

Molecules

Palladium(II) and Platinum(II) complexes bearing ONS-type pincer ligands. Synthesis, characterization and catalytic investigations.

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Supplementary material

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Table S1. Hydrogen bond parameters [\AA , $^\circ$]

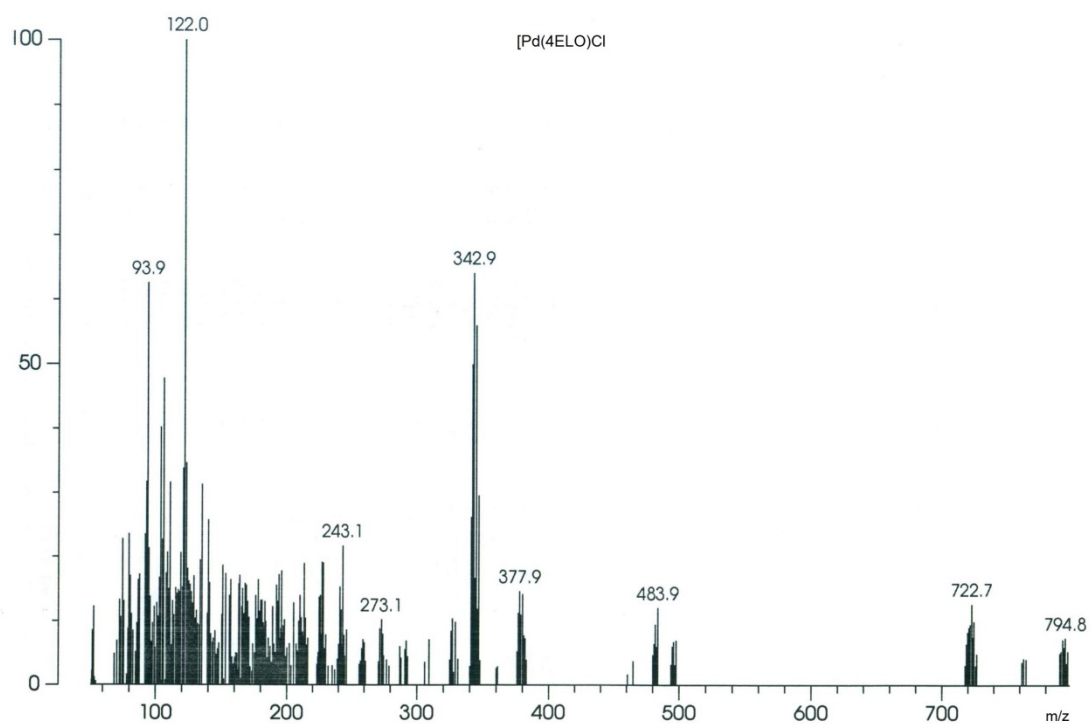
Compound	D–H \cdots A	D–H	H \cdots A	D \cdots A	\angle DHA	Symmetry
3	N(14)–H(14A) \cdots Cl(1) ^a	0.77(5)	2.80(5)	3.452(4)	144(5)	$x, -y+1/2, z+1/2$
5	N(14)–H(14A) \cdots Cl(1) ^a	0.76(4)	2.75(4)	3.500(3)	171(4)	$x-1/2, -y-1/2, z-1/2$

Table S2. Intermolecular $\pi\cdots\pi$ interaction parameters (\AA , $^\circ$)

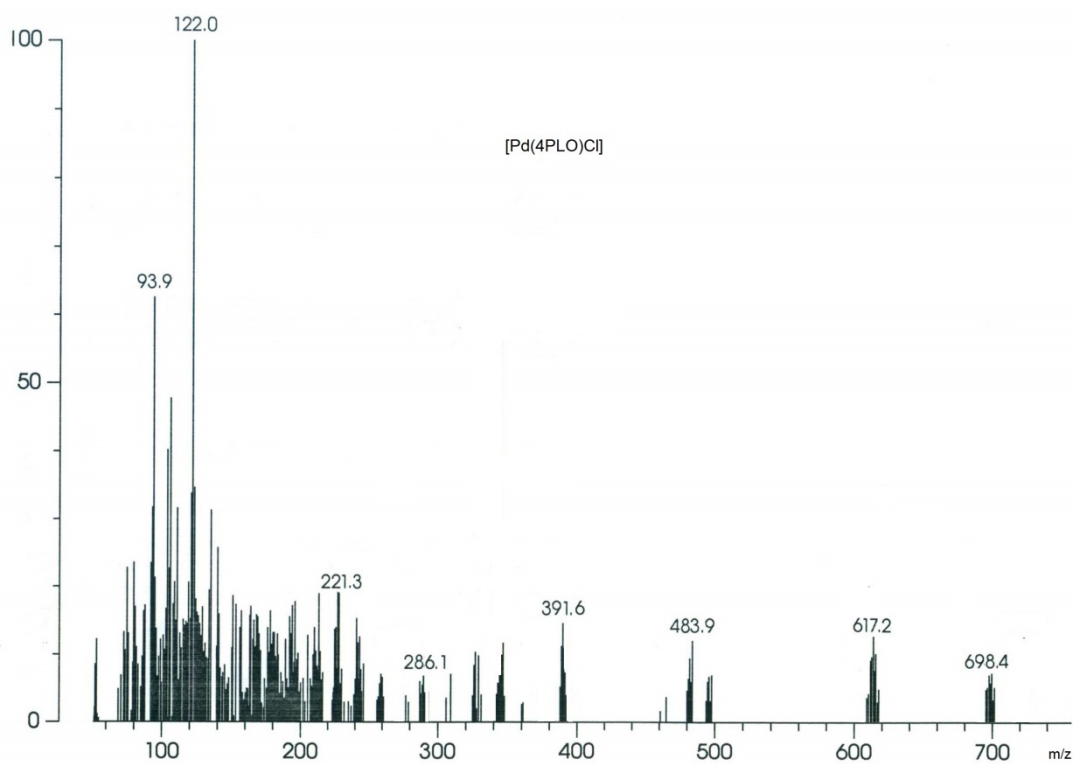
Compound	$\pi\cdots\pi$	Cg(I) \cdots Cg(J)	α
3	Cg(1) \cdots Cg(3) ^f	3.608(2)	13.38(17)
	Cg(1) ring (Pd1/S1/C17/N13/N12)		
	Cg(3) ring (N11/C11/C12/C13/C14/C15)		
	$f = 1-x, -y, -z$		
5	Cg(1) \cdots Cg(3) ^b	3.701(2)	13.27(15)
	Cg(3) \cdots Cg(4) ^c	3.623(2)	8.56(19)
	Cg(1) ring (Pd1/S1/C17/N13/N12)		
	Cg(3) ring (N11/C11/C12/C13/C14/C22)		
	Cg(5) ring (C14/C15/C16/C17/C21/C22)		
	$b = -x, -y, -z$		
	$c = -x+1, -y, -z$		

Cg(I) \cdots Cg(J): Distance between ring centroids; α : Dihedral angle between planes I and J. For details, see Janiak, C. A critical account on π – π stacking in metal complexes with aromatic nitrogen-containing ligands. *J. Chem. Soc. Dalton Trans.* **2000**, 3885–3898.

