Design of a Flexible Organometallic Tecton: Host−Guest Chemistry with Picric Acid and Self-assembly of Platina Macrocycles

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Supporting Information

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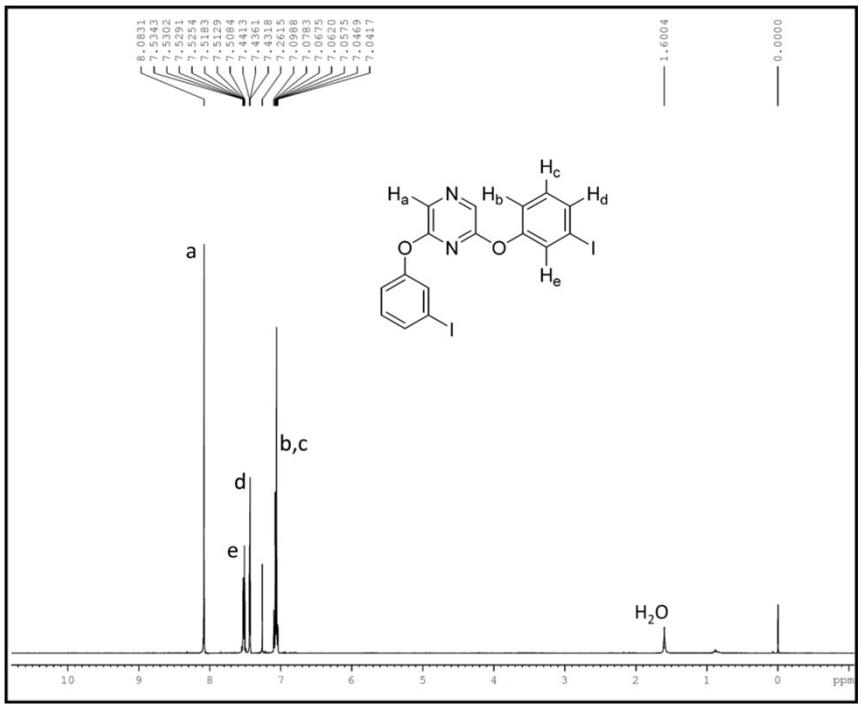
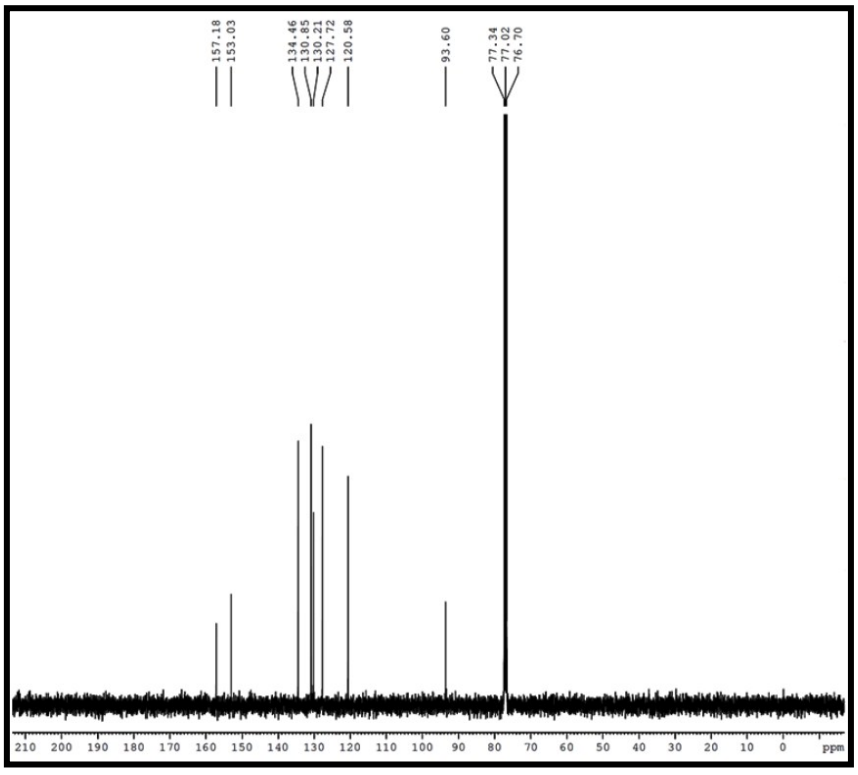
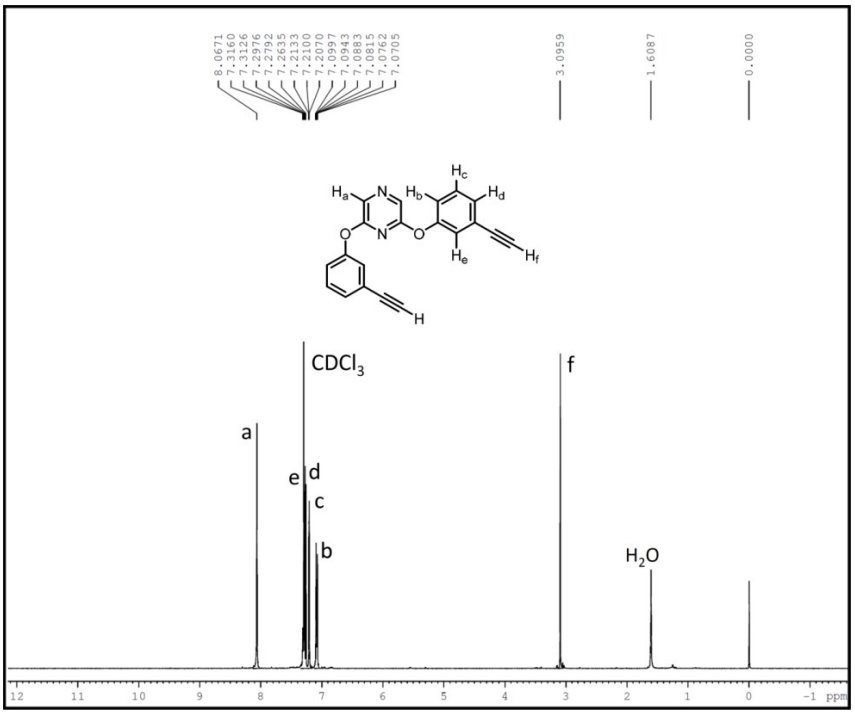
^{1}H NMR spectrum of 1 (2,6-bis(3-iodophenoxy)pyrazine):



