Metal-Assisted Conversion of a N-ylide Mesomeric Betaine into its Carbenic Tautomer: Generation of N-(fluoren-9-yl)imidazol-2-ylidene Complexes

Laure Benhamou,[a,b] Stéphanie Bastin,[a,b] Noël Lugan,[a,b] Guy Lavigne*[a,b] and Vincent César*[a,b]

[a] CNRS, LCC (laboratoire de Chimie de Coordination), 205 route de Narbonne, F-31077 Toulouse Cedex 4, France
E-mail: vincent.cesar@lcc-toulouse.fr, guy.lavigne@lcc-toulouse.fr
[b] Université de Toulouse, UPS, INPT, 31077 Toulouse, France

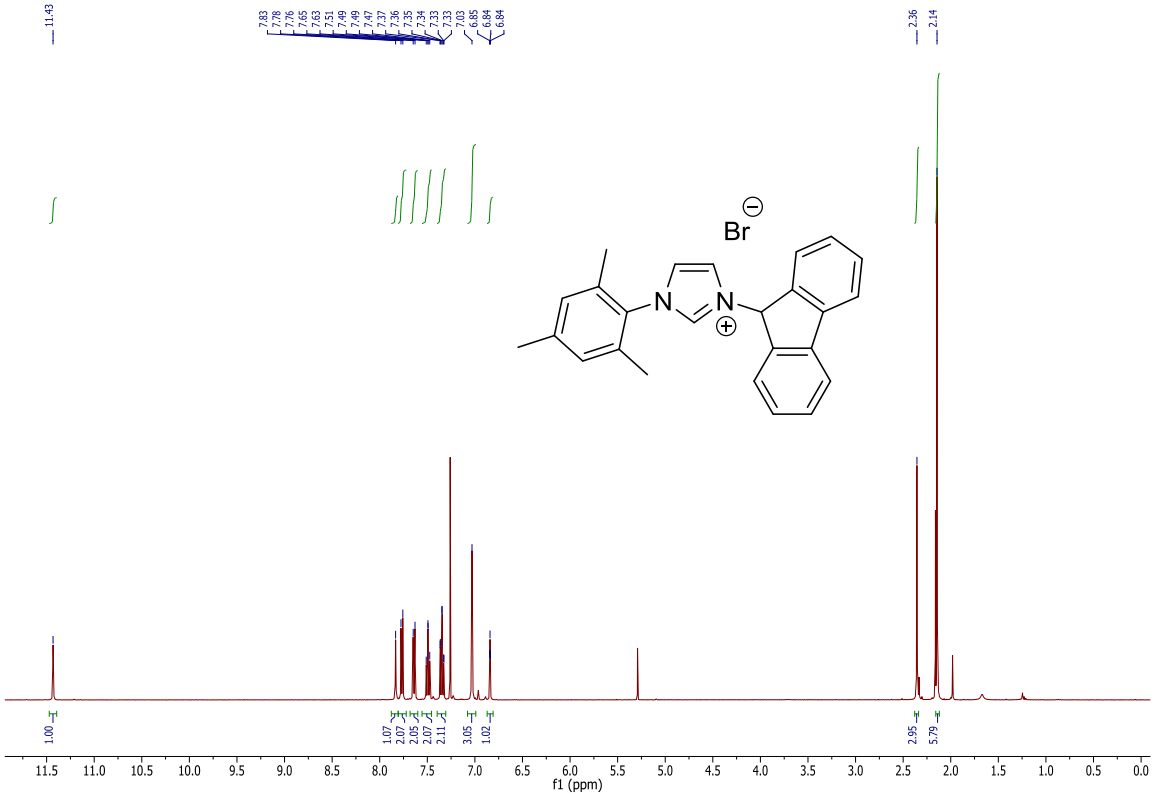
Supporting Information

Contents

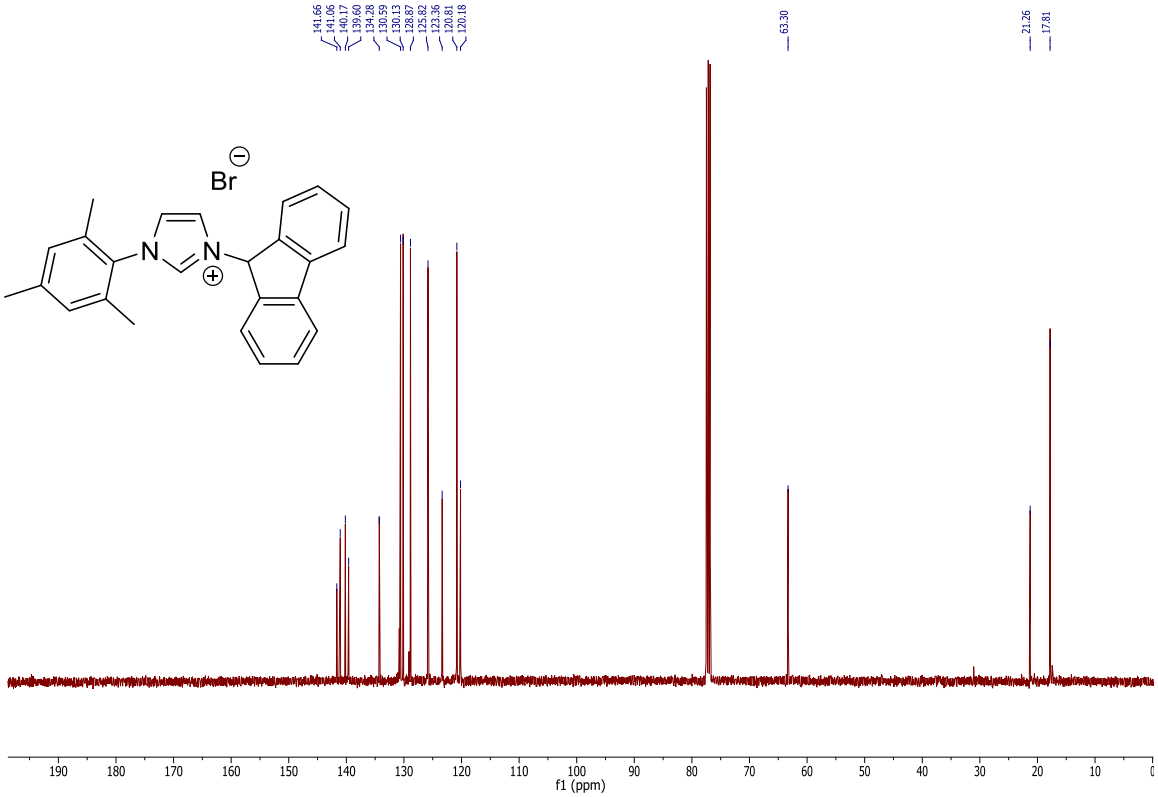
Table S1. Crystals data and structures refinments for complexes **4, 5, 6,** and **7**.

complex	**4**	**5.CHCl$_3$**	**6**	**7**
empirical formula	$C_{25}H_{22}AuClN_2$	$C_{33}H_{34}ClNRh$, $CHCl_3$	$C_{25}H_{22}AgBrN_2$	$C_{33}H_{33}N_2Rh$
molecular weight (g)	582.86	716.35	818.81	560.52
temperature (K)	100	180	100	173
λ (Å)	0.71069	0.71069	0.71069	0.71069
crystal system	monoclinic	monoclinic	monoclinic	
space group	C 2/c (#15)	$P2_1/n$ (#14)	P -1 (#2)	$P2_1/n$ (#14)
a (Å)	27.8036(11)	12.688(3)	10.4907(13)	17.2079(8)
b (Å)	8.4332(3)	16.274(3)	11.3717(10)	9.2276(9)
c (Å)	12.041(4)	16.218(3)	20.0840(19)	17.4436(11)
α(°)			101.272(8)	
β (°)	102.572(1)	106.45(3)	102.156(12)	103.472(4)
γ(°)			93.563(9)	
volume (Å^3)	4343.1(3)	3211.7(12)	4481.5(7)	2693.6(3)
Z	8	4	2	4
$D_{calcd.}$ (g.cm^{-3})	1.783	1.481	1.565	1.372
μ (mm^{-1})	6.911	0.891	2.645	0.657
F_{000}	2256	1464	1072	1160
θ_{max} (°)	26.4	26.4	28.8	26.4
completeness to θ_{max}	99	99	99	99

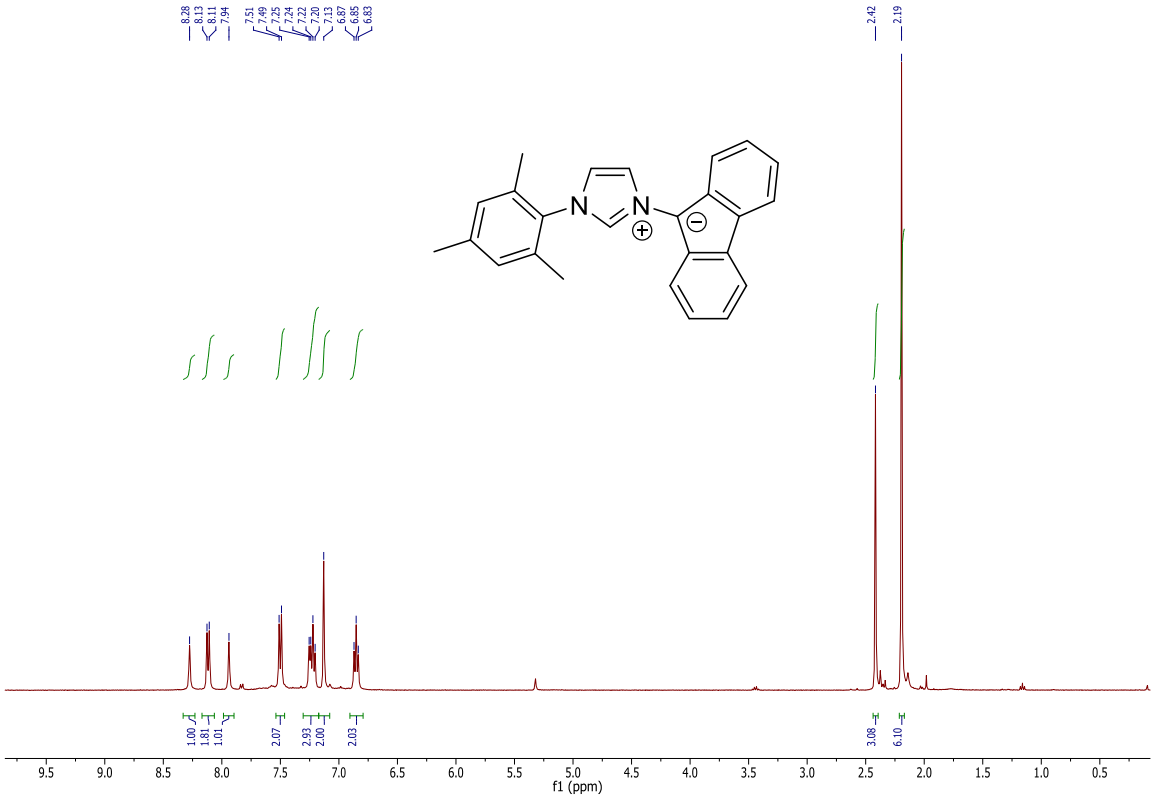
^{1}H NMR spectrum of **1** (400MHz, $CDCl_3$)



