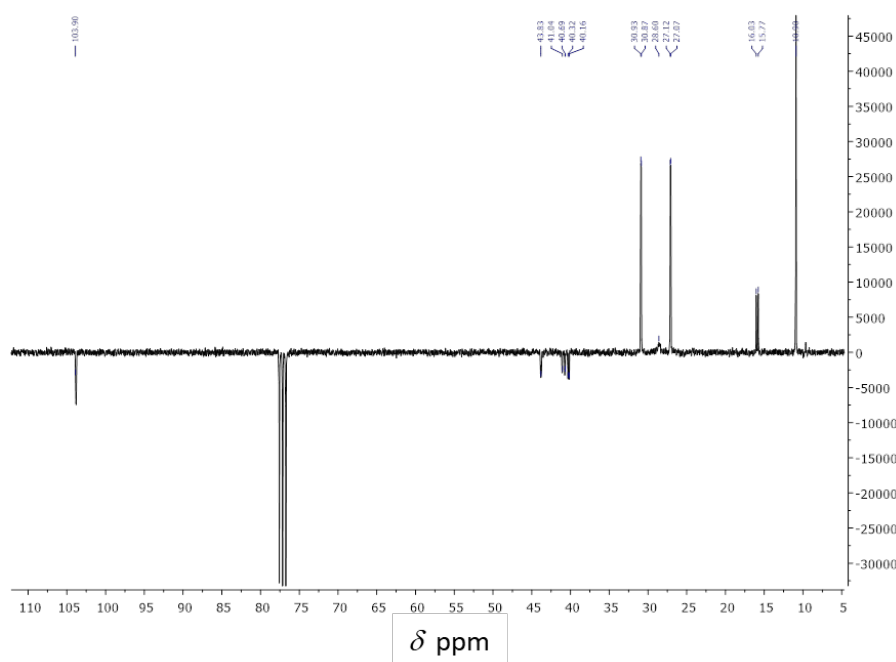
Complex 1

$^{31}\text{P}\{^1\text{H}\}$ -NMR (121.42 MHz, CDCl_3 , 298 K)



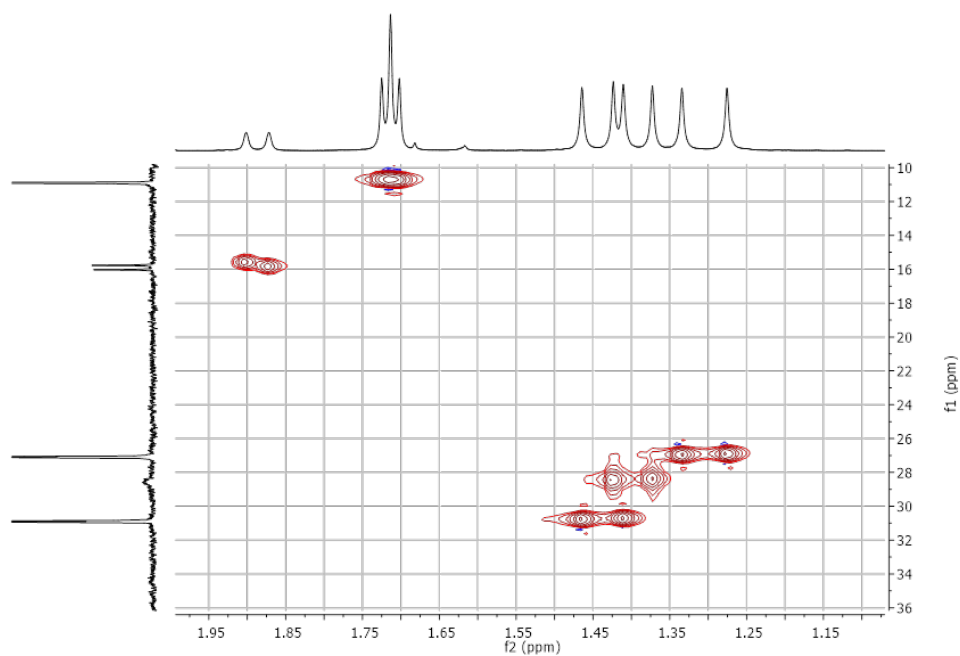
Complex 1

$^{13}\text{C}\{^1\text{H}\}$ -APT (75.48 MHz, CDCl_3 , 298 K)



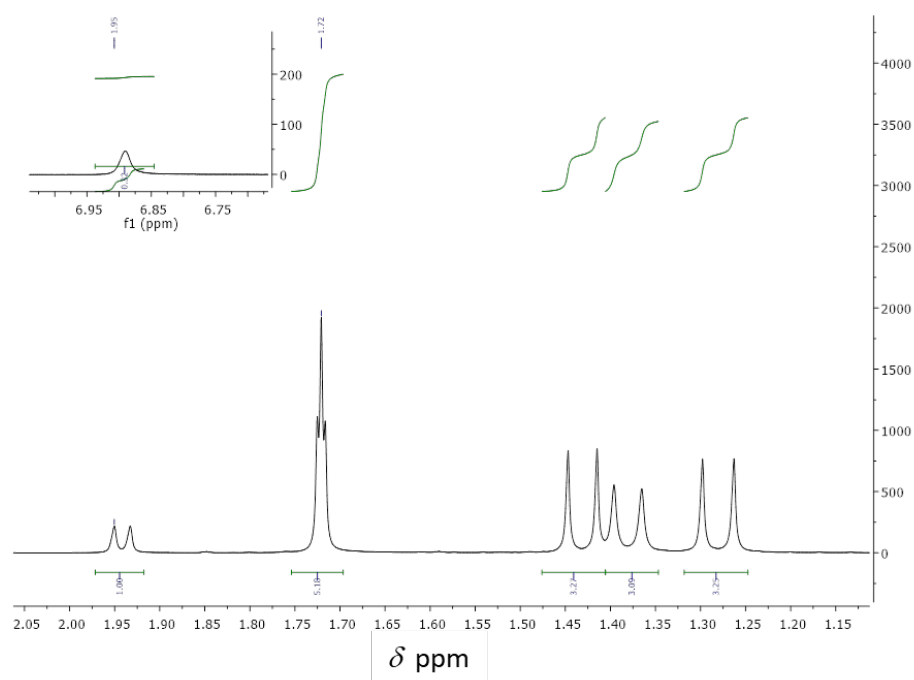
Complex 1

^1H - ^{13}C HSQC (CDCl_3 , 298 K)



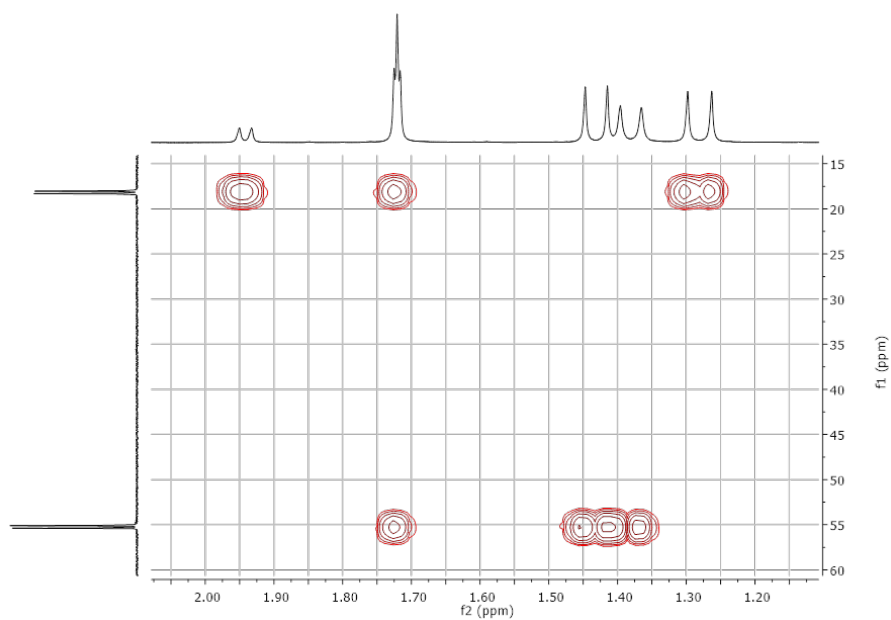
Complex 2

^1H -NMR (500.13 MHz, CDCl_3 , 298 K)



Complex 2

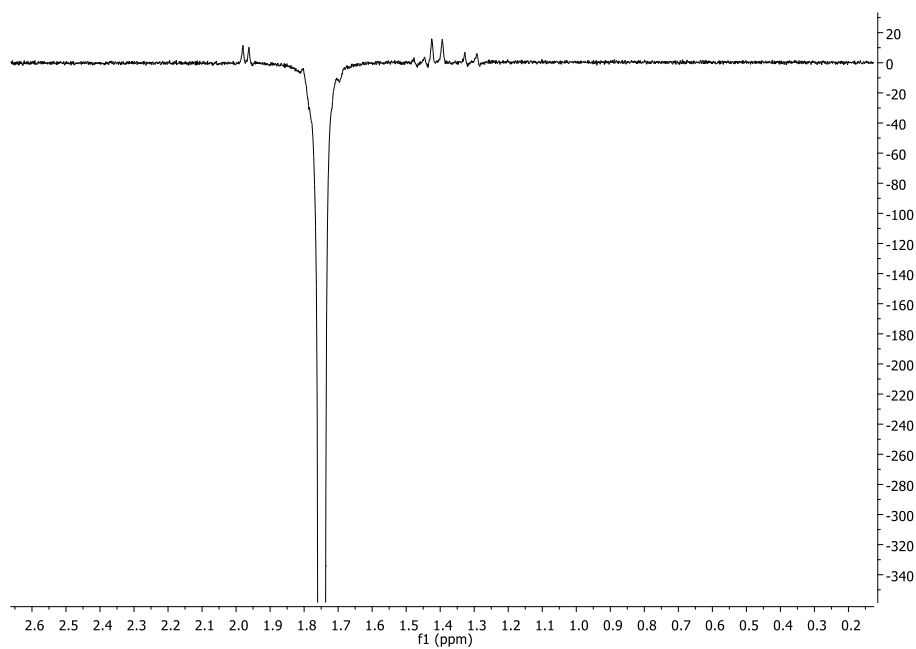
^1H - ^{31}P HMBC (CDCl_3 , 298 K)



Complex 2

NOE (500.13 MHz, CDCl₃, 298 K)