Figure S1. Mass spectra of the complexes (FAB).

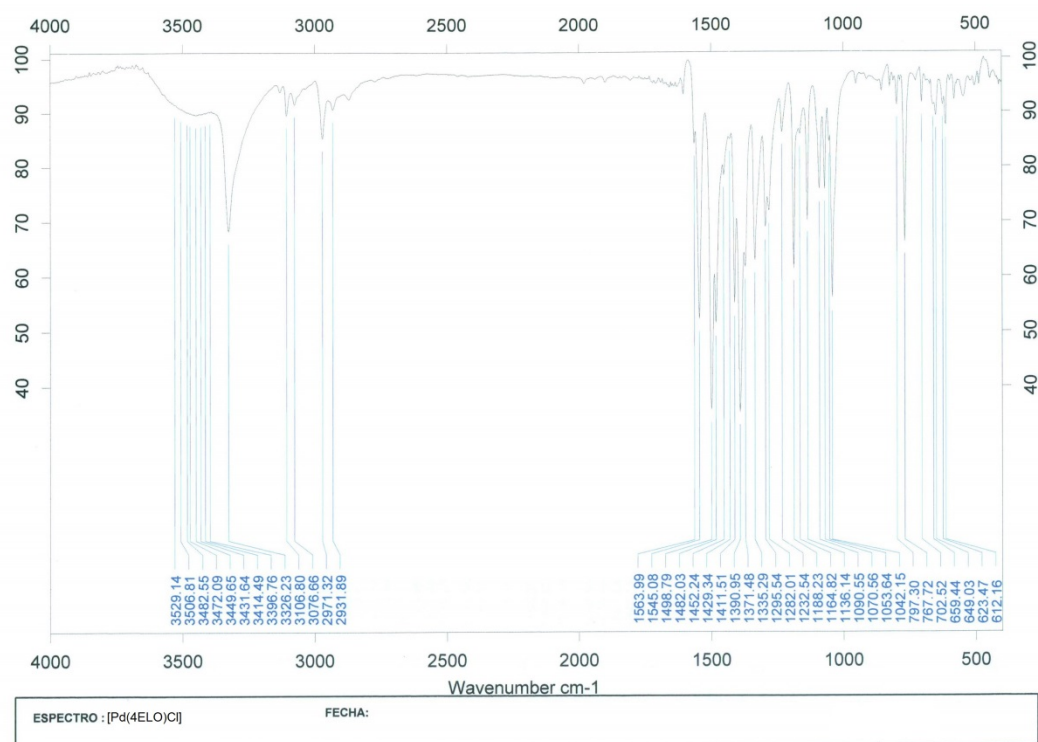


$[Pd(4ELO)Cl]$ (3)

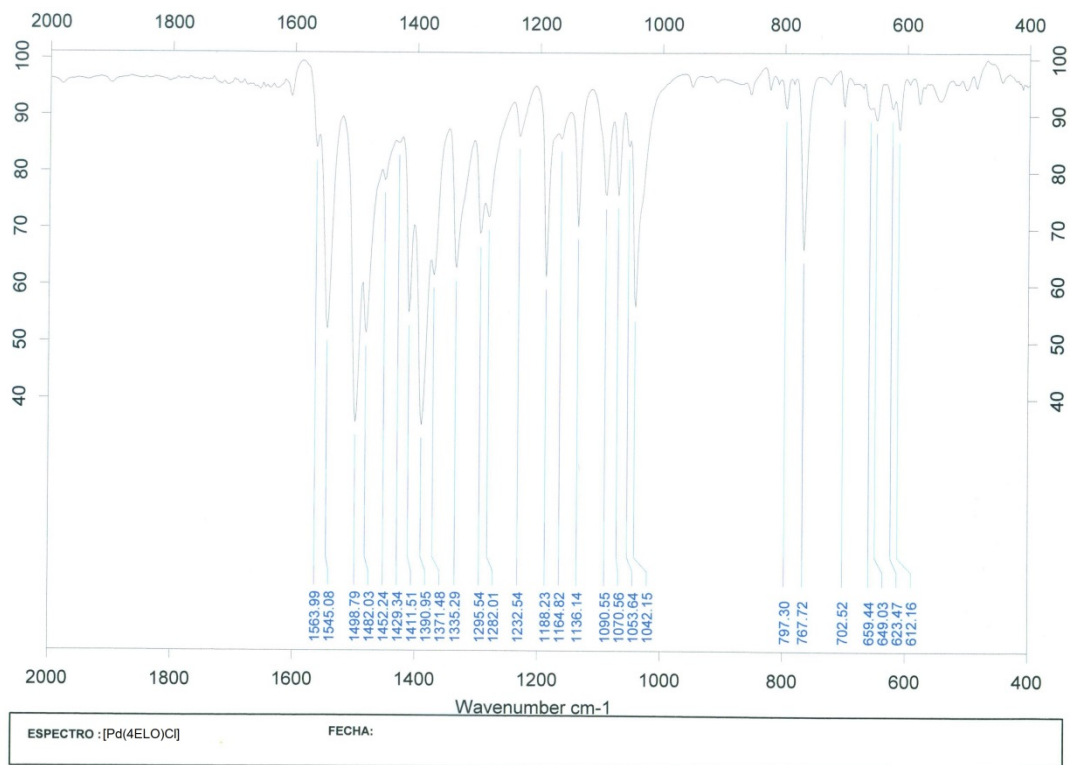


$[Pd(4PLO)Cl]$ (5)

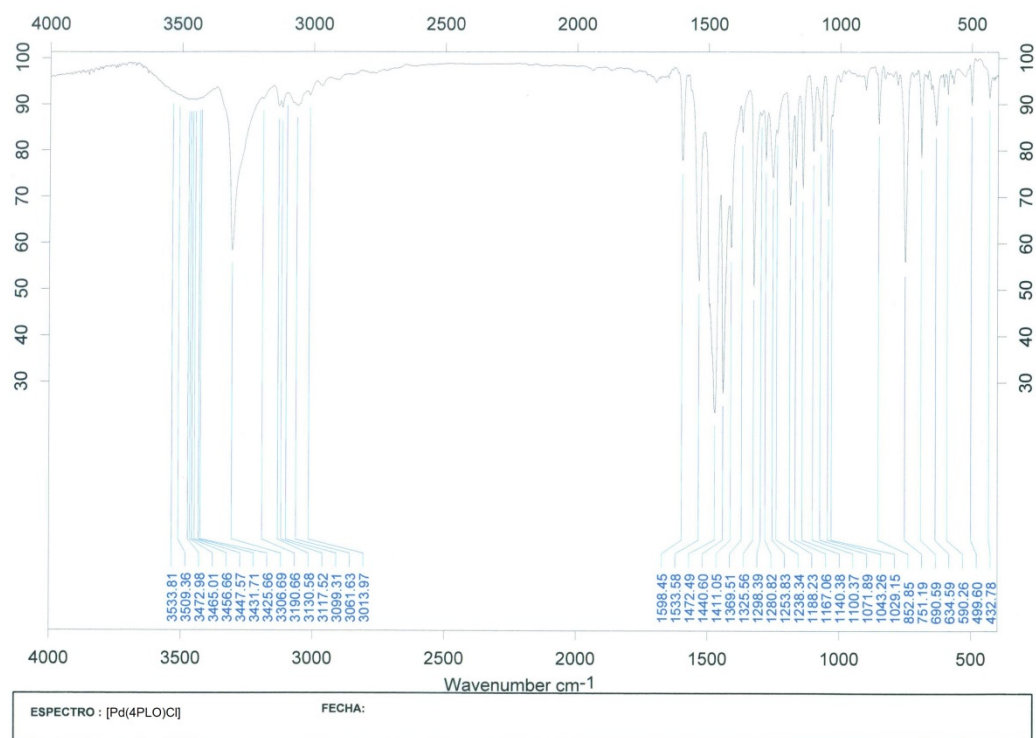
Figure S2. FT-IR spectra in the region 4000-500 cm^{-1}