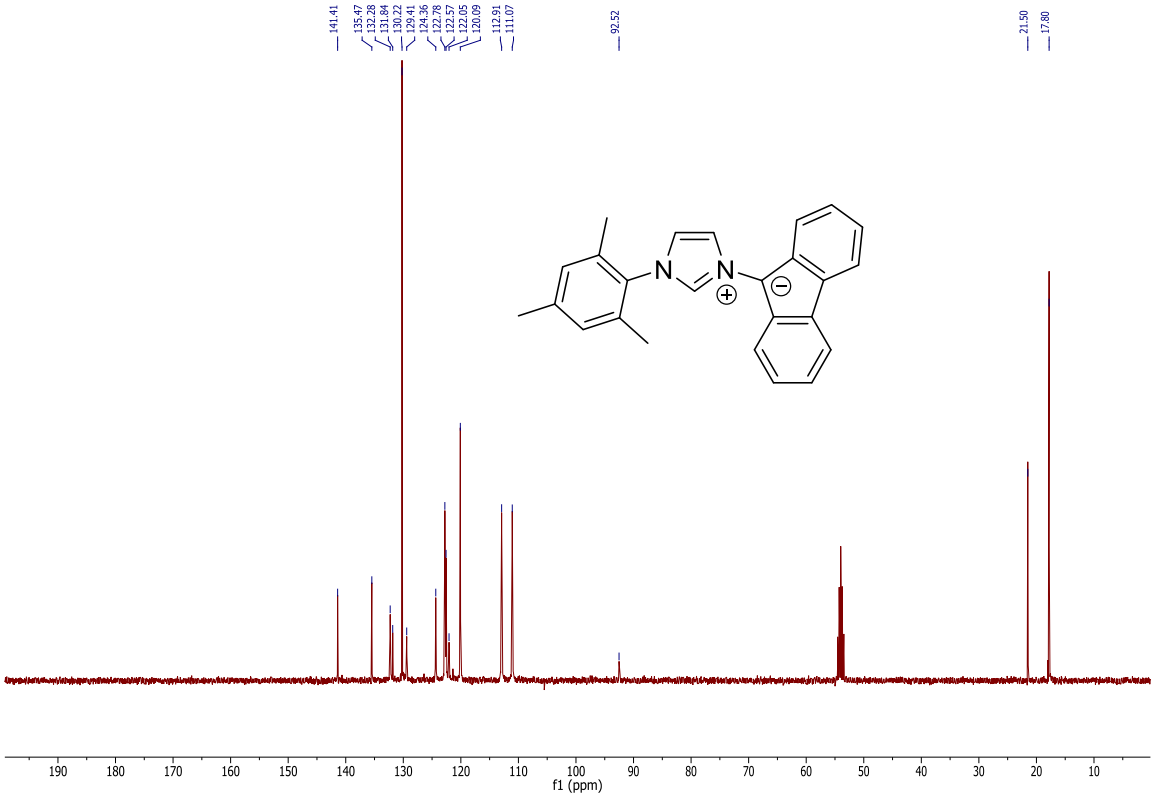
^{13}C{^{1}H} NMR spectrum of **1** (100.6 MHz, $CDCl_3$)



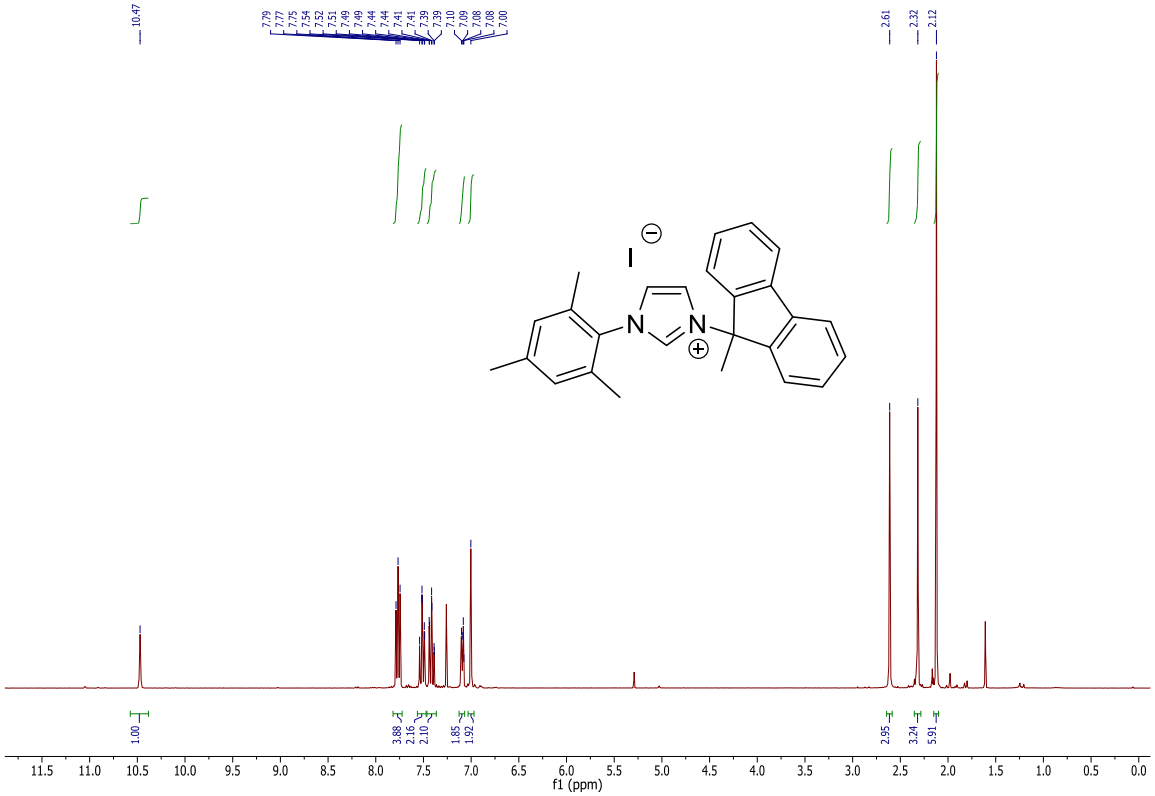
^{1}H NMR spectrum of **2** (400MHz, CD_2Cl_2)



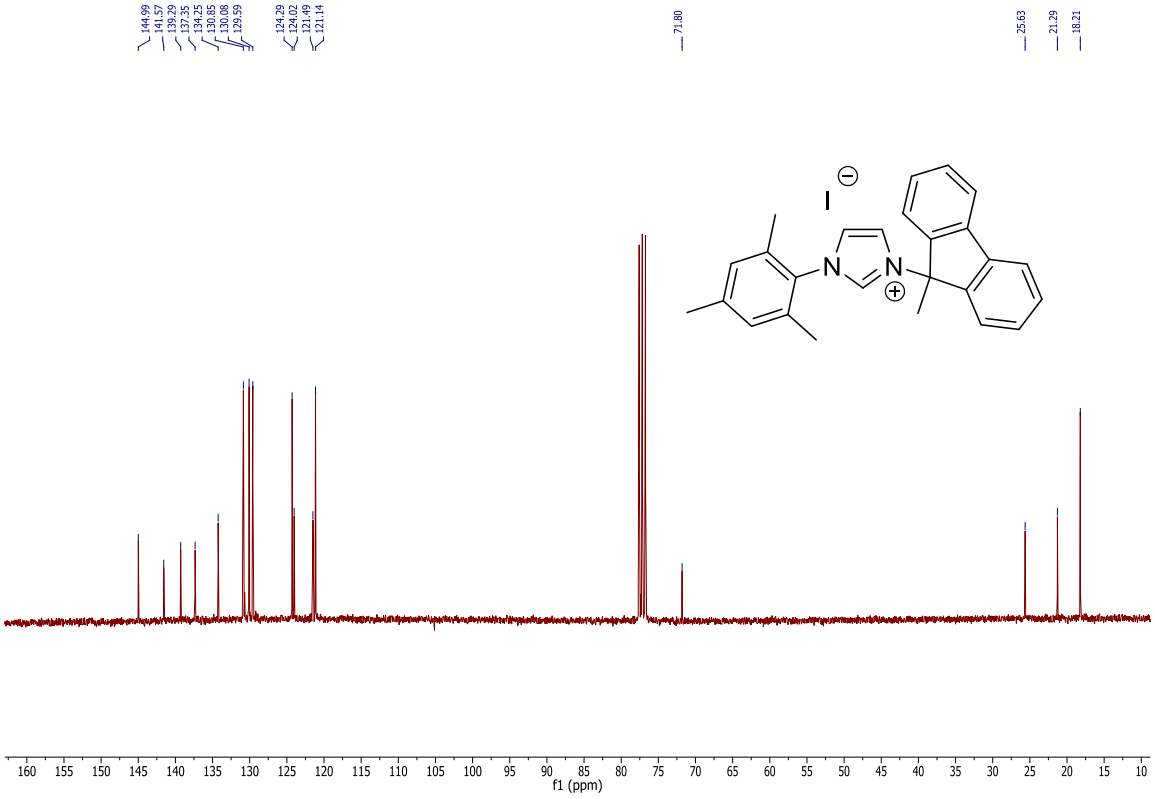
^{13}C{^{1}H} NMR spectrum of **2** (100.6 MHz, CD_2Cl_2)