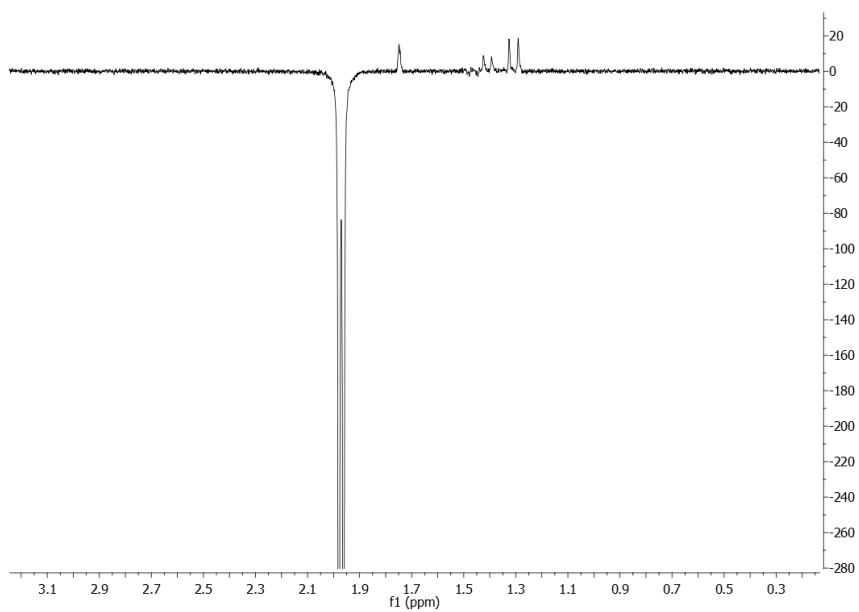
Irradiation of the C₅Me₅ signal



Complex 2

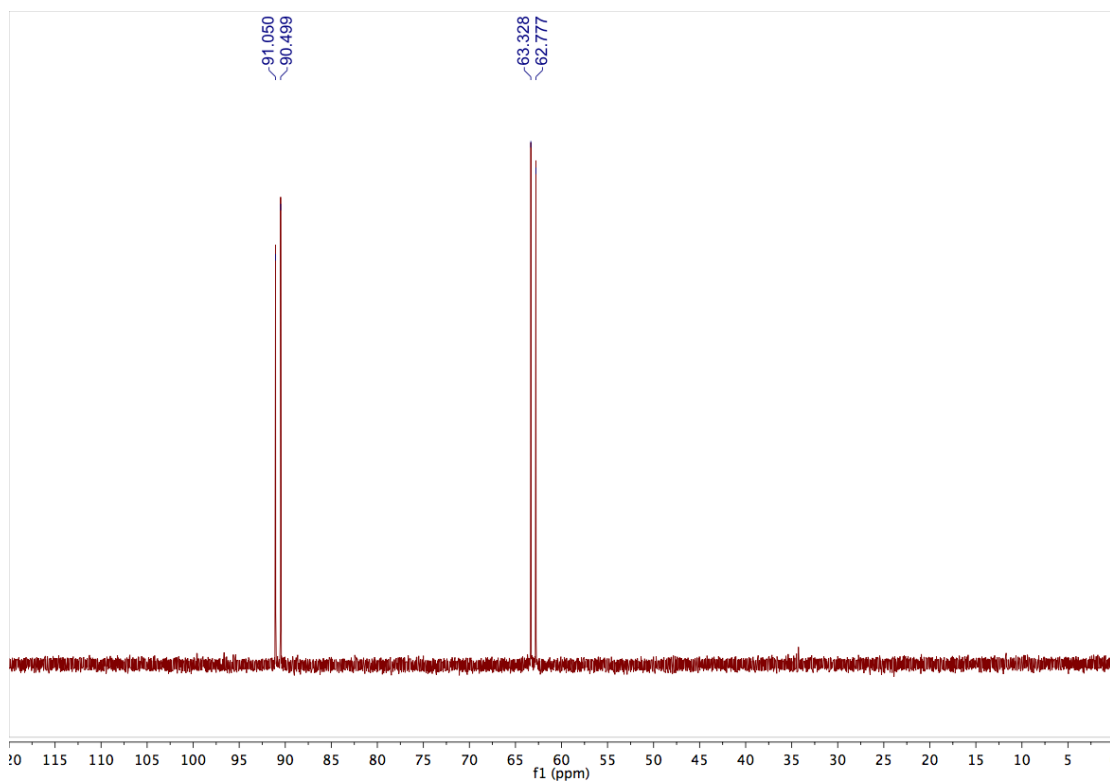
NOE (500.13 MHz, CDCl₃, 298 K)

Irradiation of the P¹Me signal



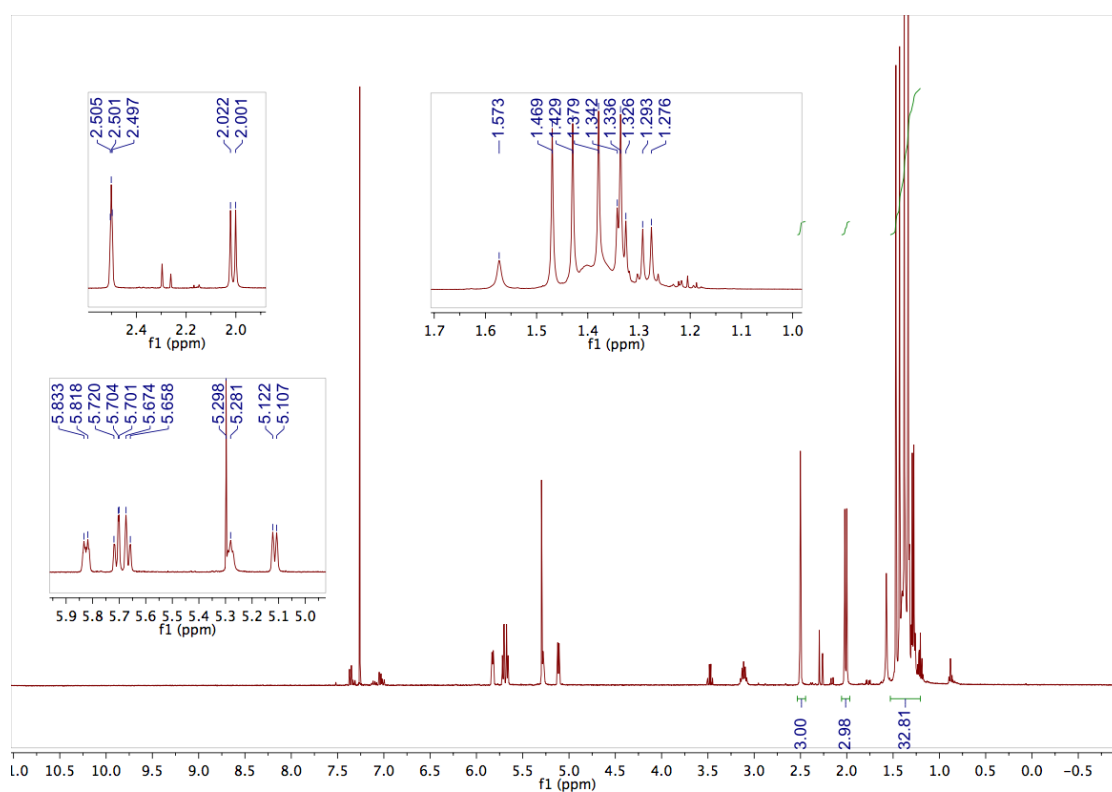
Complex 3

$^{31}\text{P}\{^1\text{H}\}$ -NMR (161.9 MHz, CDCl_3 , 298 K)



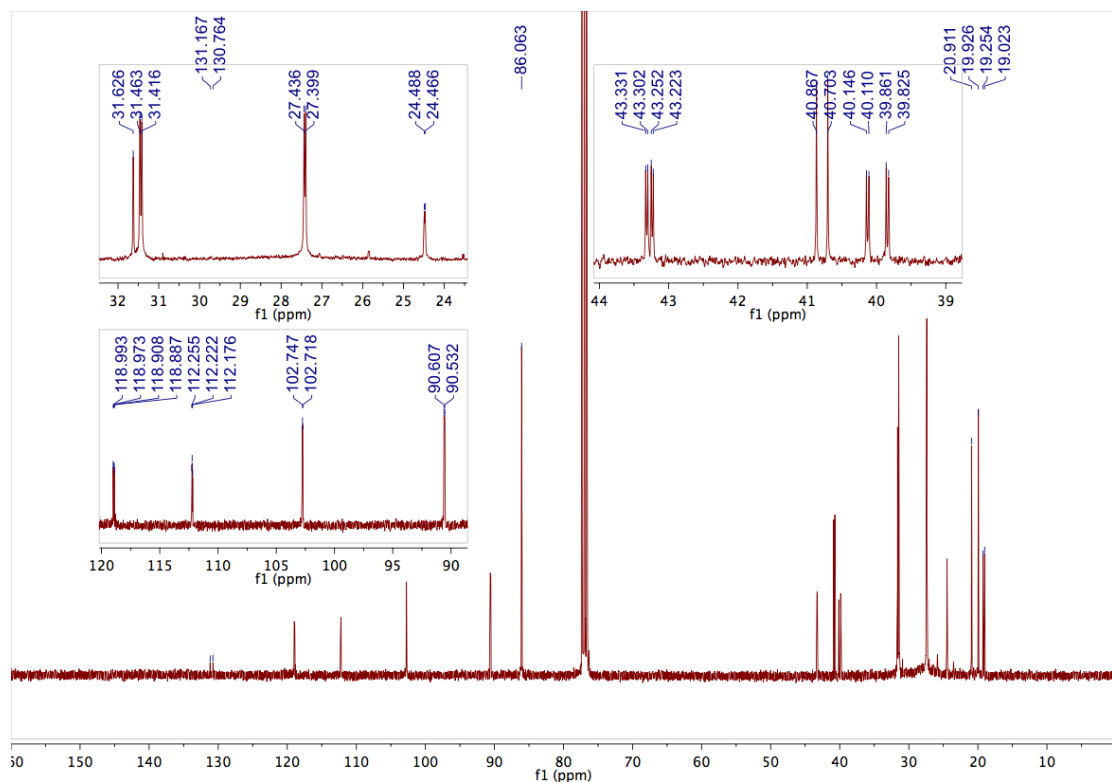
Complex 3

^1H -NMR (400.13 MHz, CDCl_3 , 298 K)