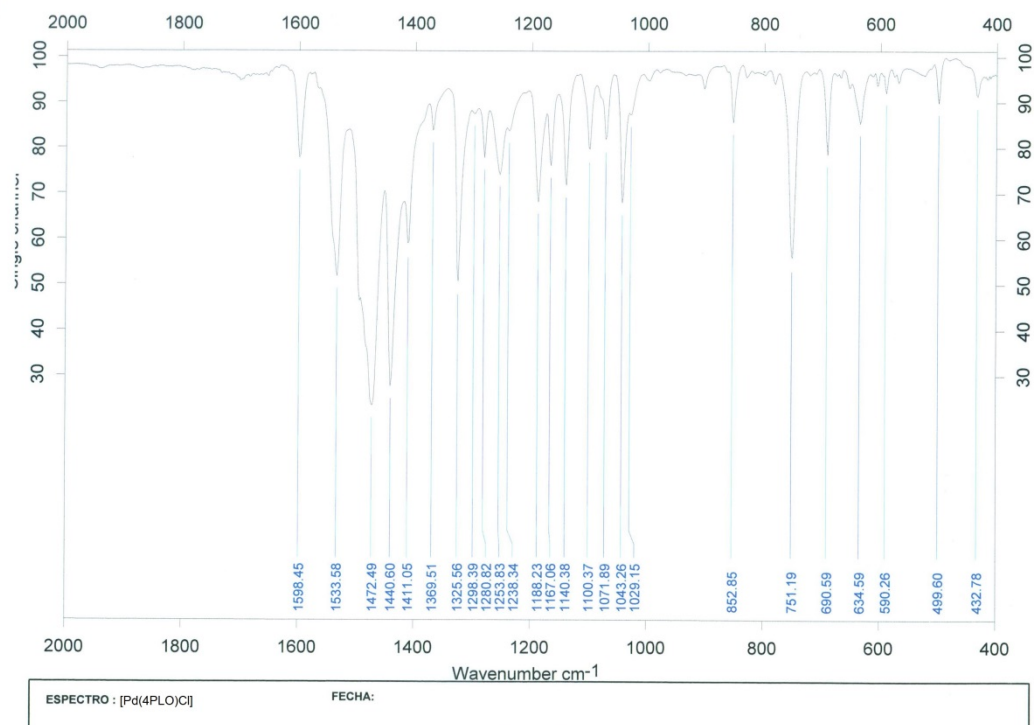
[Pd(4ELO)Cl](3)



[Pd(4ELO)Cl (3)

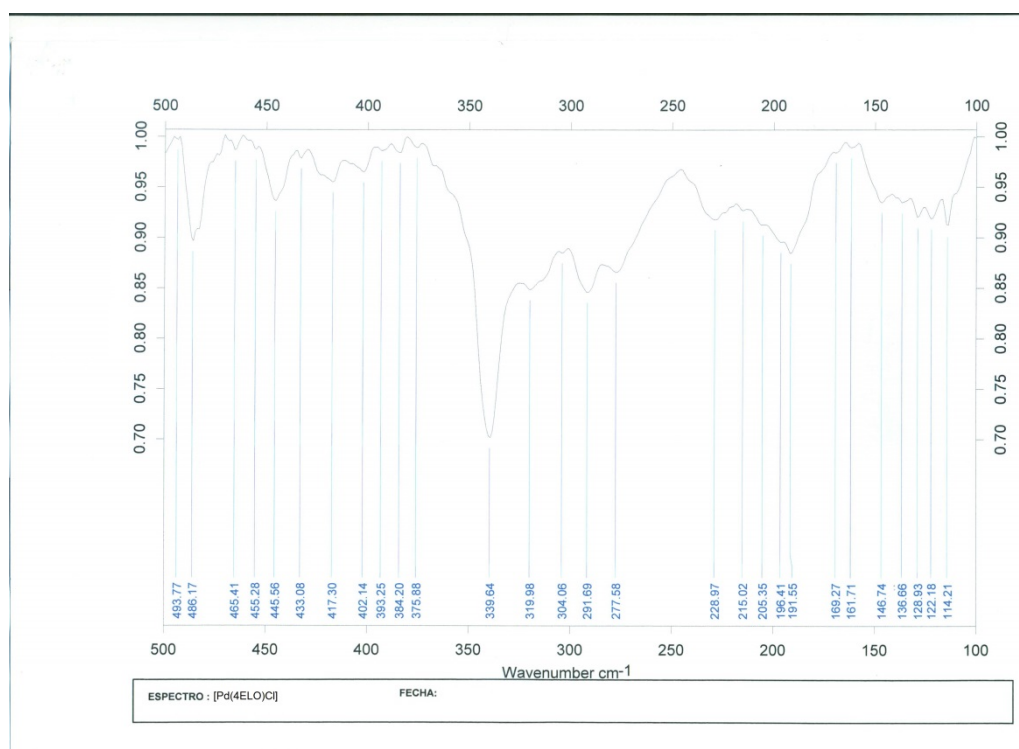


$[Pd(4PLO)Cl]$ (5)