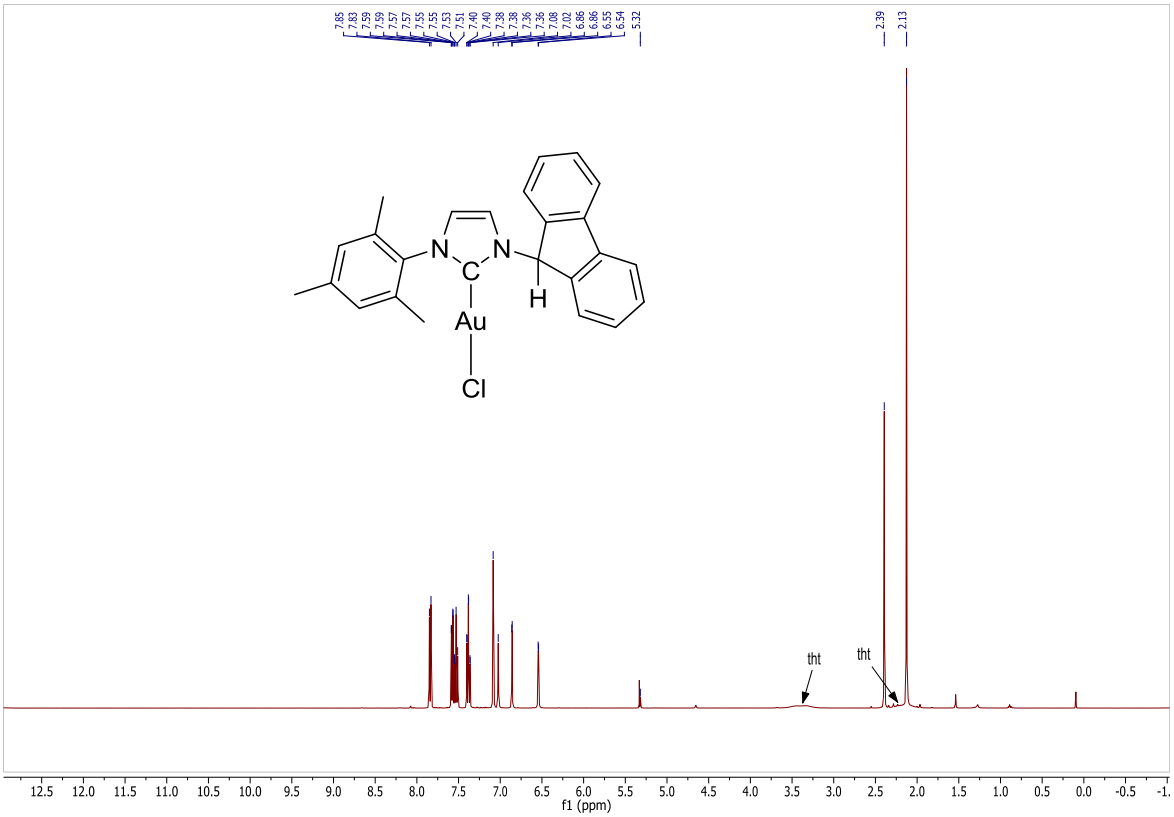
^{1}H NMR spectrum of **3** (300MHz, $CDCl_3$)



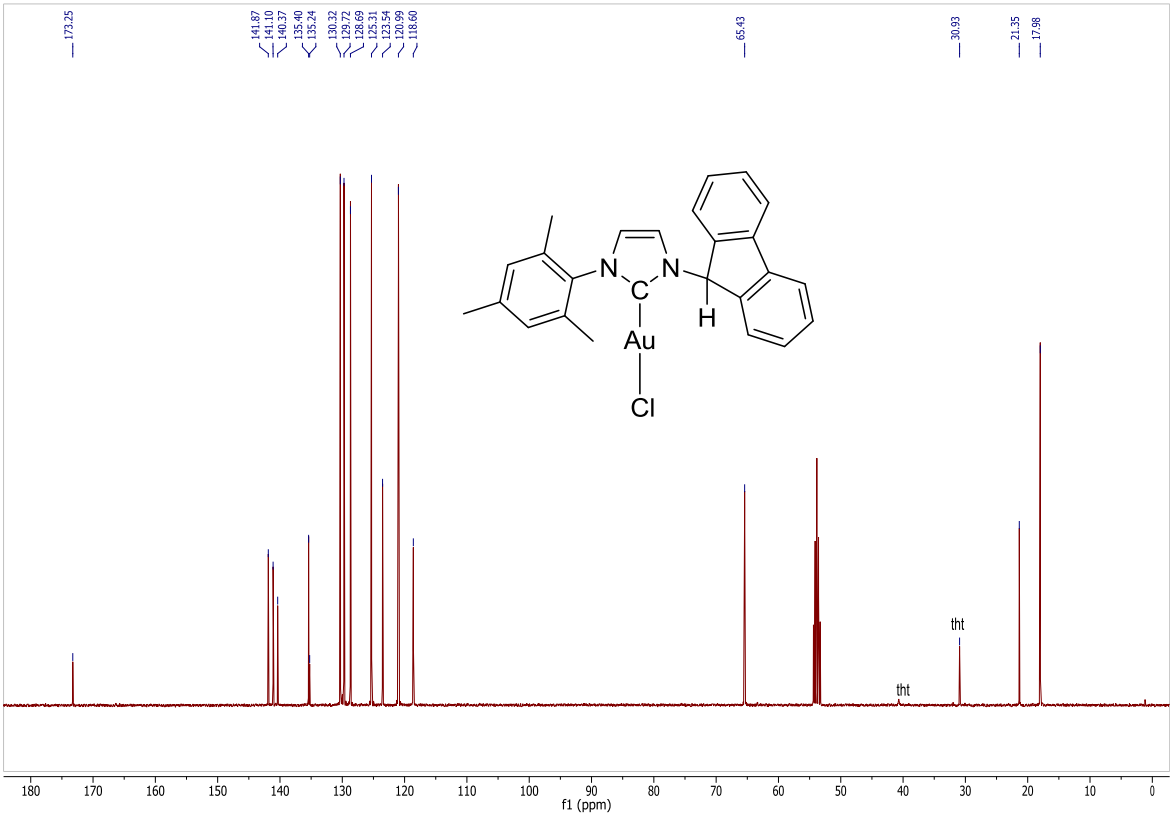
^{13}C{^{1}H} NMR spectrum of **3** (75.5 MHz, $CDCl_3$)



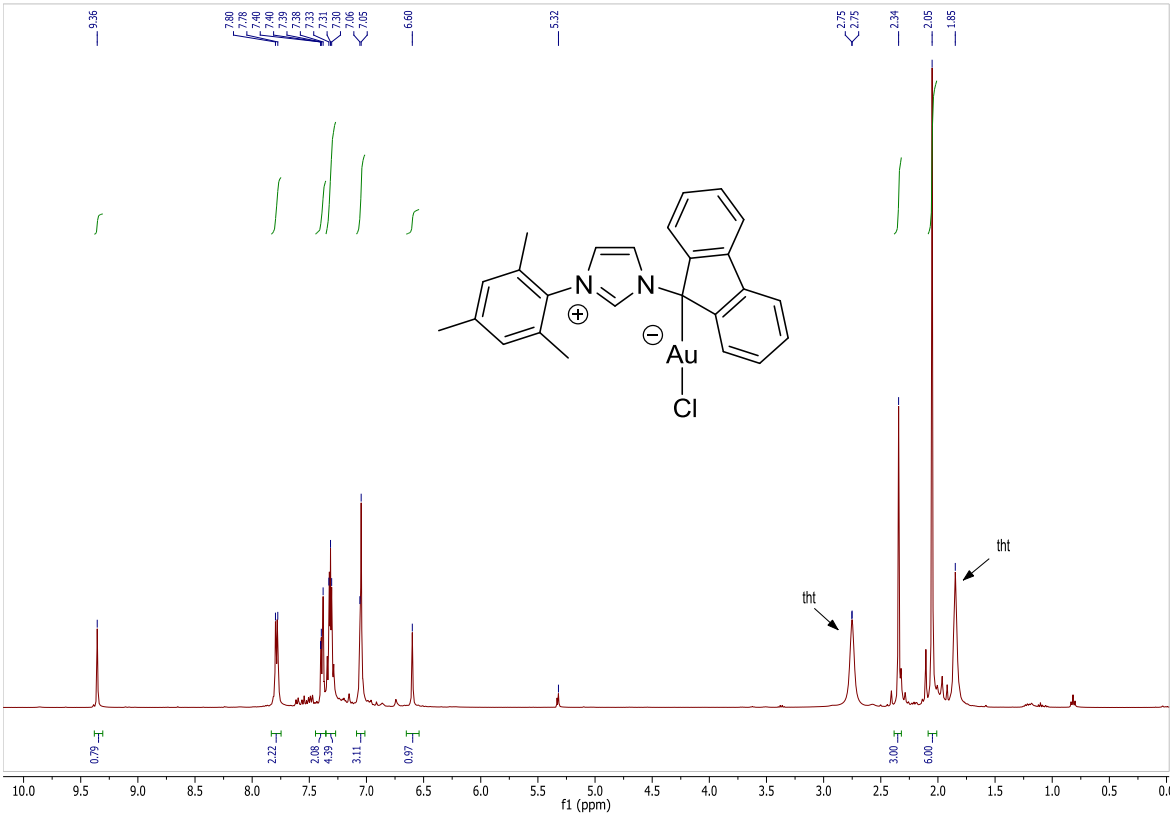
^{1}H NMR spectrum of **4** (400 MHz, CD_2Cl_2)