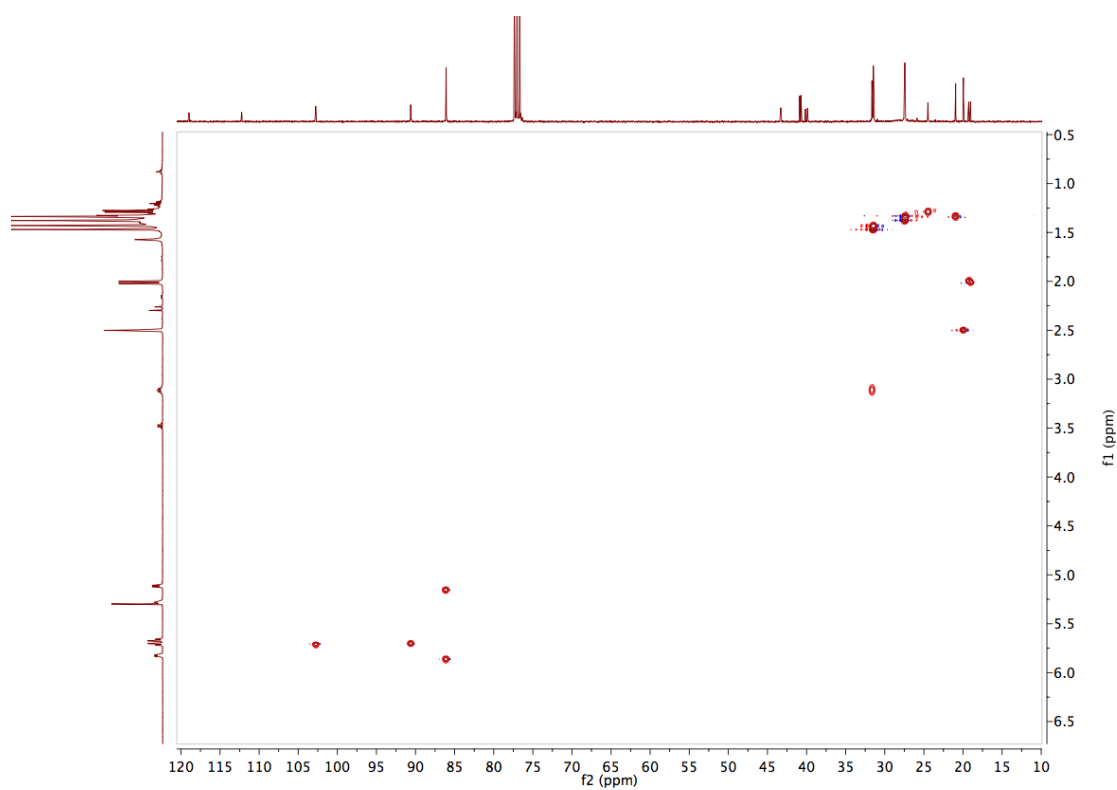
Complex 3

$^{13}\text{C}\{^1\text{H}\}$ -NMR (100.5 MHz, CDCl_3 , 298 K)



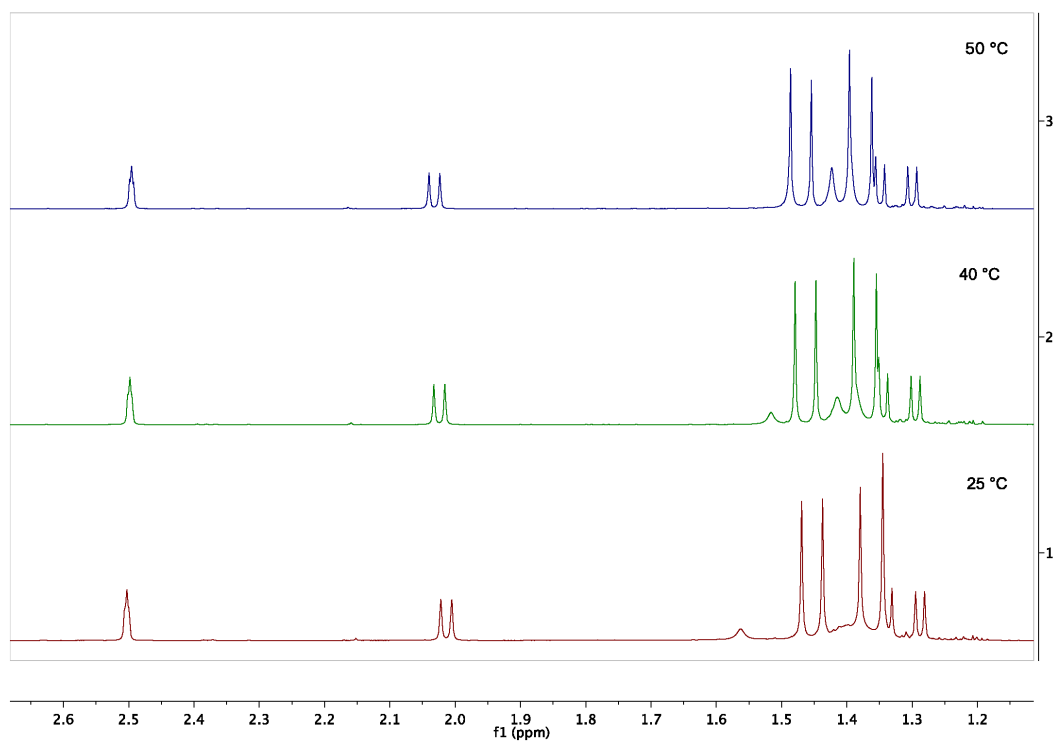
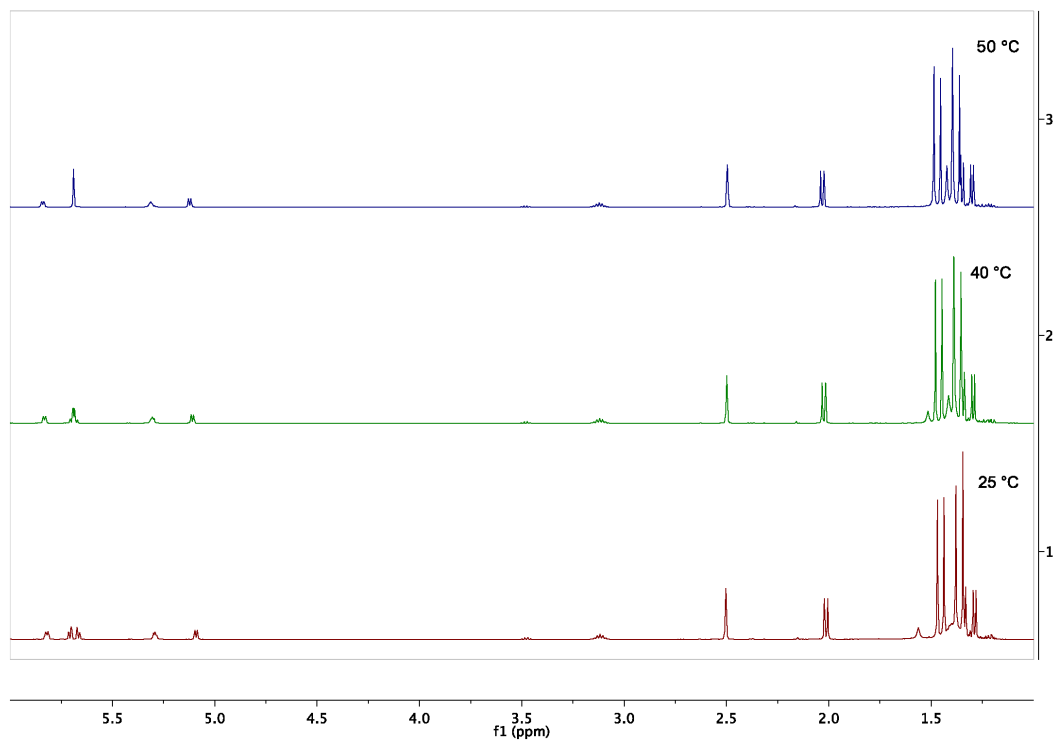
Complex 3

^1H - ^{13}C HSQC (CDCl_3 , 298 K)



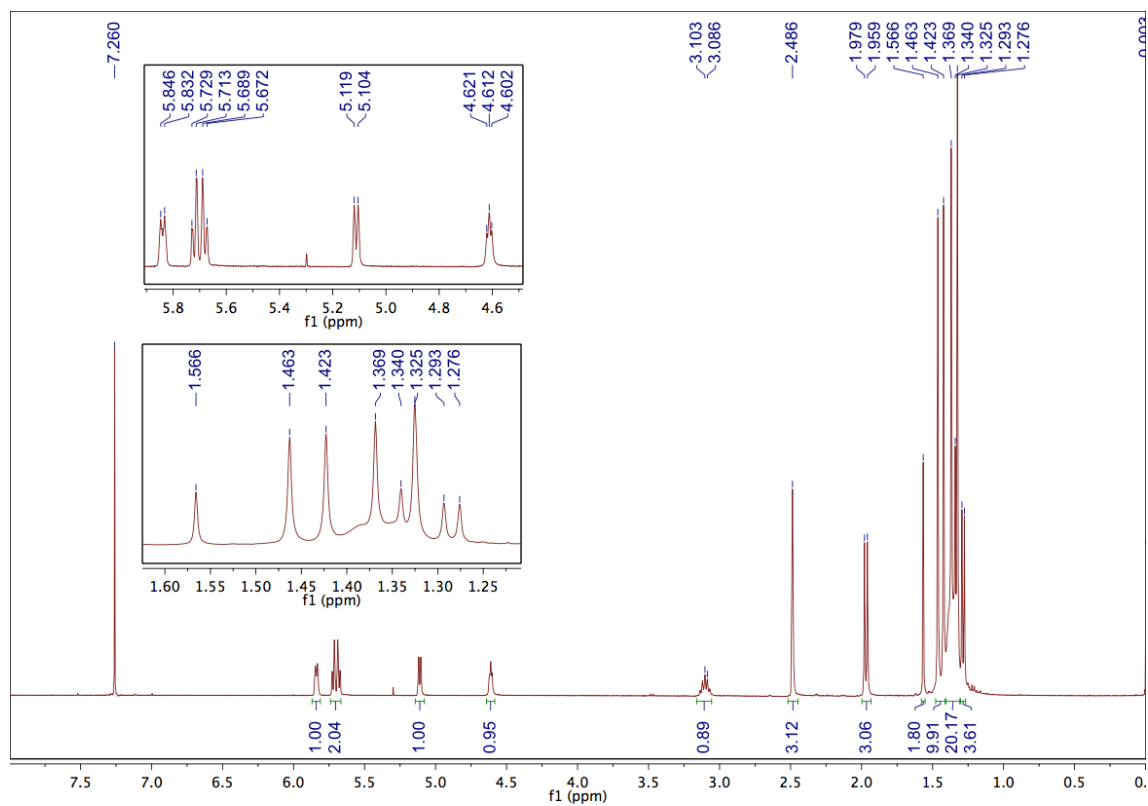
Complex 3

^1H -NMR Variable temperature measurements (400.13 MHz, CDCl_3 , 298 K)