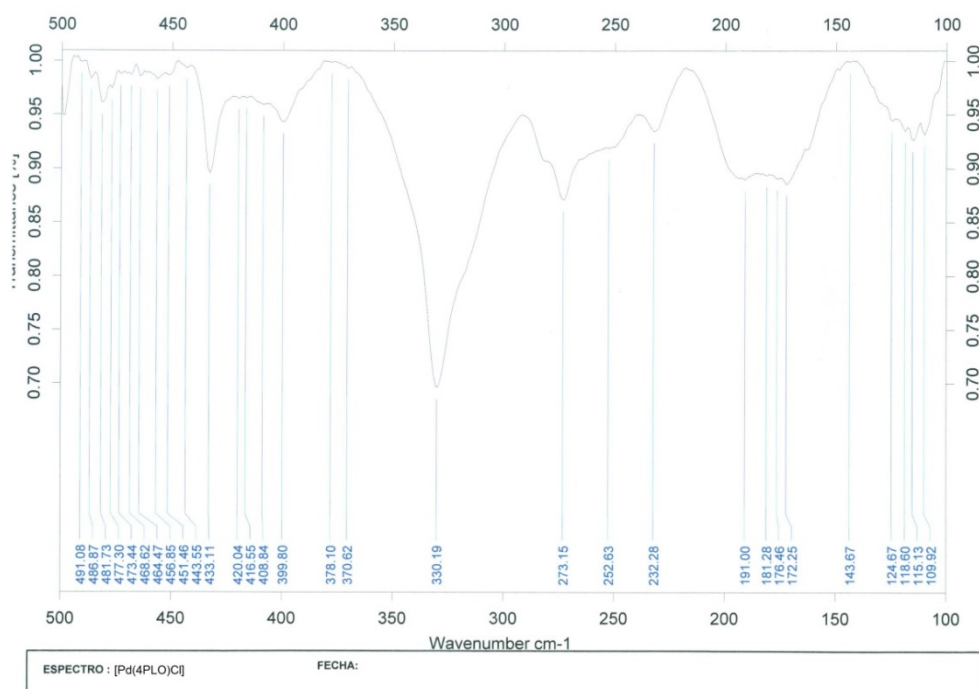


$[Pd(4PLO)Cl]$ (5)

Figure S3. FT-IR spectra in the region 500-100 cm^{-1}

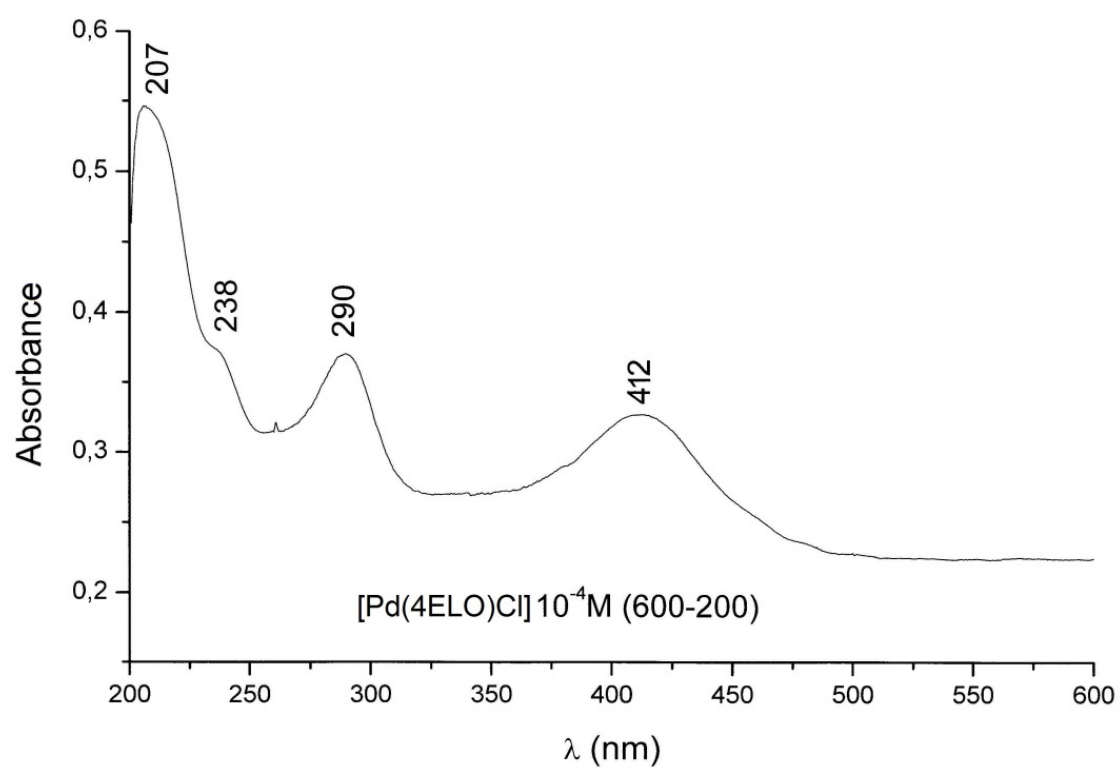


[Pd(4ELO)Cl] (3)

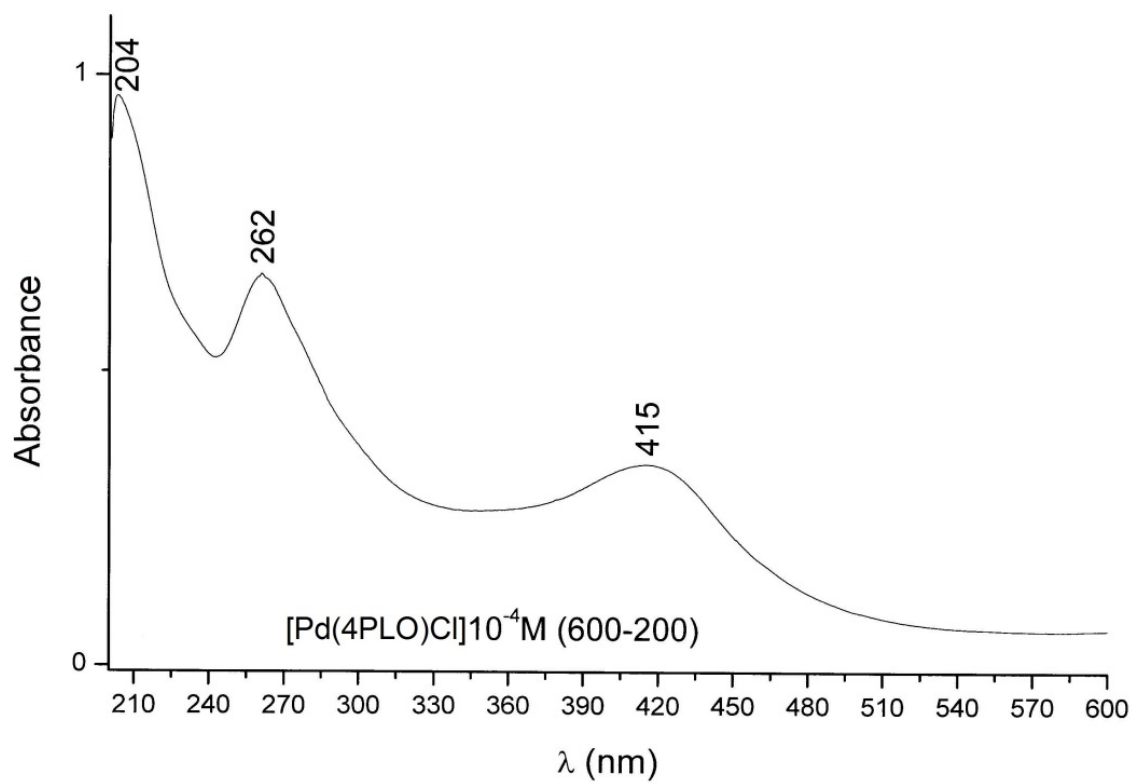


[Pd(4PLO)Cl] (5)