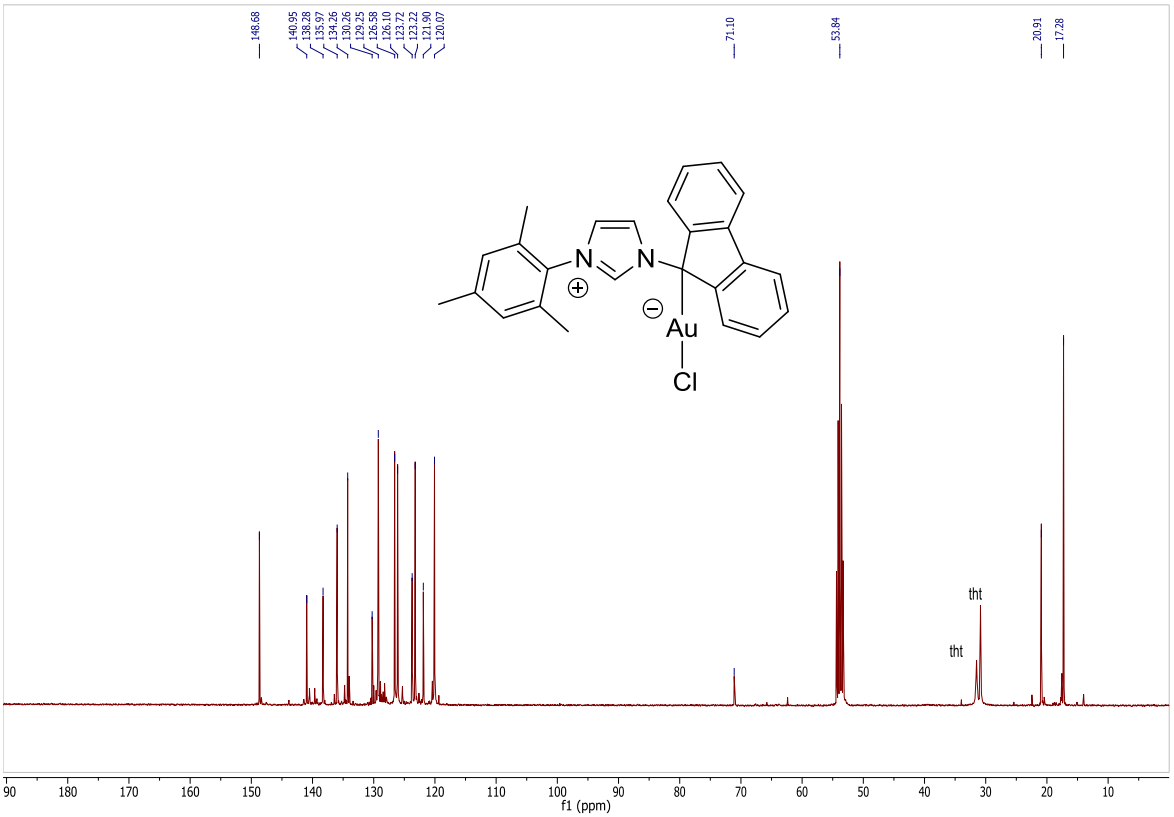
^{13}C{^{1}H} NMR of **4** (105.5 MHz, CD_2Cl_2)



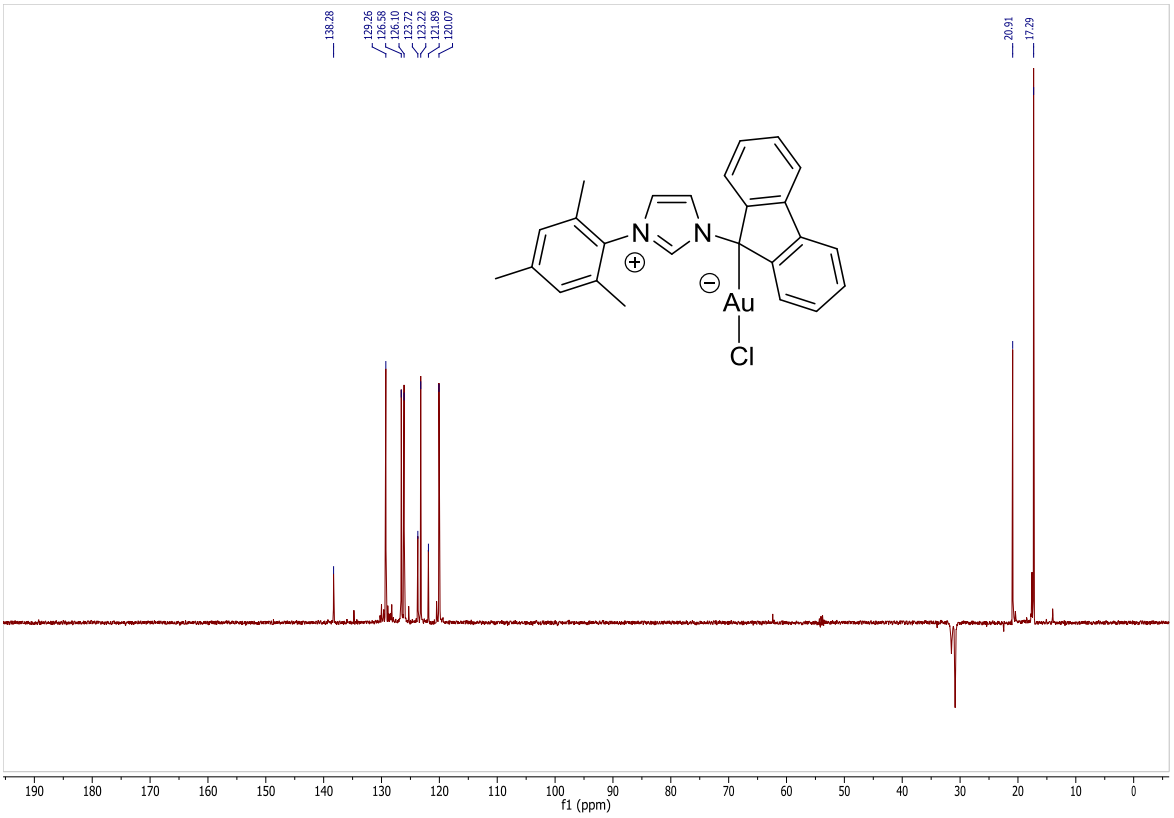
^{1}H NMR spectrum of **4'** (400 MHz, CD_2Cl_2, 214 K)



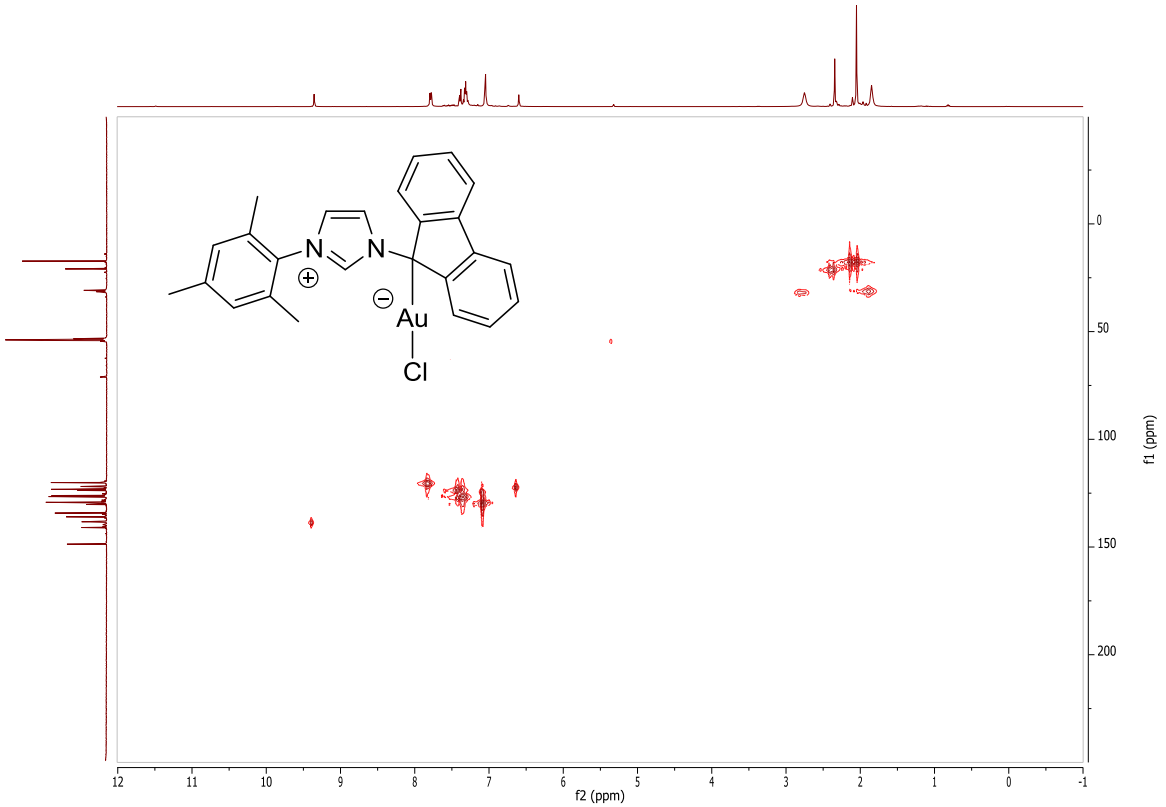
^{13}C{^{1}H} NMR spectrum of **4'** (105.5 MHz, CD_2Cl_2, 214 K)