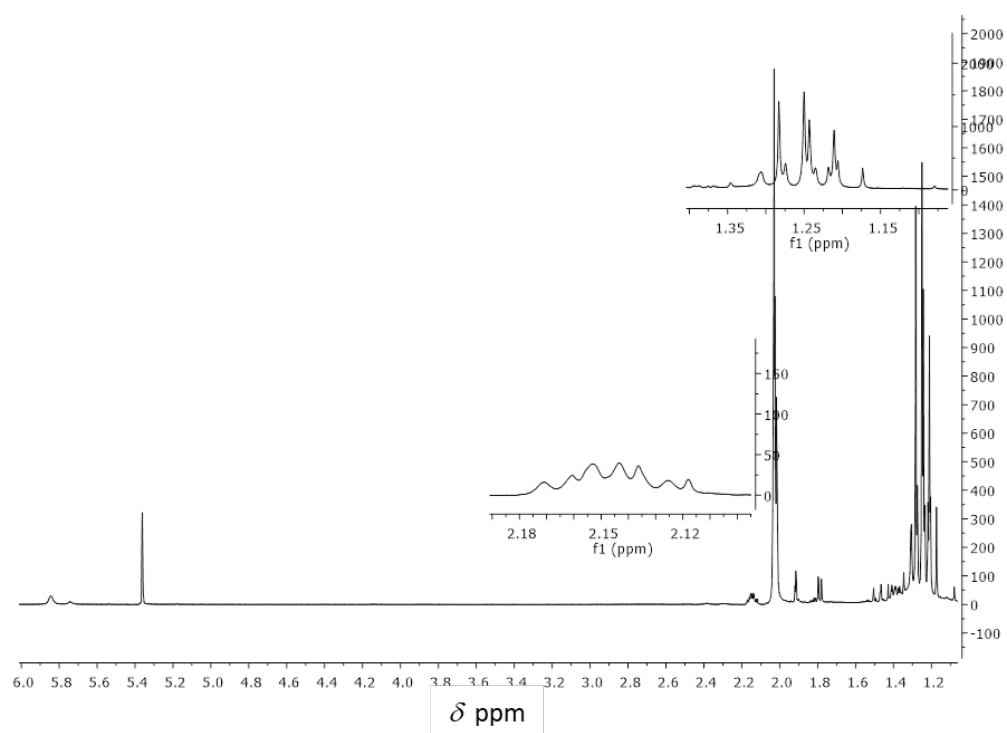
Complex 3'

^1H -NMR (400.13 MHz, CDCl_3 , 298 K)



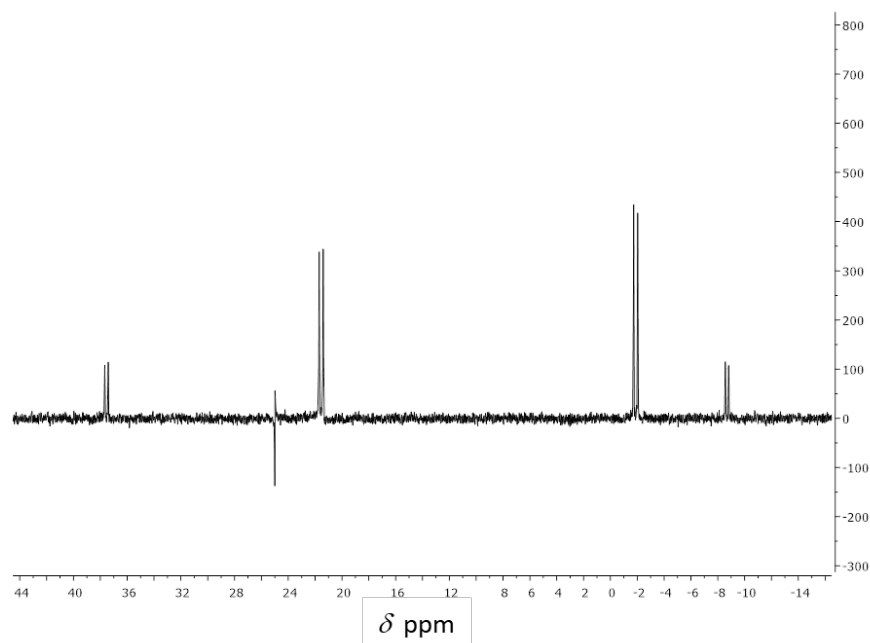
Complex 4

^1H -NMR (500.13 MHz, CD_2Cl_2 , 298 K)



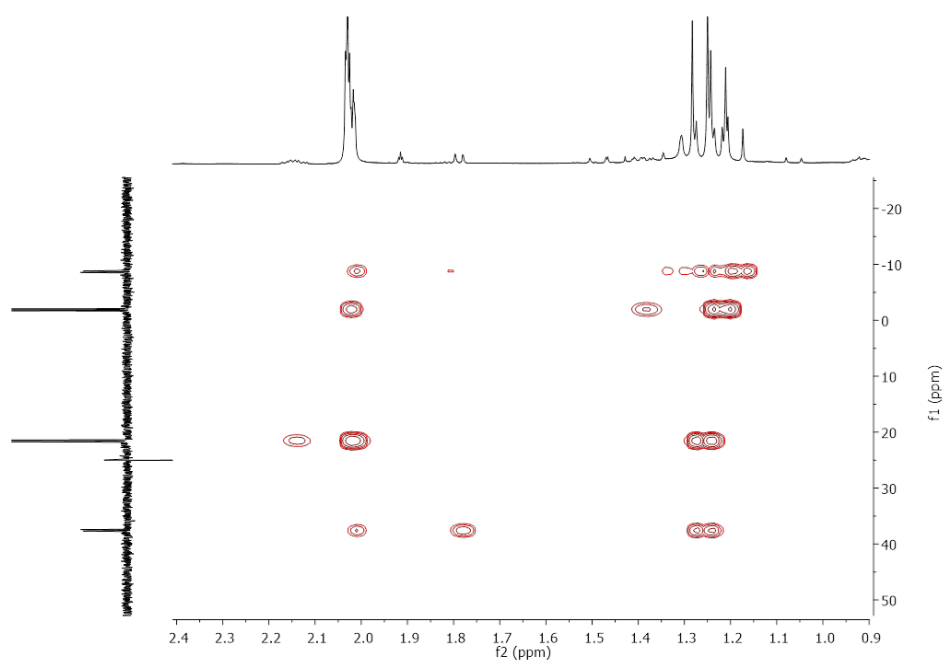
Complex 4

$^{31}\text{P}\{^1\text{H}\}$ -NMR (202.46 MHz, CD_2Cl_2 , 298 K)



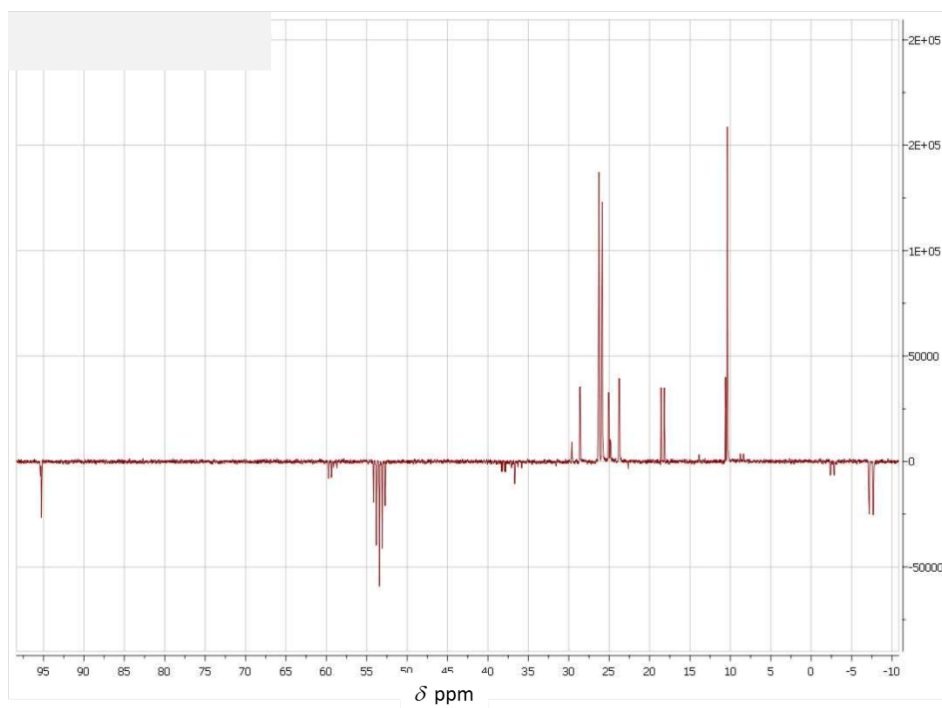
Complex 4

^1H - ^{31}P HMBC (CD_2Cl_2 , 298 K)



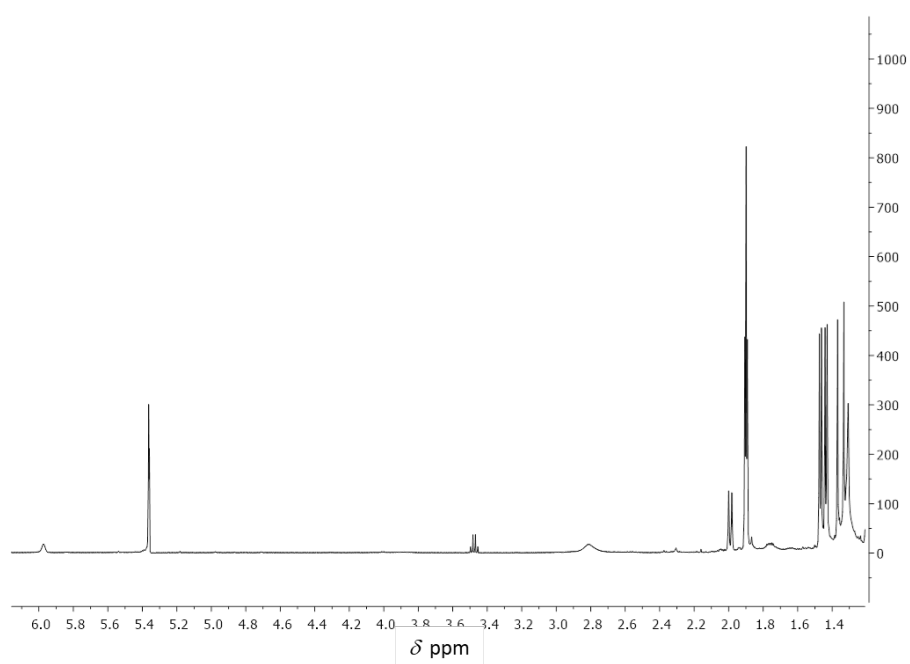
Complex 4

$^{13}\text{C}\{^1\text{H}\}$ -APT (75.48 MHz, CD_2Cl_2 , 298 K)