Figure S4. UV-visible Spectra

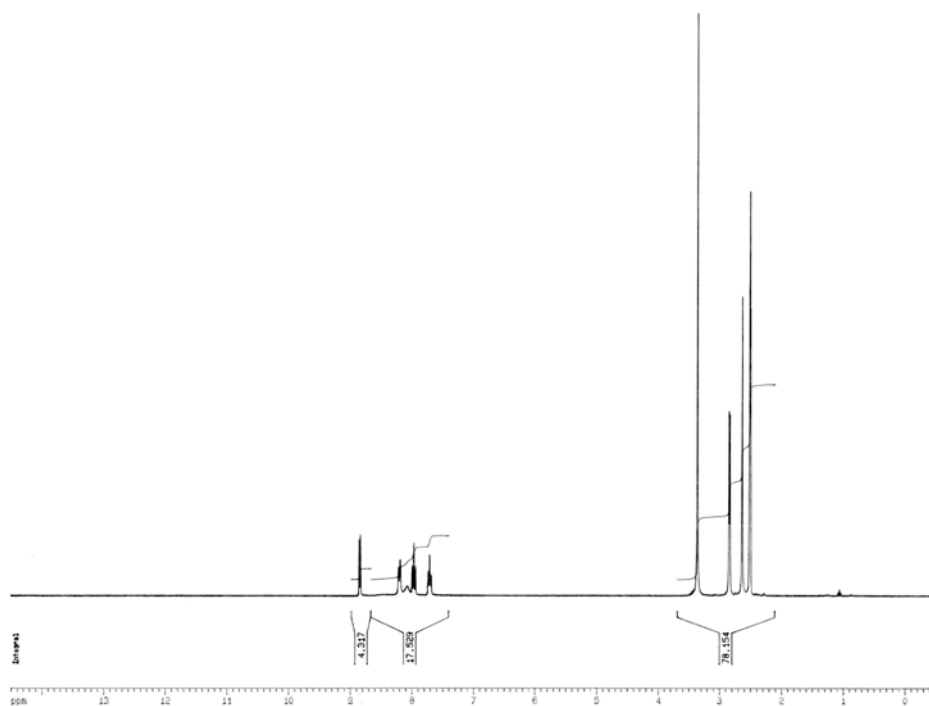


$[Pd(4ELO)Cl]$ (3)

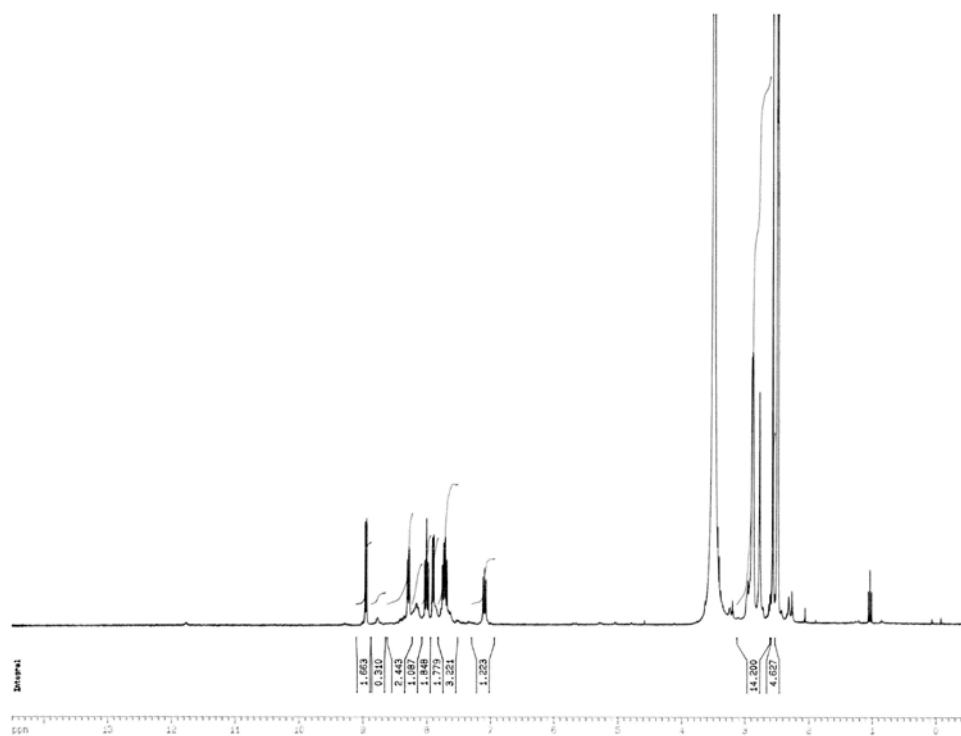


$[Pd(4PLO)Cl]$ (5)