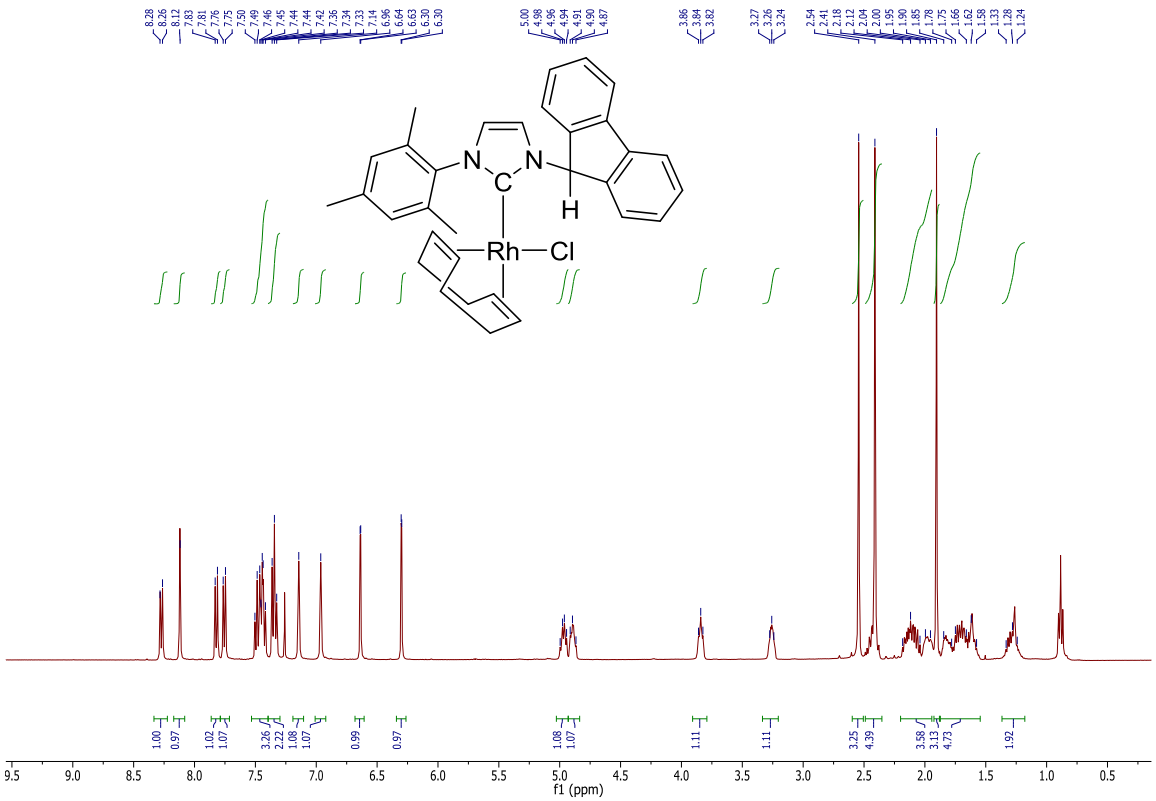
^{13}C DEPT135 NMR of **4'**(105.5 MHz, CD_2Cl_2, 214 K)



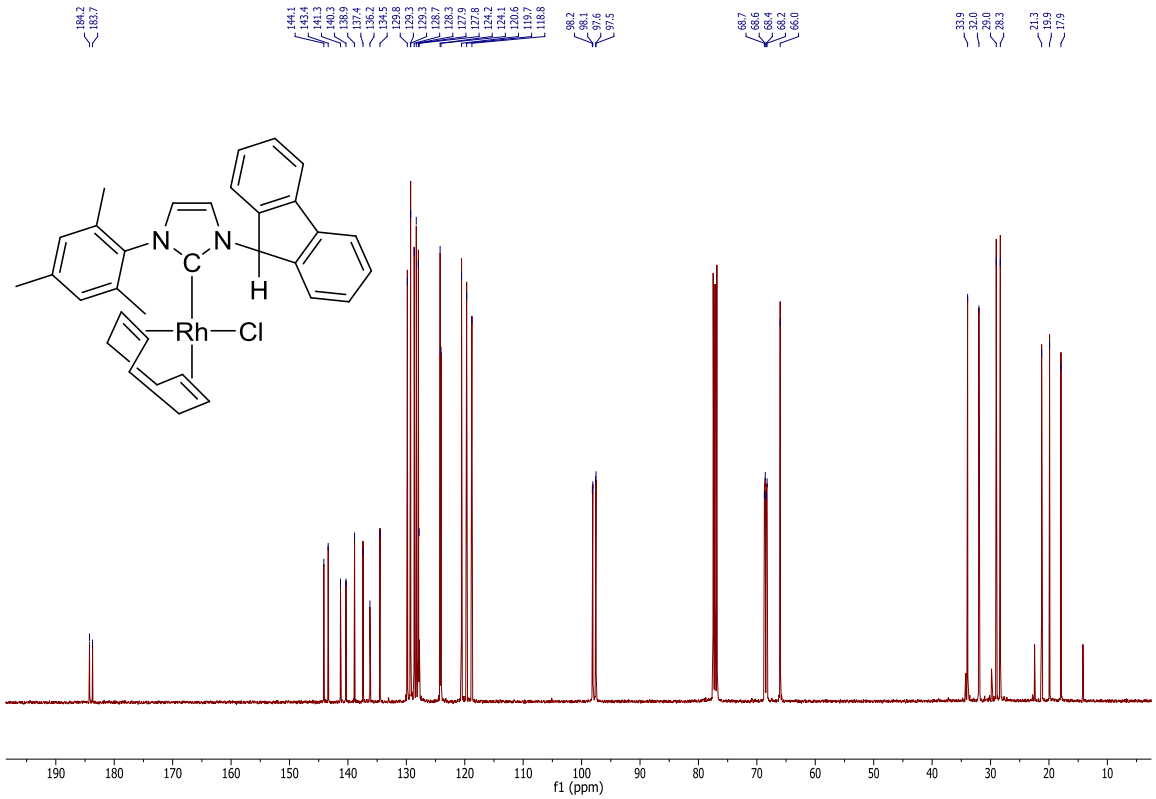
{^{13}C-^{1}H} HMQC NMR of **4'**(105.5 MHz, CD_2Cl_2, 214 K)



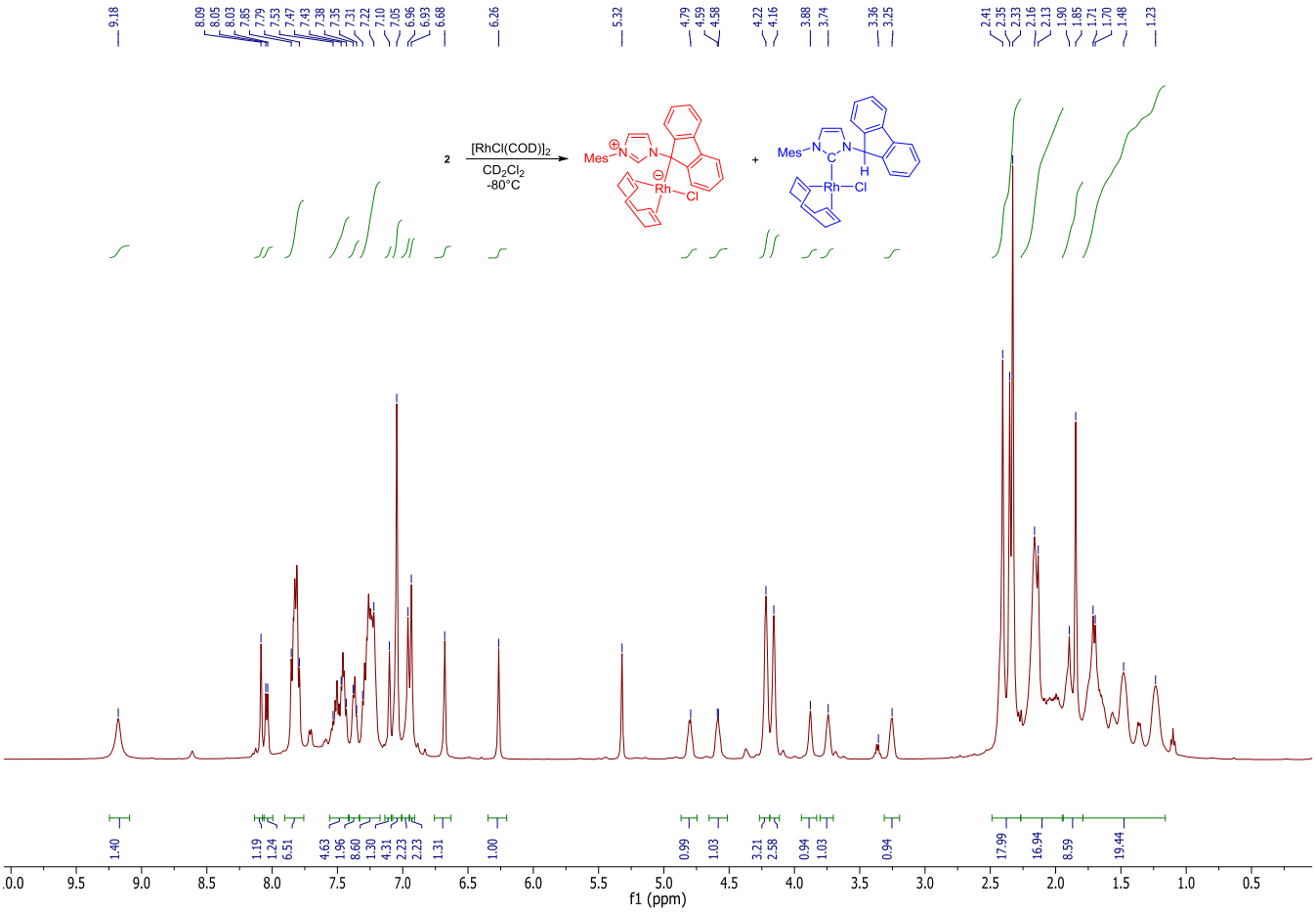
^{1}H NMR spectrum of **5** (400MHz, $CDCl_3$)



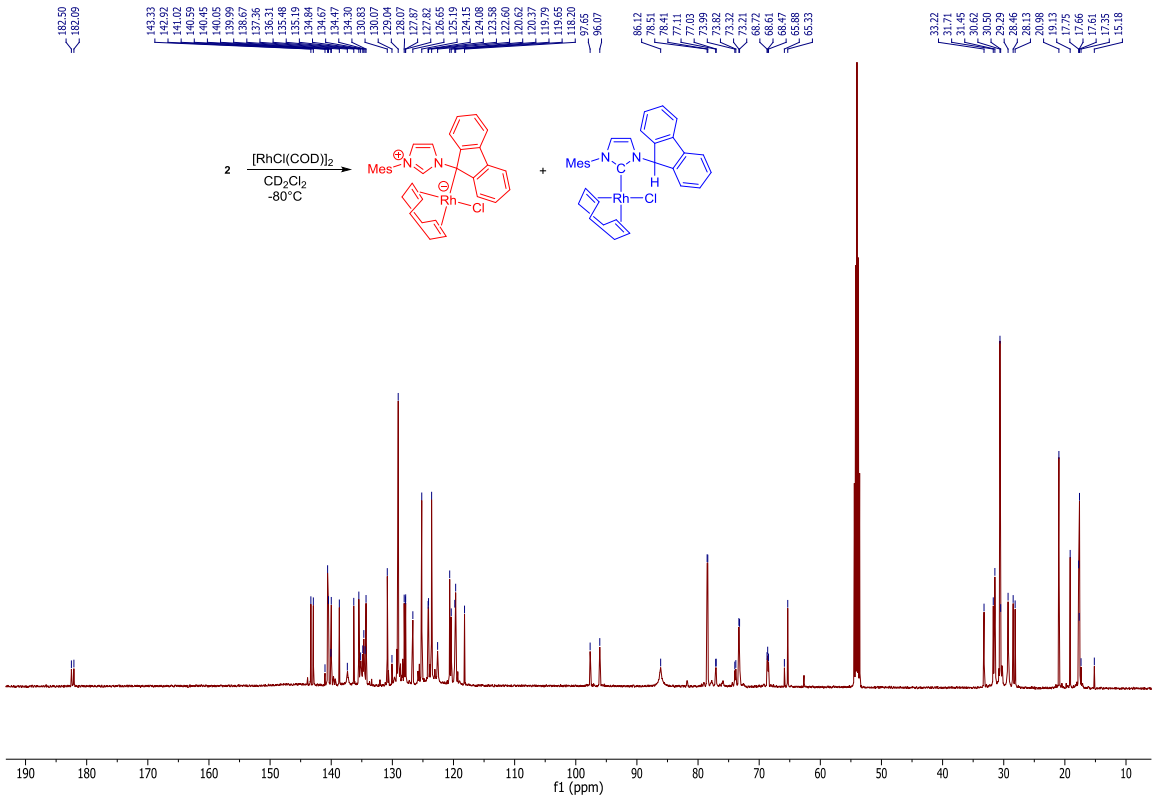
^{13}C{^{1}H} NMR spectrum of **5** (100.6 MHz, $CDCl_3$)