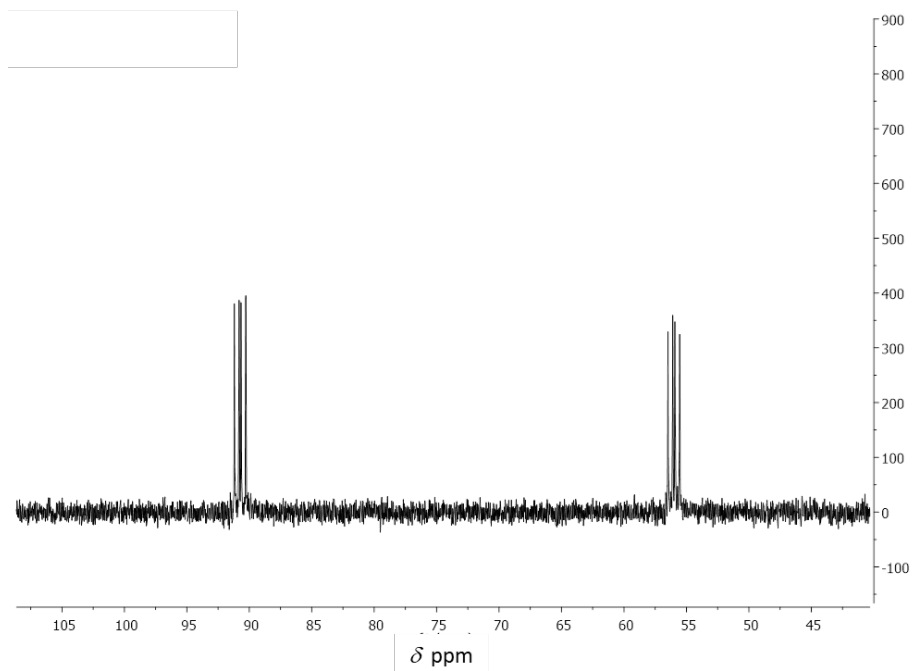
Complex 5

^1H -NMR (500.13 MHz, CD_2Cl_2 , 298 K)



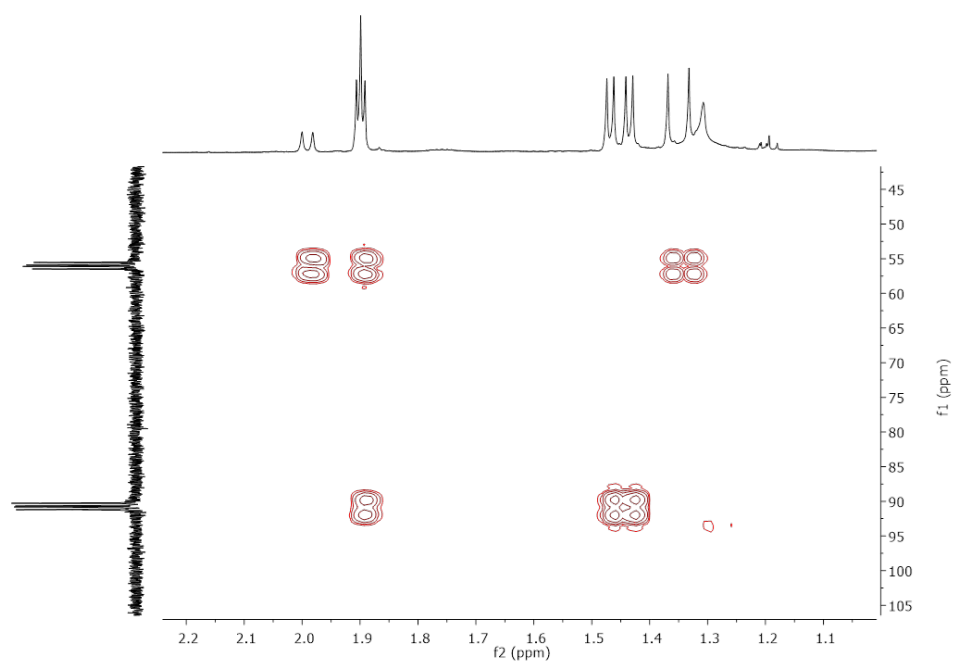
Complex 5

$^{31}\text{P}\{^1\text{H}\}$ -NMR (202.46 MHz, CD_2Cl_2 , 298 K)



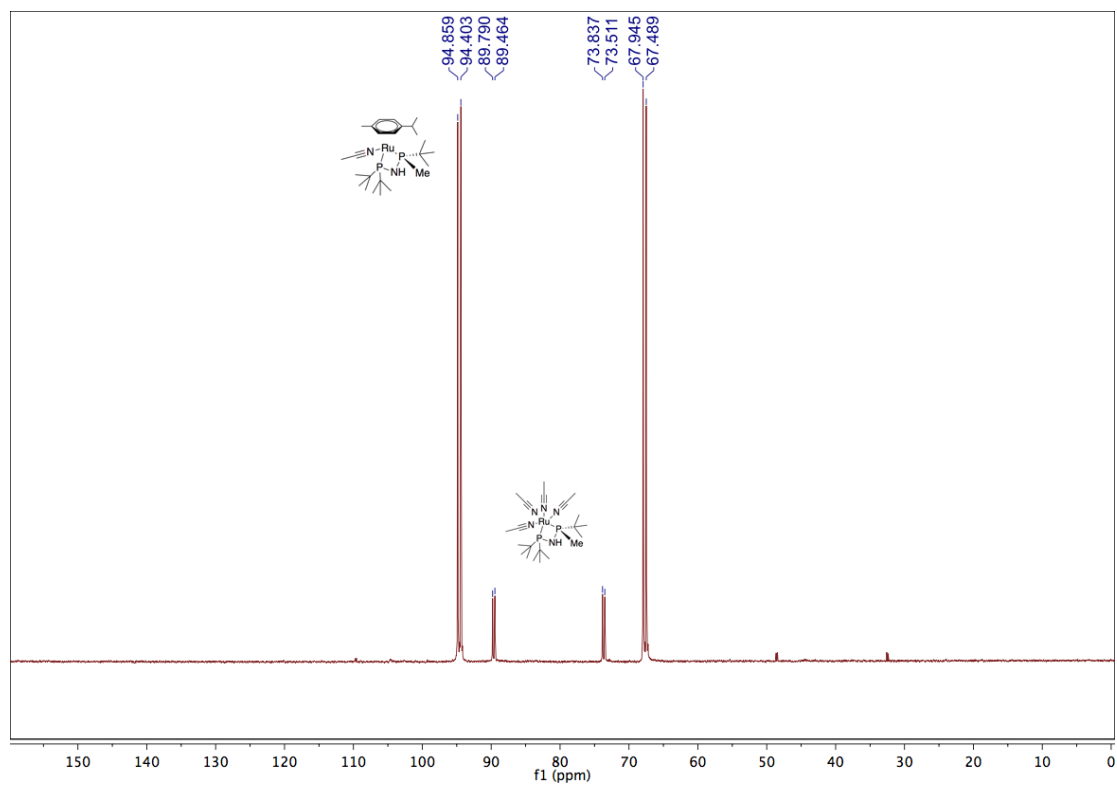
Complex 5

^1H - ^{31}P HMBC (CD_2Cl_2 , 298 K)



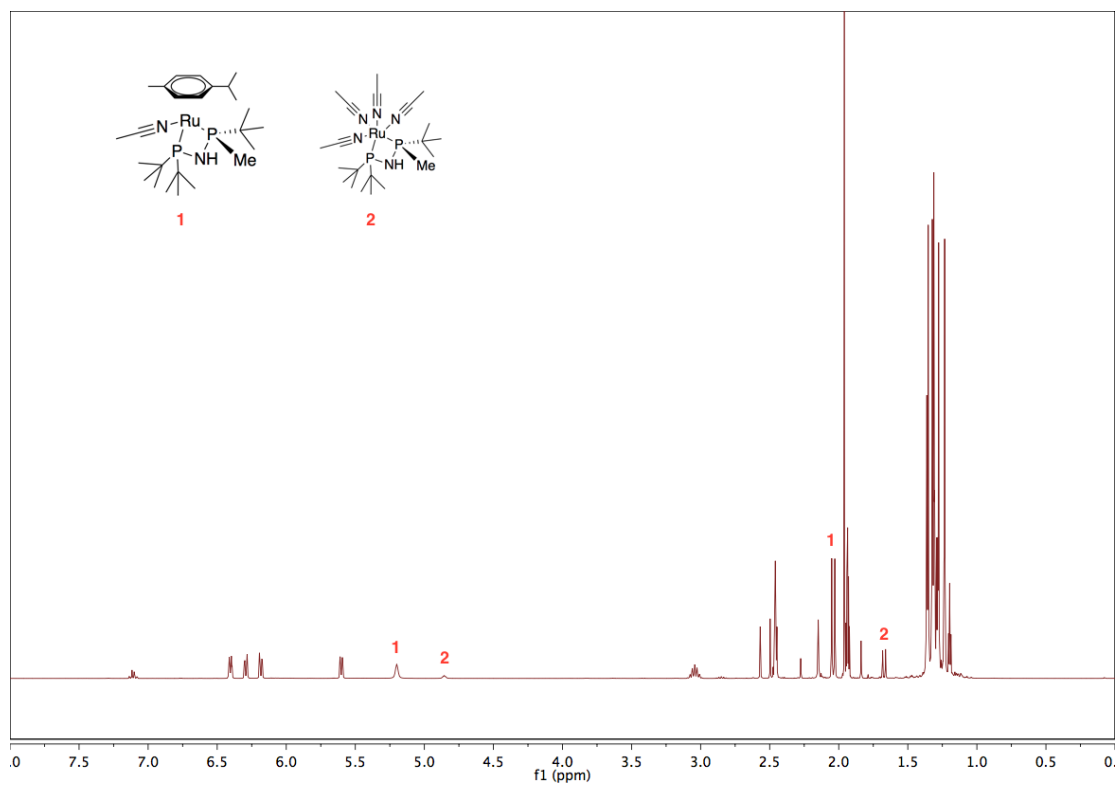
Complex 6

$^{31}\text{P}\{^1\text{H}\}$ -NMR (161.9 MHz, CH_3CN , 298 K)