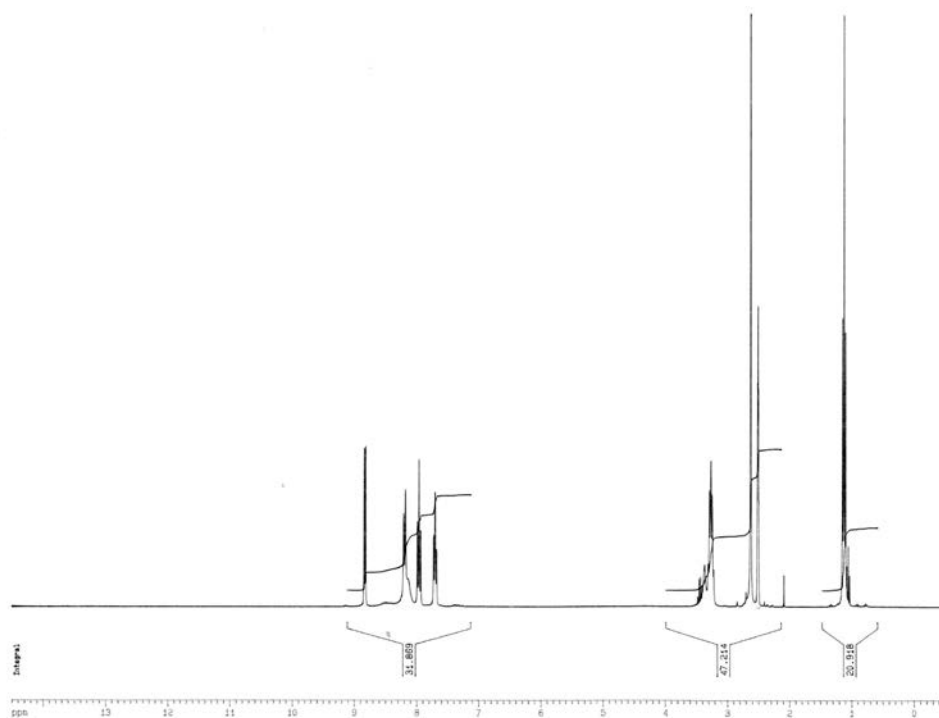
Figure S5. ^1H NMR spectra



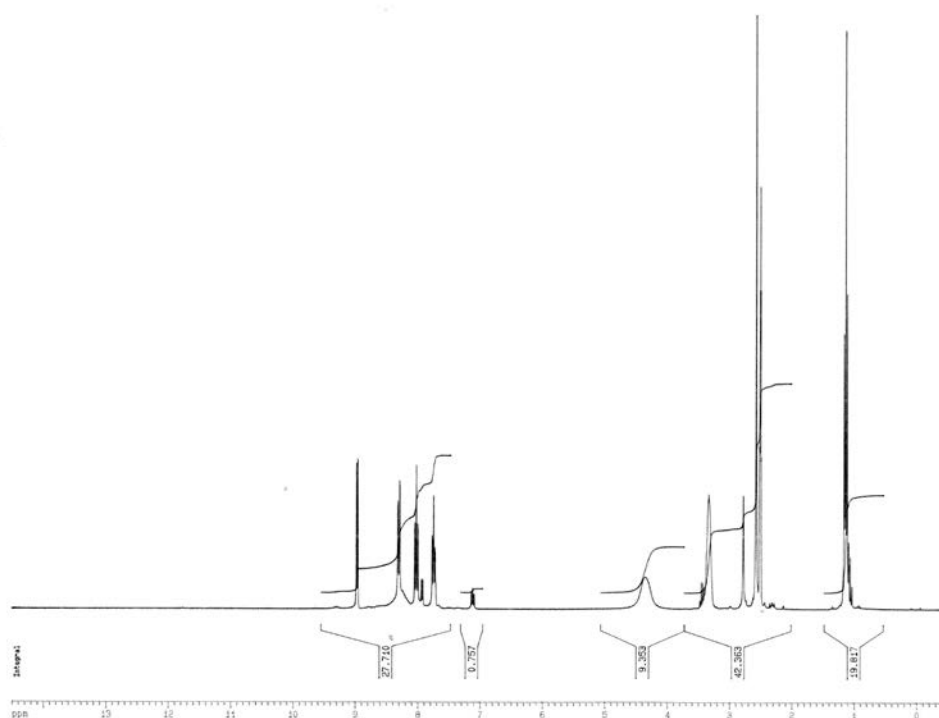
$[\text{Pd}(\text{4MLO})\text{Cl}]$ (1)



$[\text{Pt}(\text{4MLO})\text{Cl}]$ (2)

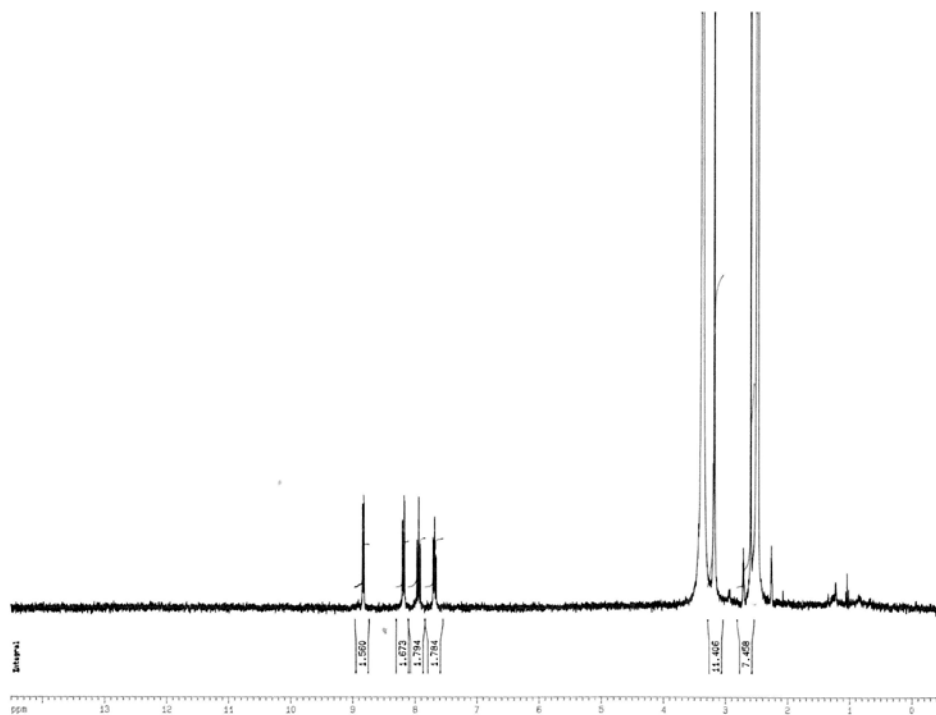


$[Pd(4ELO)Cl]$ (3)

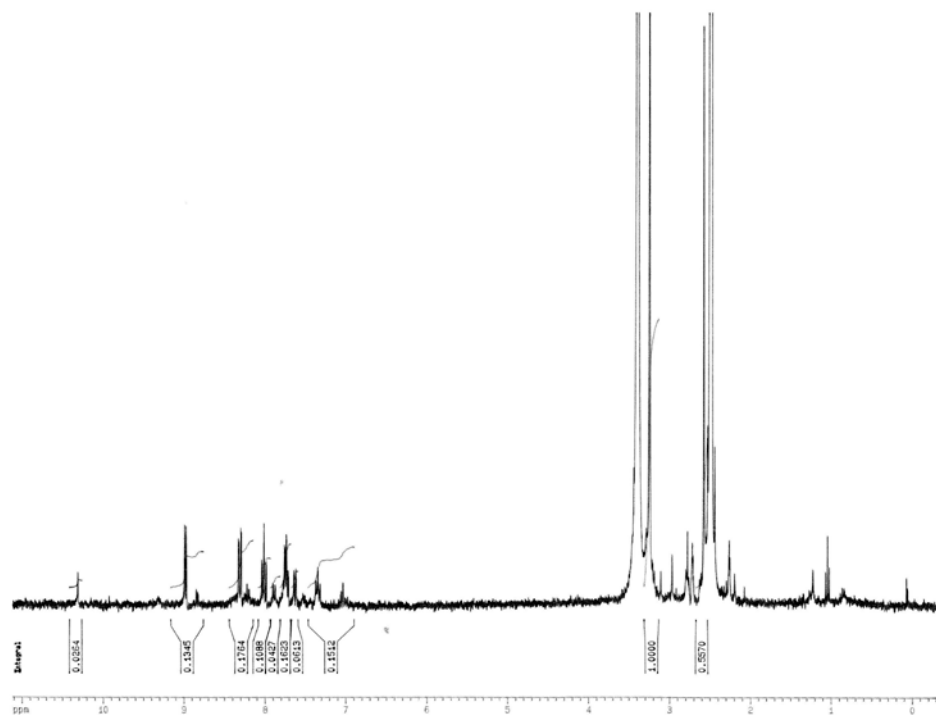


$[Pt(4ELO)Cl]$ (4)