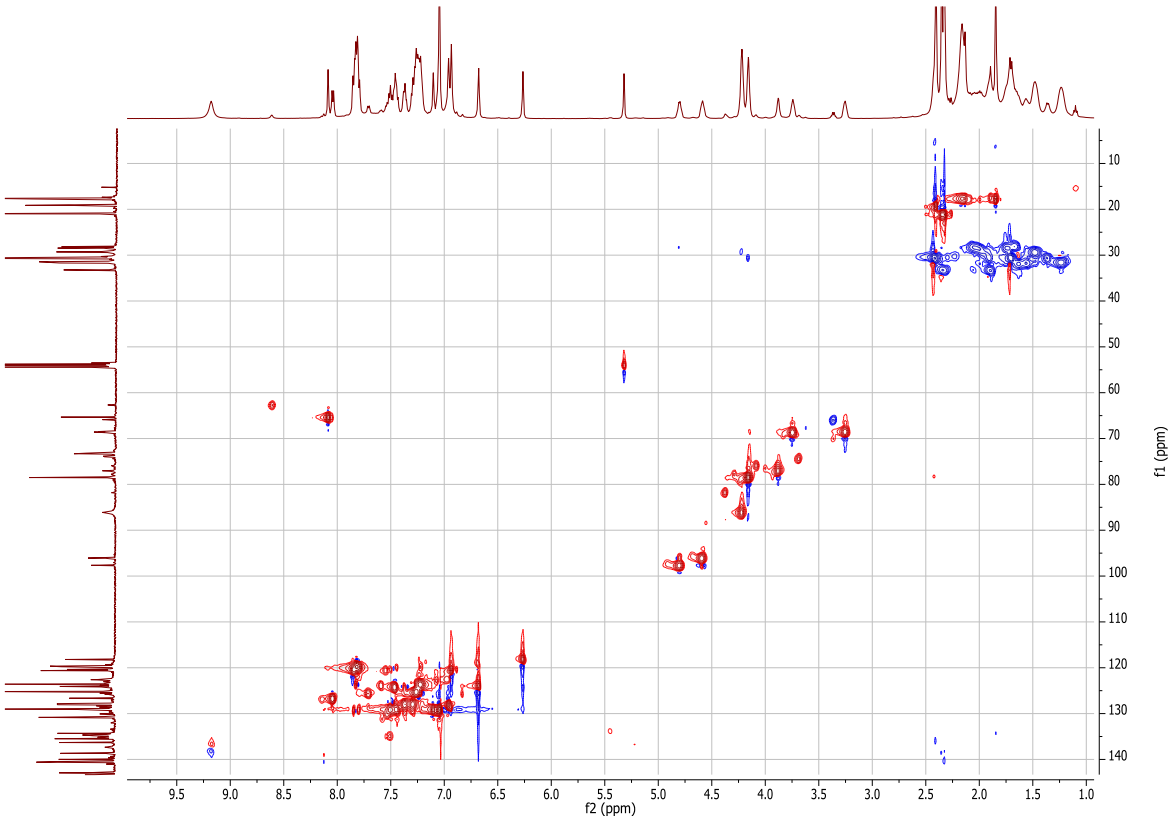
^{1}H NMR spectrum of the mixture of **5'**, **5** and $[RhCl(COD)]_2$ (500 MHz, CD_2Cl_2, 193 K)



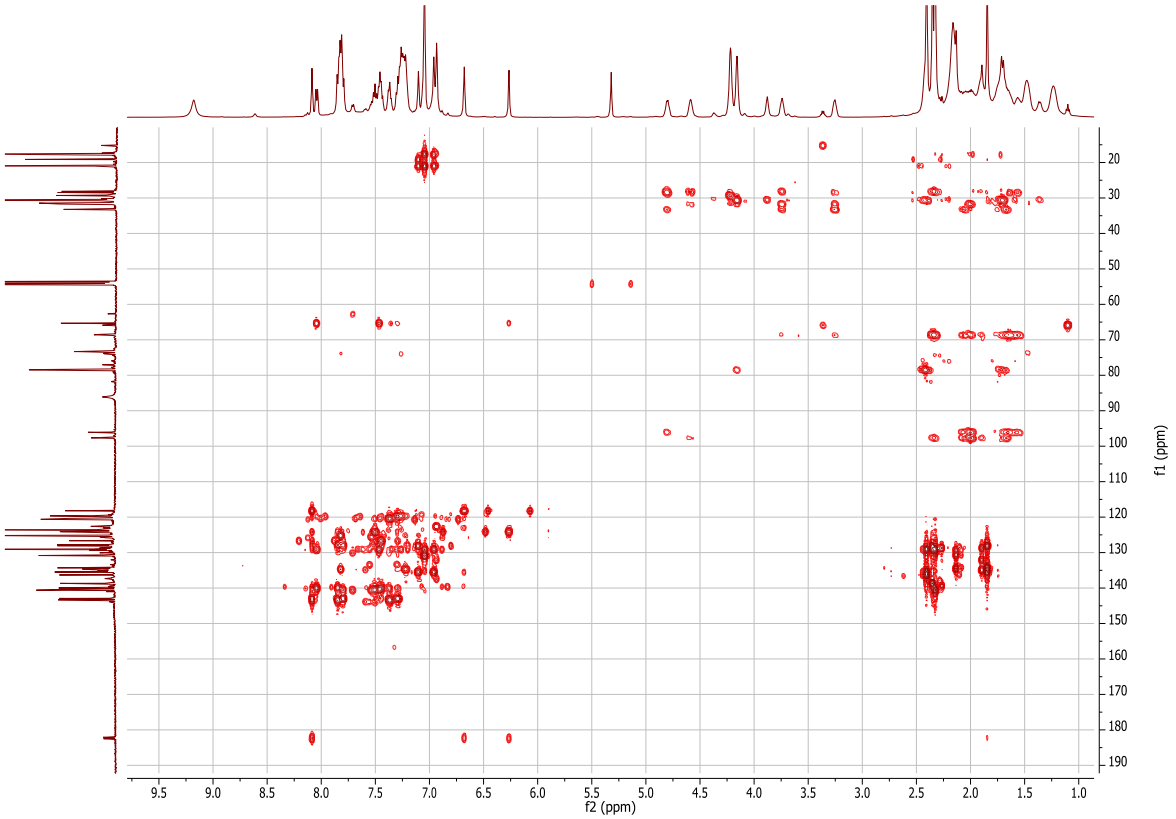
^{13}C{^{1}H} NMR spectrum of the mixture of **5'**, **5** and $[RhCl(COD)]_2$ (125.8 MHz, CD_2Cl_2, 193 K)



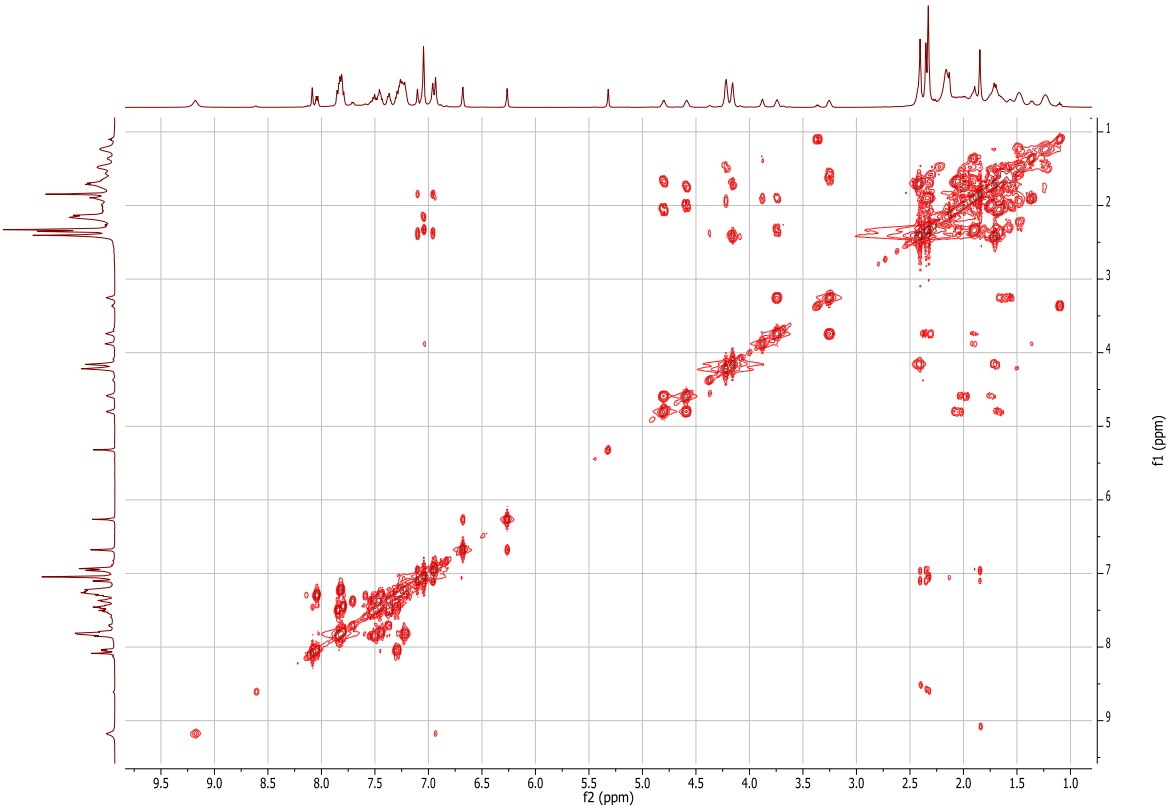
{^{13}C-^{1}H} HSQC NMR of the mixture of **5'**, **5** and [RhCl(COD)]$_2$ (500 MHz, CD_2Cl_2, 193 K)