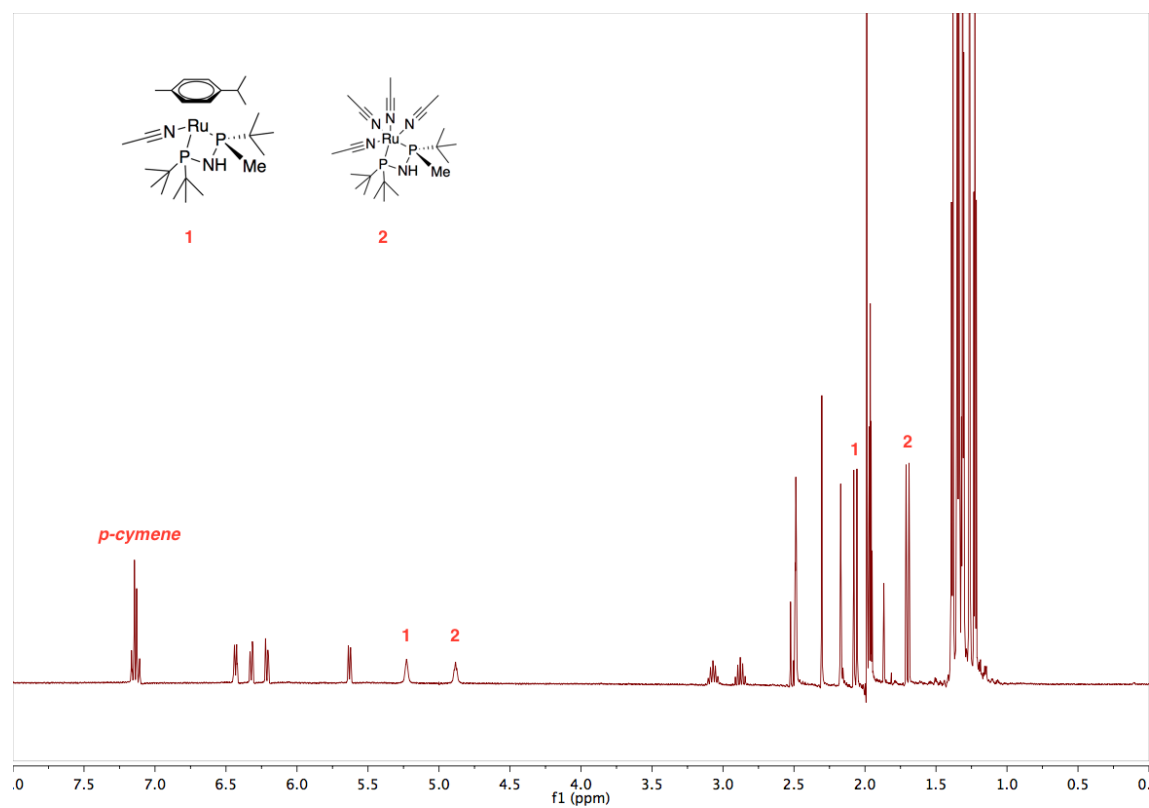


Complex 6

^1H -NMR (400.13 MHz, CH_3CN , 298 K)