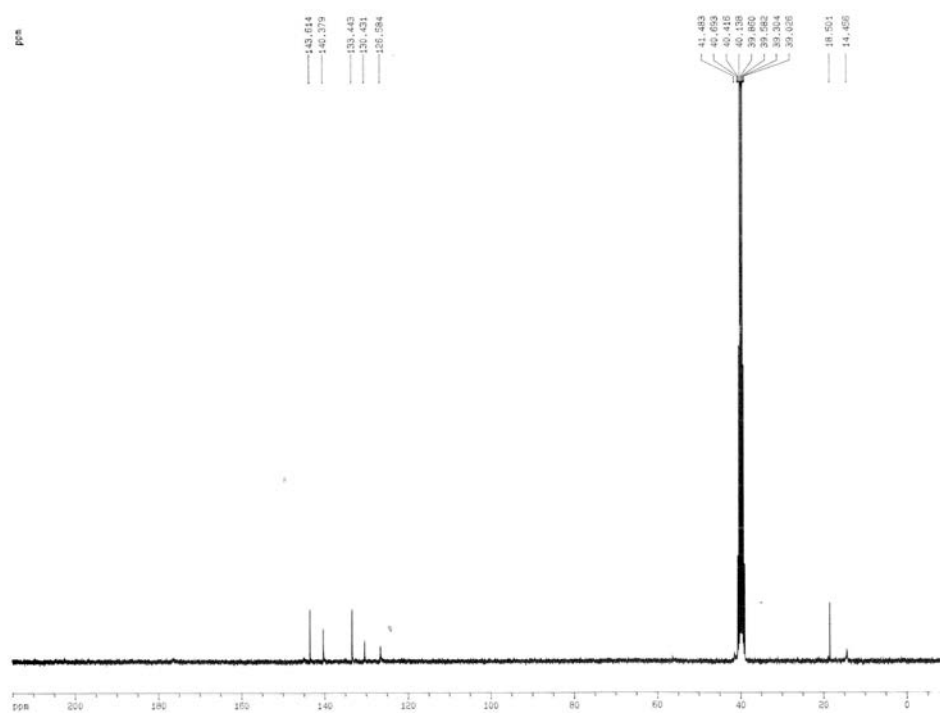


[Pd(4DMLO)Cl] (7)

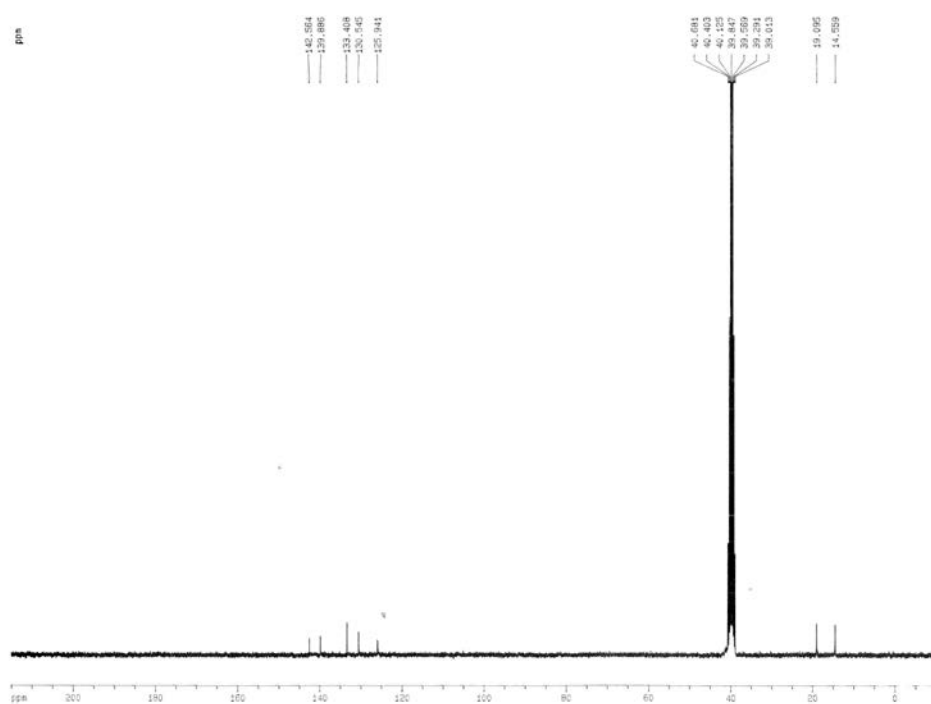


[Pt(4DMLO)Cl] (8)