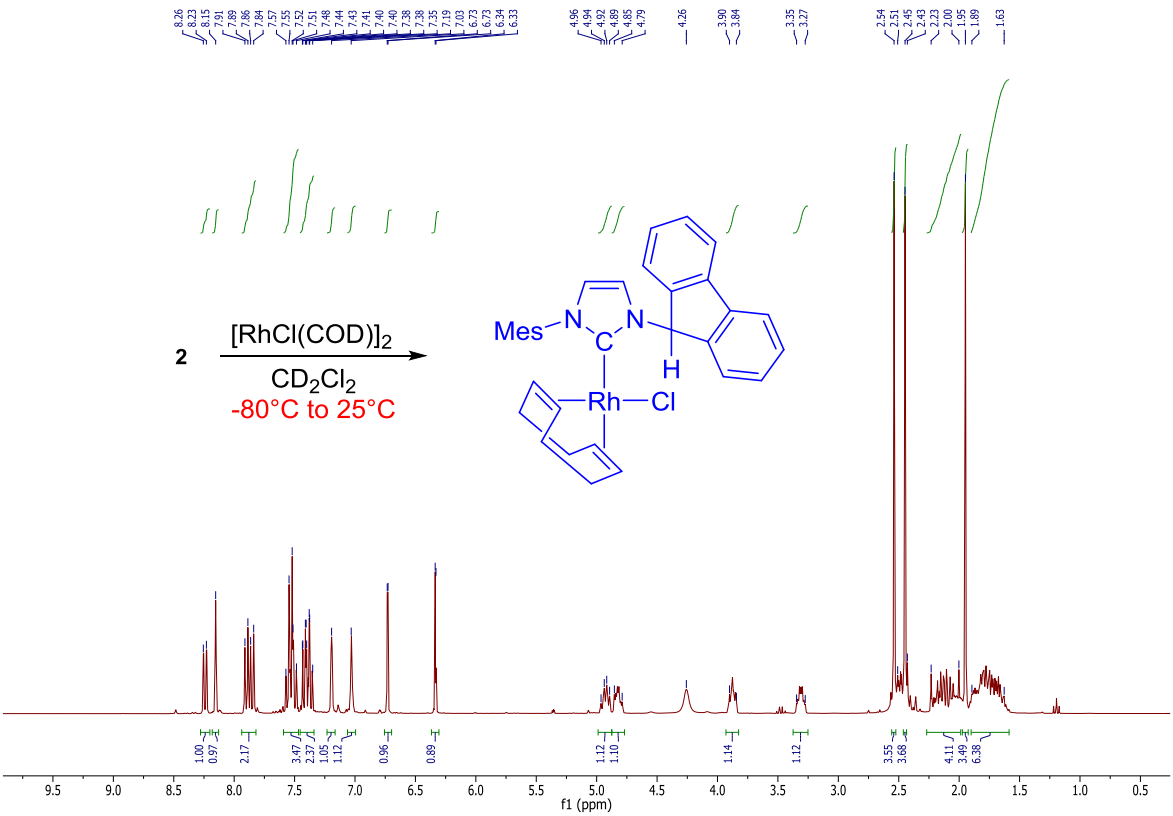
{^{13}C-^{1}H} HMBC NMR of the mixture of **5'**, **5** and [RhCl(COD)]$_2$ (500 MHz, CD_2Cl_2, 193 K)



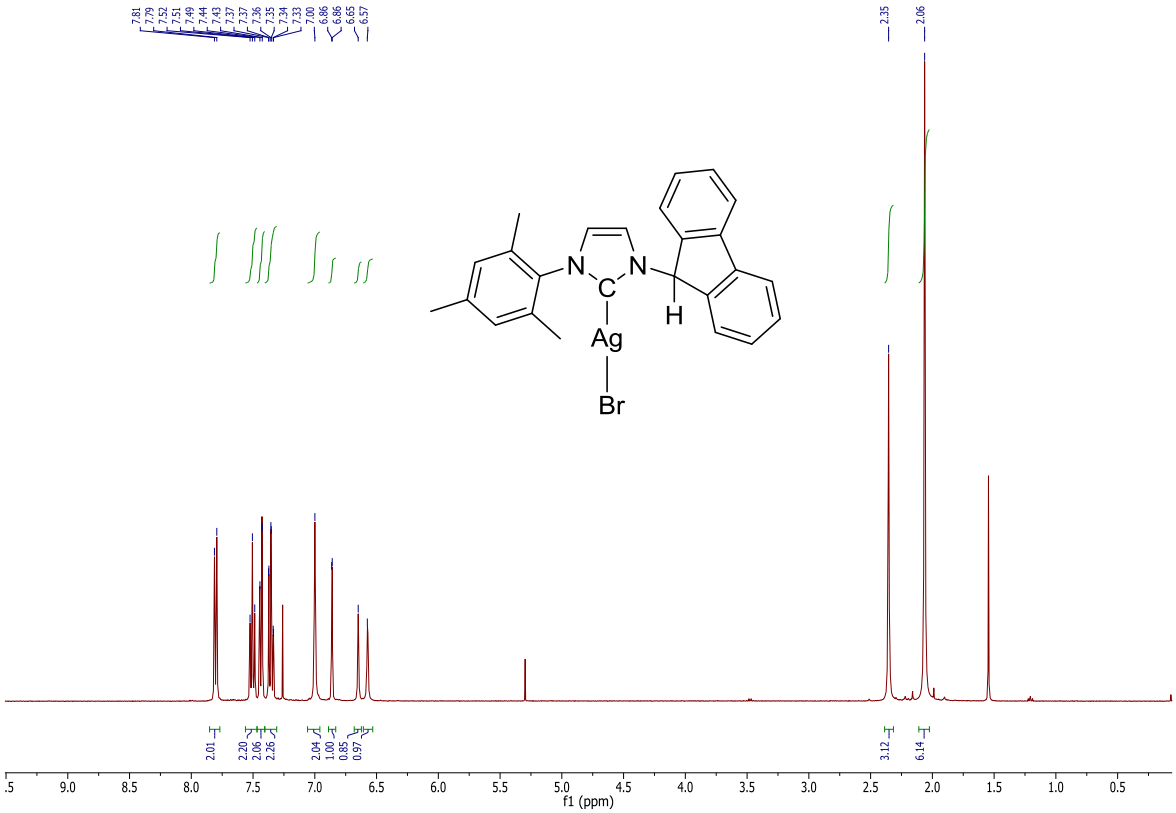
{^{1}H-^{1}H} COSY NMR of the mixture of **5'**, **5** and [RhCl(COD)]$_2$ (500 MHz, CD_2Cl_2, 193 K)



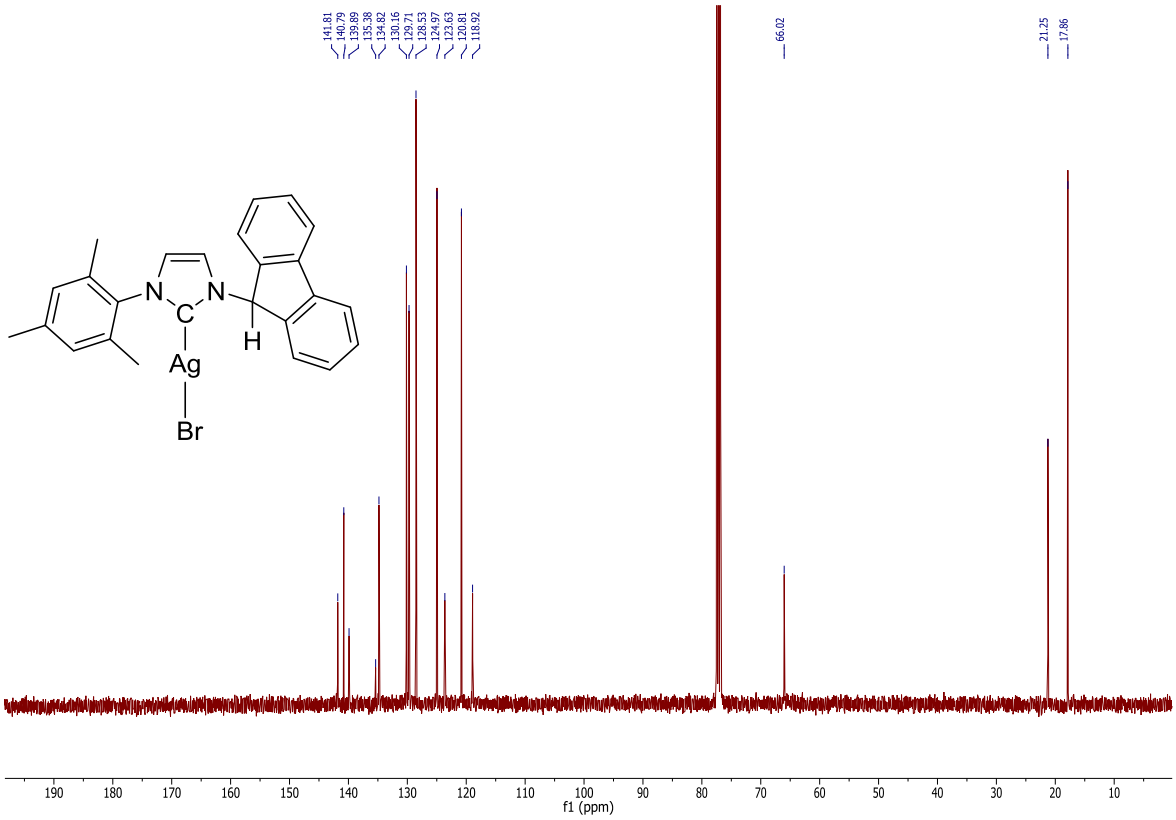
^{1}H NMR spectrum of the reaction after returning to 25°C (500 MHz, CD_2Cl_2, 298 K)