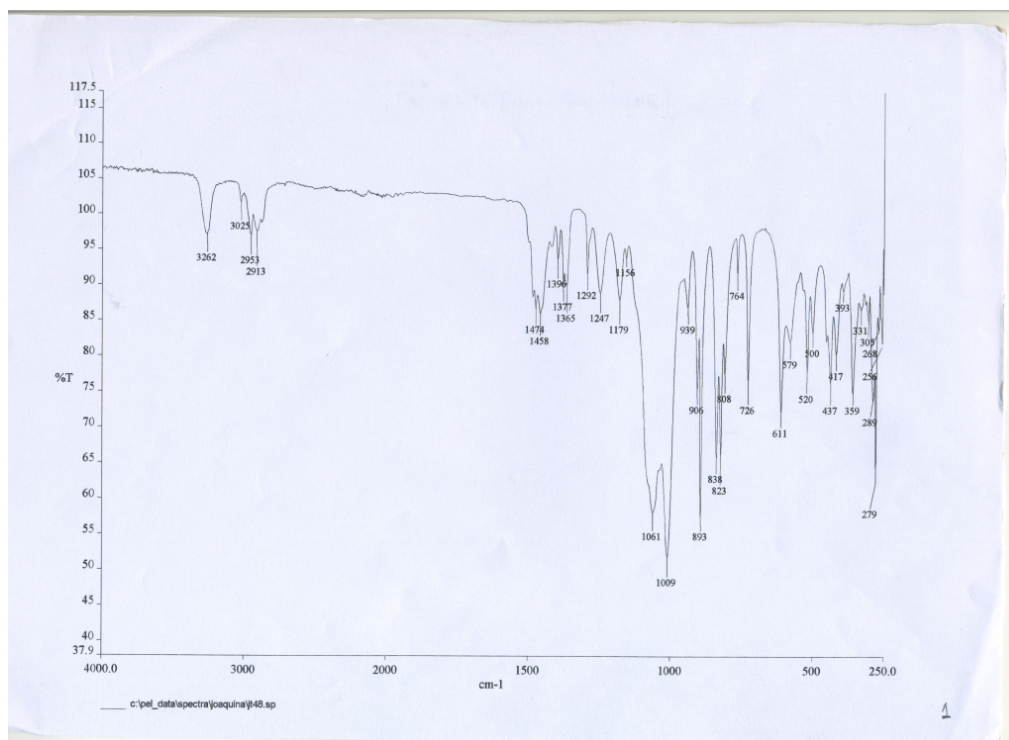


^1H -NMR (400.13 MHz, CH_3CN , 298 K) a few hours later

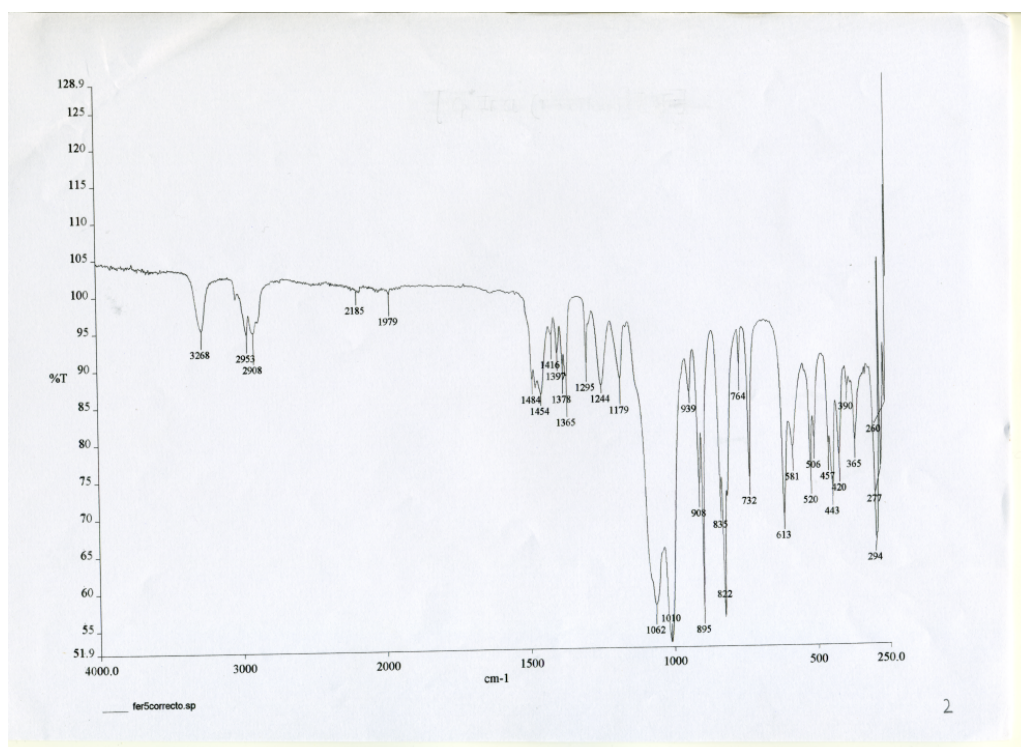


2. Selected IR spectra

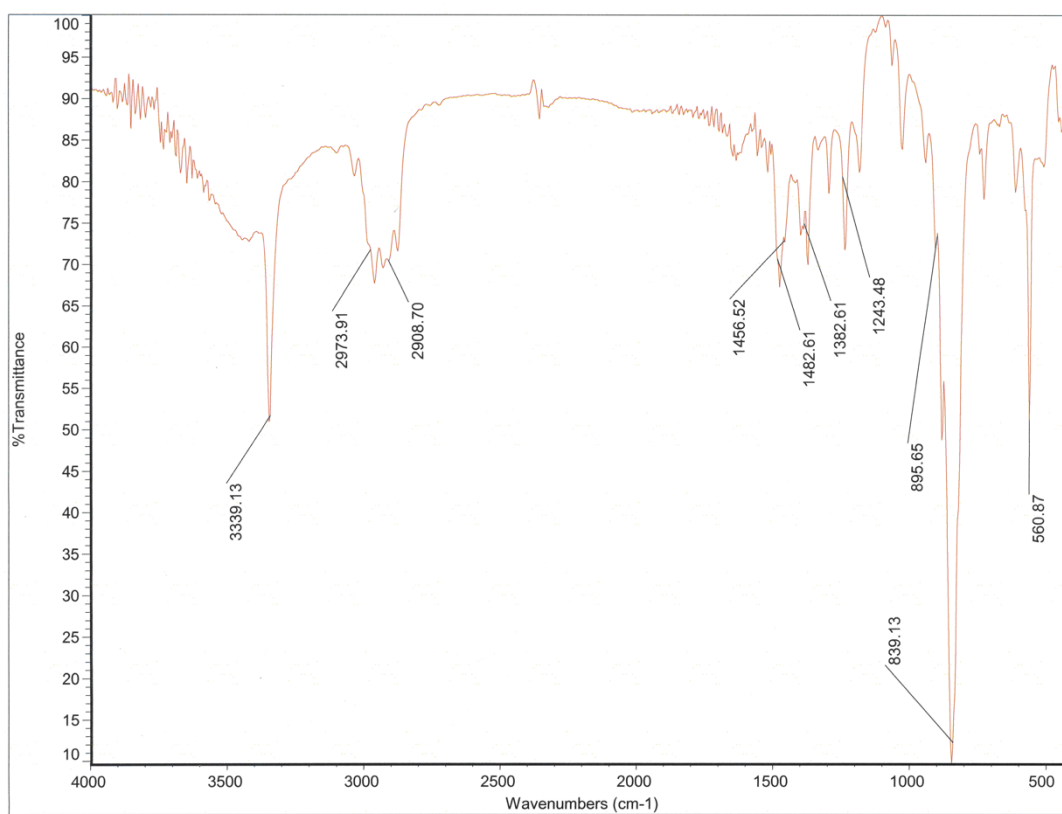
Complex 1



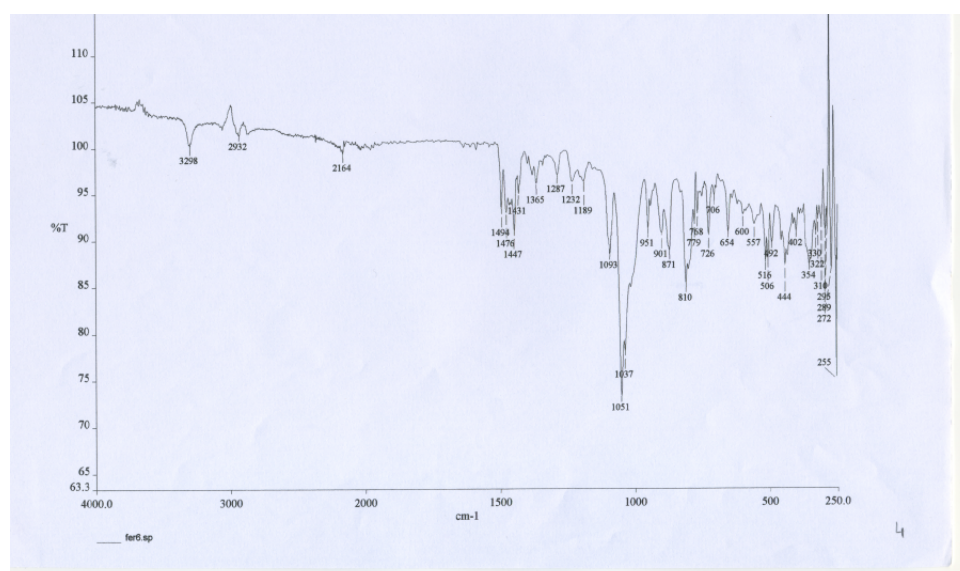
Complex 2



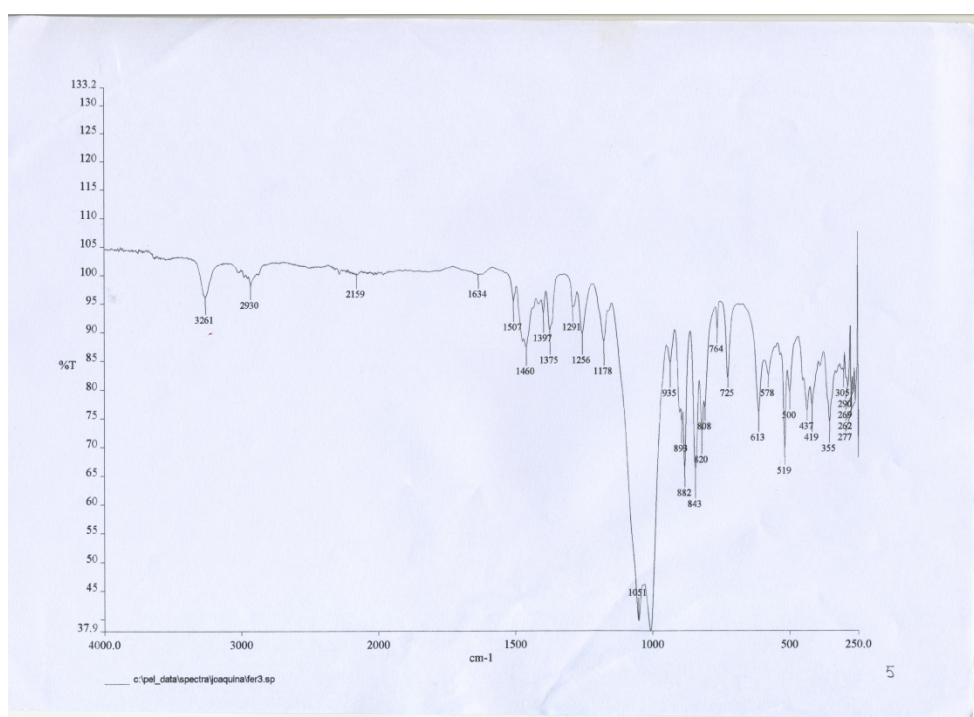
Complex 3'



Complex 4

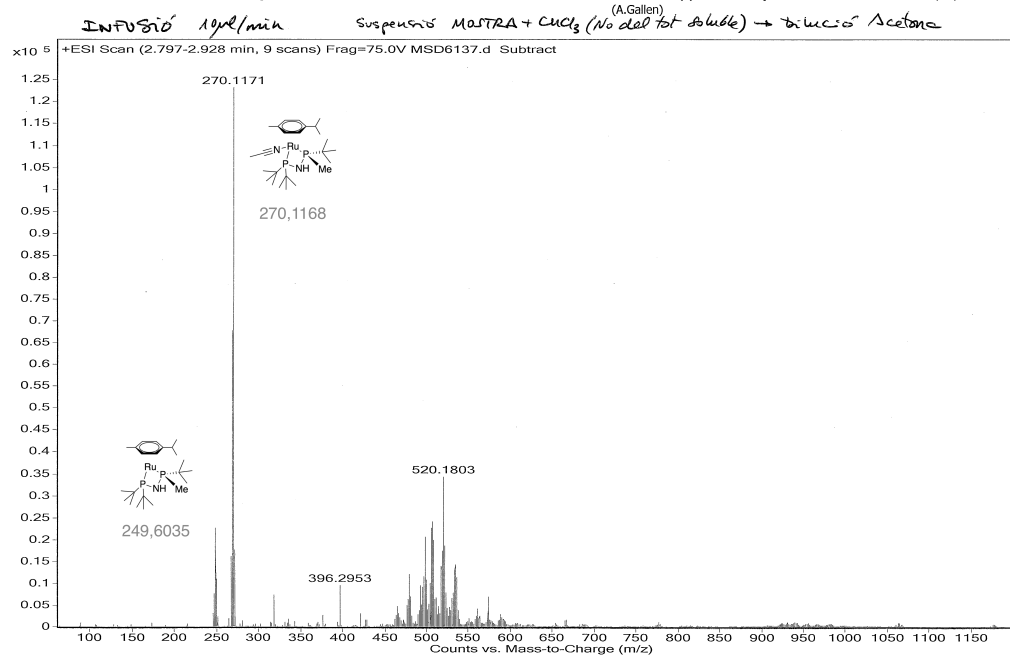


Complex 5

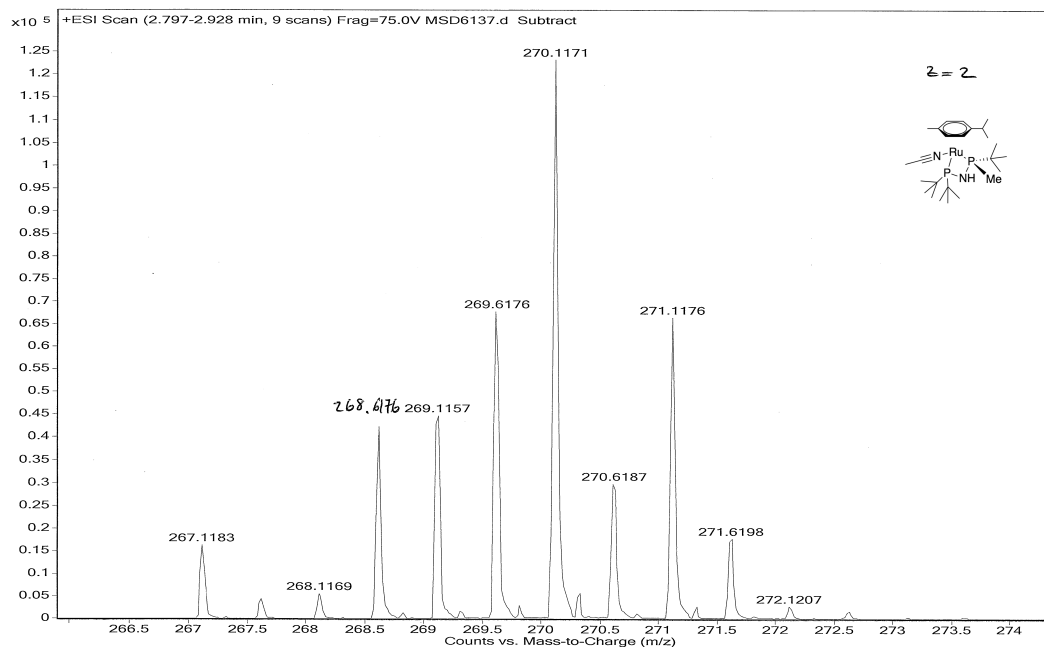


3. Mass spectra of complex 6

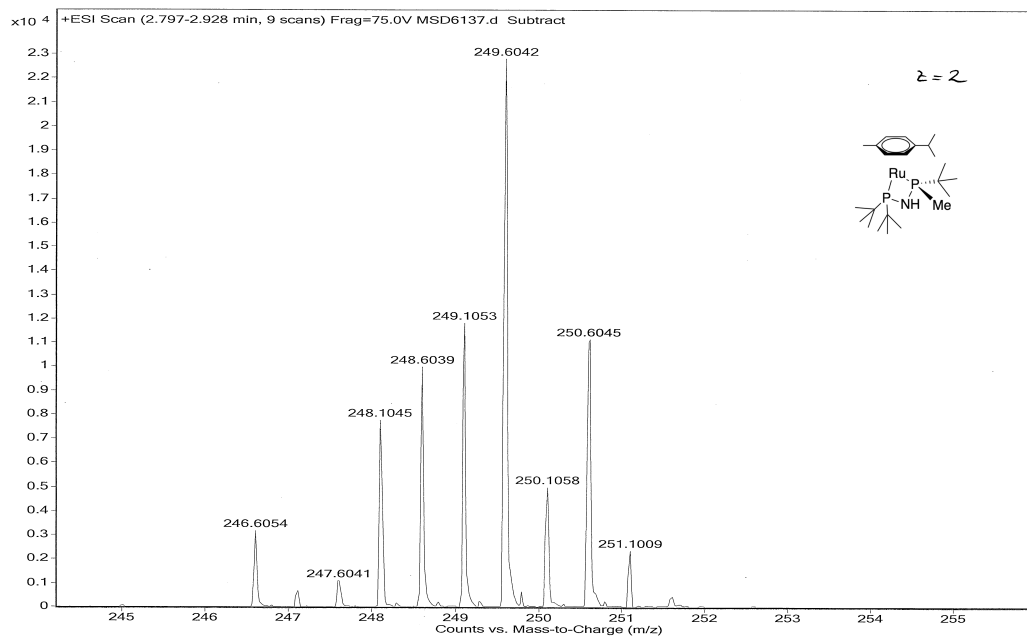
Sample Name	EM3787	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MSD6137.d	ACQ Method		Comment	AGO 86 BF4 (2) (A.Gallen)	Acquired Time	2/20/2017 11:44:02 AM