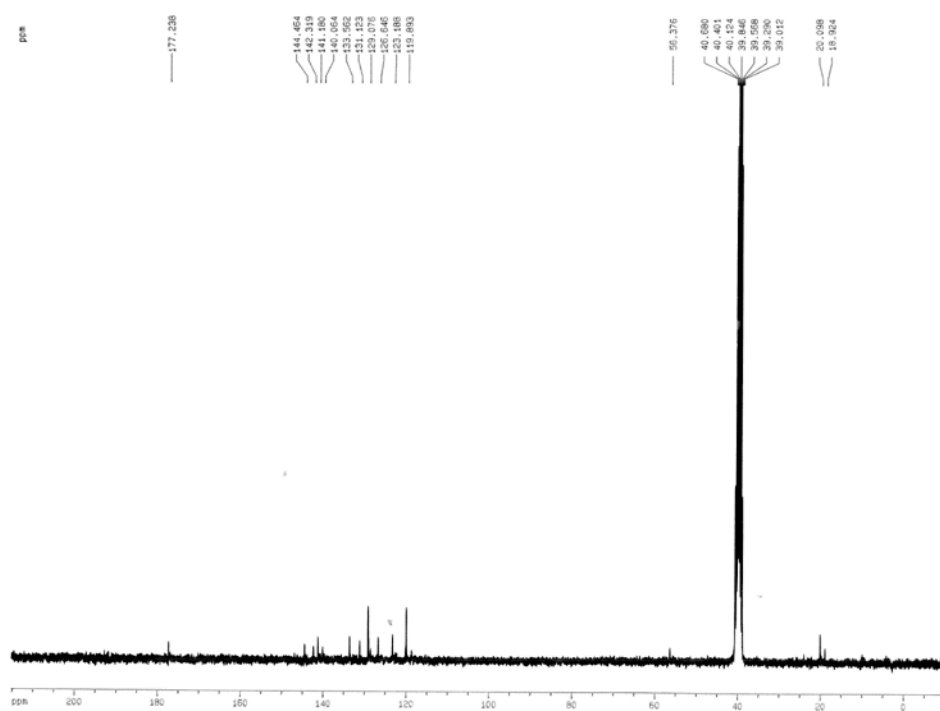
Figure S6. ^{13}C NMR spectra



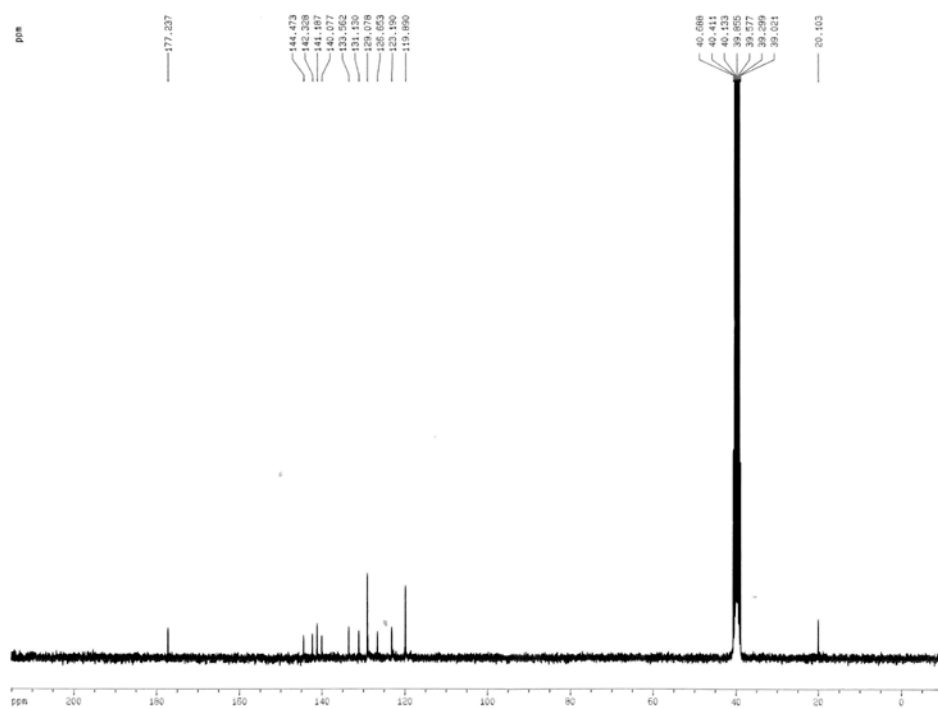
$[\text{Pd}(\text{4ELO})\text{Cl}]$ (3)



$[\text{Pt}(\text{4ELO})\text{Cl}]$ (4)

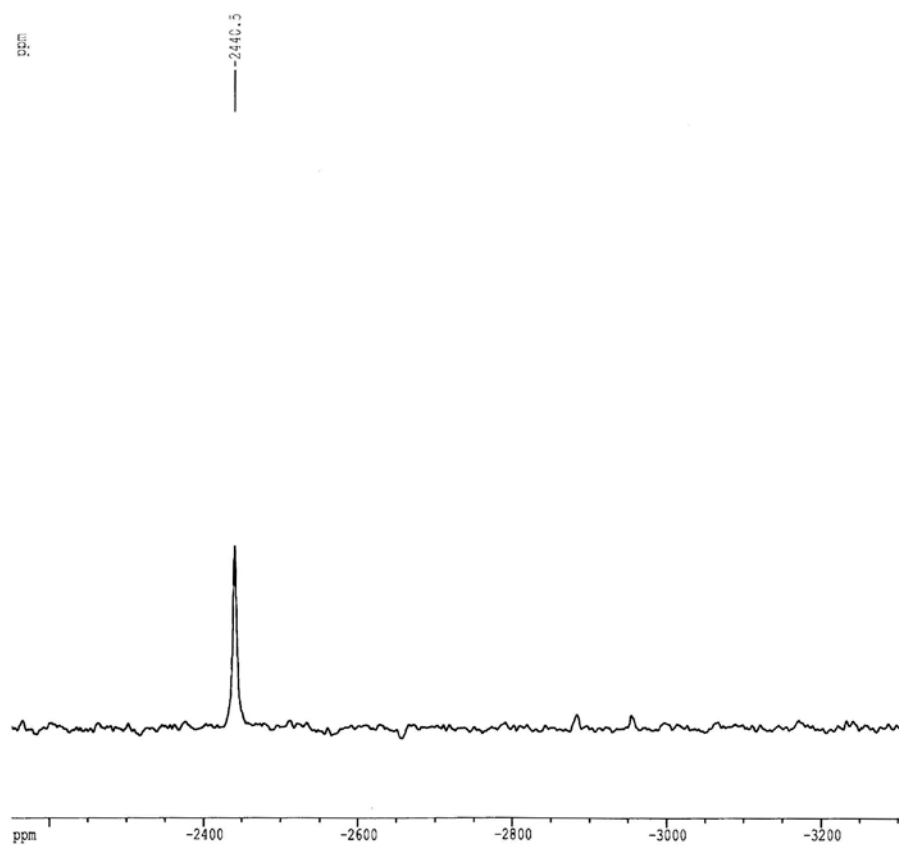


$[Pd(4PLO)Cl]$ (5)

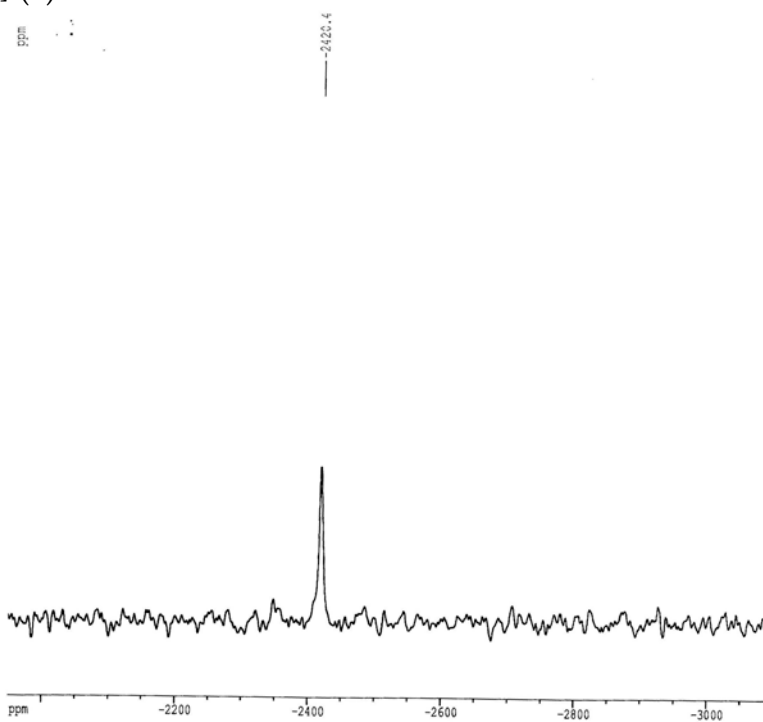


$[Pt(4PLO)Cl]$ (6)

Figure S7. ^{195}Pt NMR spectra



$[\text{Pt}(\text{4PLO})\text{Cl}]$ (6)



$[\text{Pt}(\text{4DMLO})\text{Cl}]$ (8)