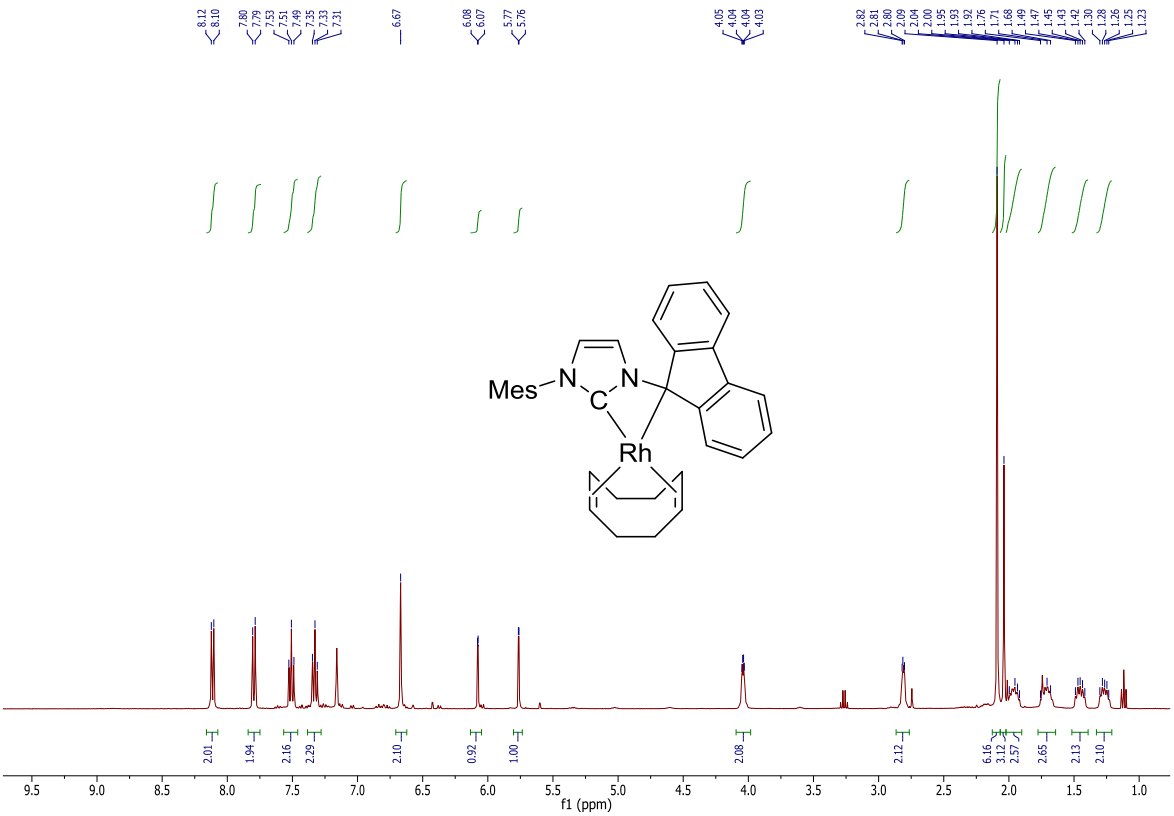
^{1}H NMR spectrum of **6** (400MHz, $CDCl_3$)



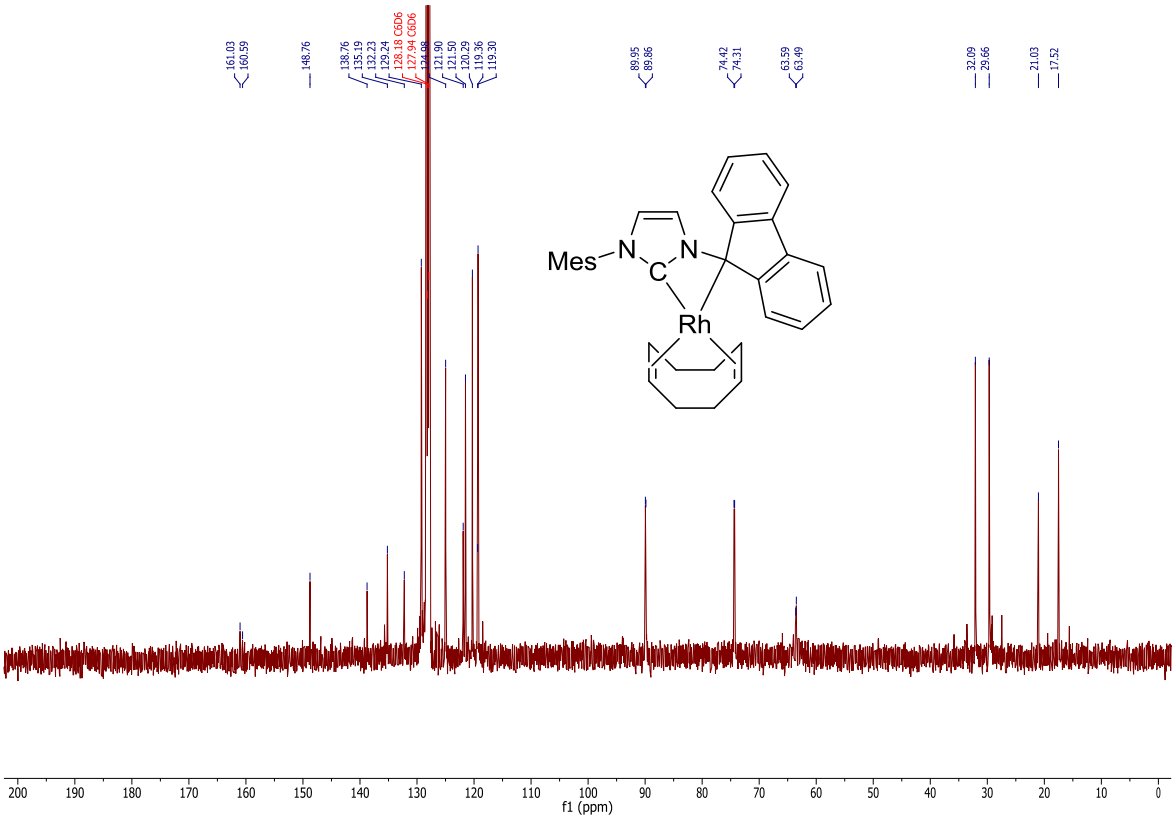
^{13}C{^{1}H} NMR spectrum of **6** (100.6 MHz, $CDCl_3$)



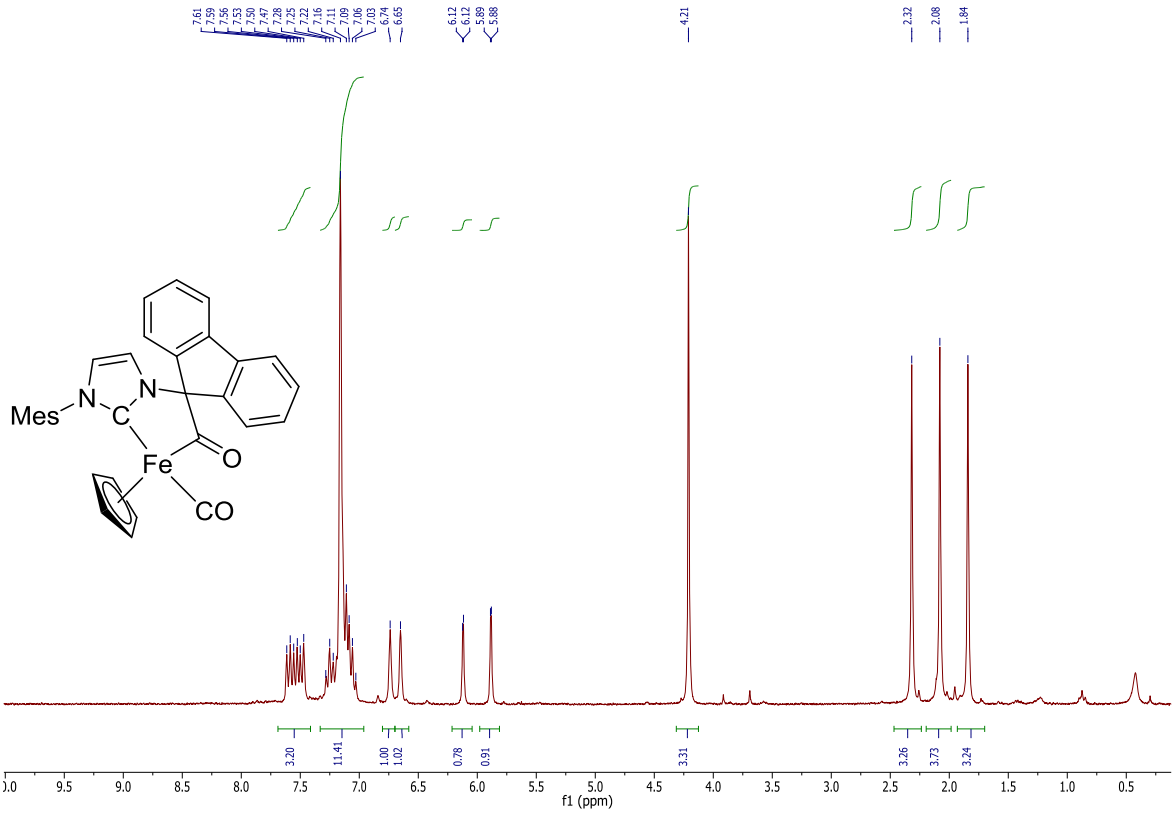
^{1}H NMR spectrum of **7** (400MHz, C_6D_6)



^{13}C{^{1}H} NMR spectrum of **7** (100.6 MHz, C_6D_6)



^{1}H NMR spectrum of **8** (250 MHz, C_6D_6)



^{13}C{^{1}H} NMR spectrum of **8** (100.6 MHz, C_6D_6)