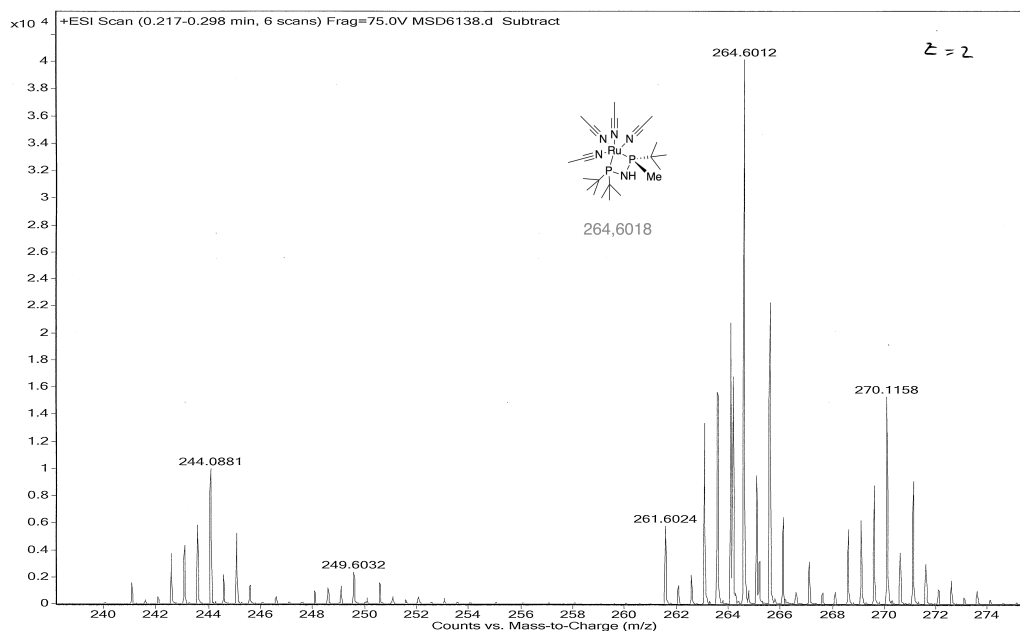
Sample Name	EM3787	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MSD6137.d	ACQ Method		Comment	AGO 86 BF4 (2) (A.Gallen)	Acquired Time	2/20/2017 11:44:02 AM



Sample Name	EM3787	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MSD6137.d	ACQ Method		Comment	AGO 86 BF4 (2) (A.Gallen)	Acquired Time	2/20/2017 11:44:02 AM

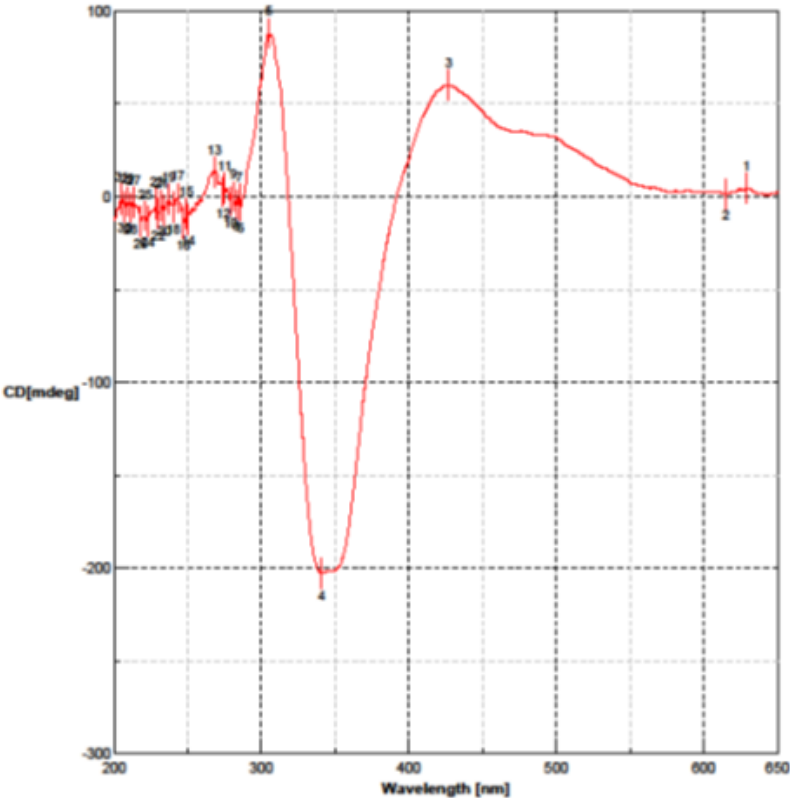


Sample Name	EM3787	Position	P1-A1	Instrument Name	Instrument 1	User Name	
Inj Vol	0.2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MSD6138.d	ACQ Method	ESIpos.m	Comment	AG086BF4 (2) (A.Gallen)	Acquired Time	2/20/2017 11:56:06 AM



4. Selected CD spectra

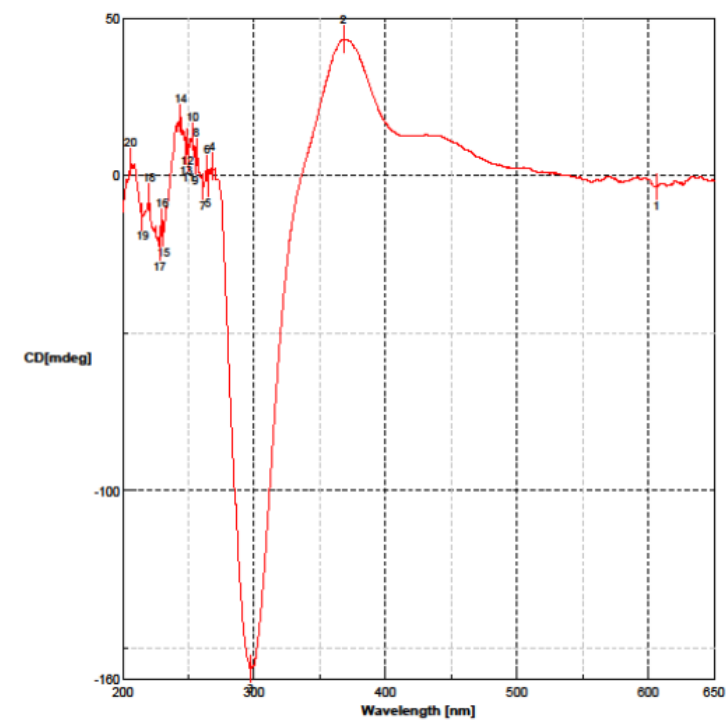
Complex 1



Date/Time 14/10/2016 10:27
Operator Laboratorio
File Name Memory#2
Sample Name JT-48
Comment JT-48 3.2 mg acetona correccion linea base

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	629	4.54919	2	615	1.53479	3	427	60.1623
4	341	-202.879	5	305	87.9883	6	286	-5.20435
7	285	-1.19677	8	283	-4.25178	9	281	0.0722305
10	279	-2.73047	11	275	4.88647	12	274	2.64086
13	268	13.3775	14	250	-12.2072	15	249	-9.14665
16	247	-14.2381	17	243	-0.867984	18	240	-5.85209
19	237	-1.49221	20	234	-7.07185	21	232	-4.54716
22	230	-8.90752	23	229	-3.9473	24	223	-13.1523
25	221	-10.3345	26	218	-13.3325	27	213	-3.34887
28	211	-5.97302	29	209	-2.50665	30	207	-5.38283
31	205	-1.07815						

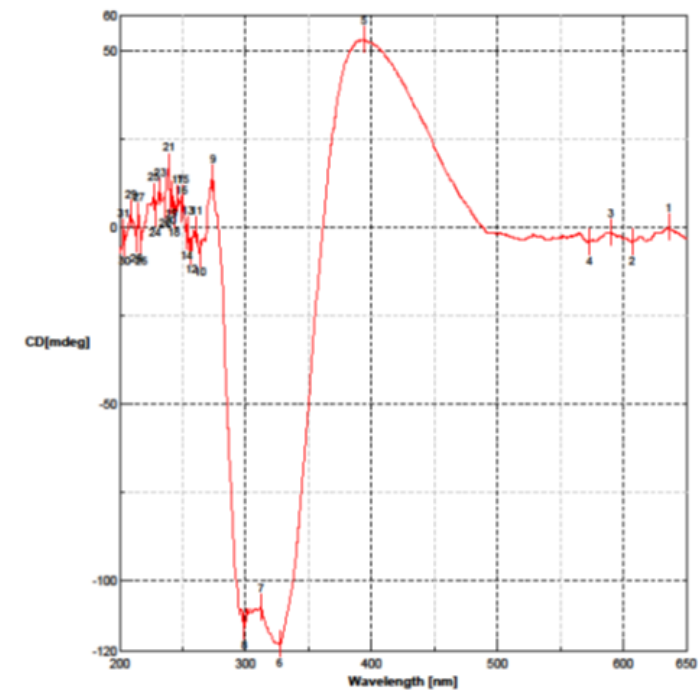
Complex 2



Date/Time 14/10/2016 10:34
Operator Laboratorio
File Name Memory#2
Sample Name FER-5
Comment FER-5 3.7 mg acetona correccion linea base

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	606	-3.35636	2	368	43.3778	3	297	-156.516
4	288	3.16385	5	265	-2.41352	6	264	2.3878
7	261	-3.39236	8	256	7.53569	9	255	4.74314
10	253	12.4214	11	250	5.71429	12	249	10.8875
13	248	8.03523	14	244	18.3441	15	231	-18.1959
16	230	-14.9042	17	228	-22.6406	18	220	-6.76608
19	215	-13.0291	20	206	4.49396			

Complex 5



Date/Time 14/10/2016 10:41
Operator Laboratorio
File Name Memory#2
Sample Name FER-3
Comment FER-3 3.5 mg acetona correccion linea base

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	636	0.11492	2	607	-4.08019	3	590	-1.42702
4	573	-4.08534	5	394	53.1769	6	327	-117.896
7	312	-107.449	8	299	-112.863	9	274	14.0662
10	264	-7.41809	11	261	-0.605603	12	257	-6.61248
13	254	-0.534705	14	253	-2.7217	15	250	8.34817
16	249	5.28281	17	246	8.35782	18	243	3.79021
19	241	9.334	20	240	7.28075	21	239	17.2756
22	236	6.42386	23	232	10.2113	24	228	3.94024
25	227	8.8663	26	217	-4.17844	27	215	3.40478
28	213	-3.25338	29	209	3.90901	30	204	-4.32326
31	203	-1.35937						