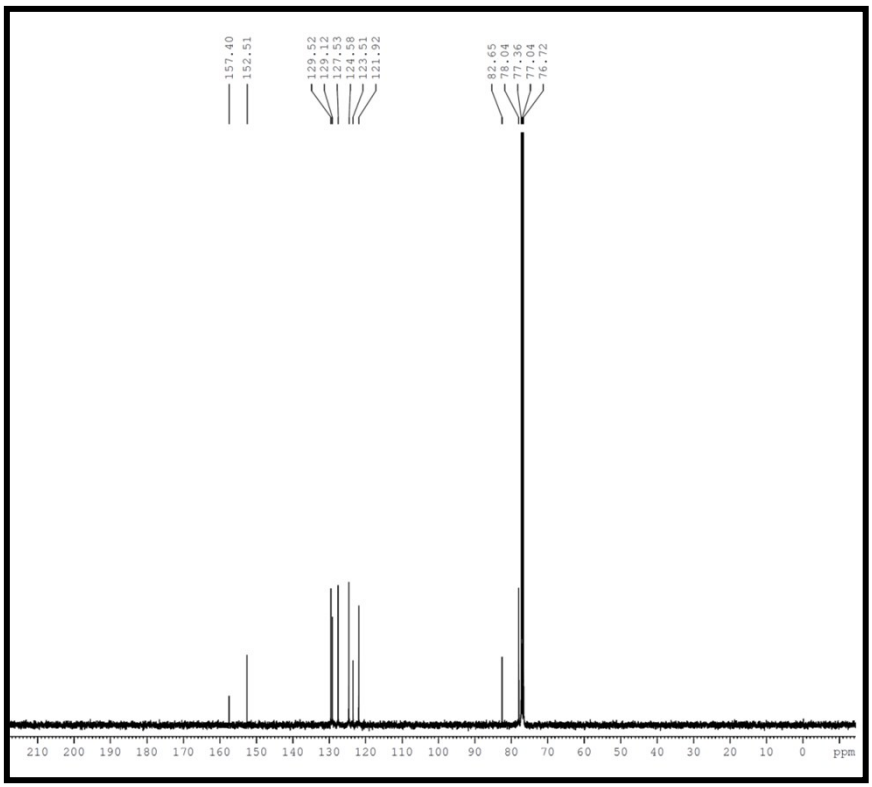
^{13}C NMR spectrum of 1 (2,6-bis(3-iodophenoxy)pyrazine):



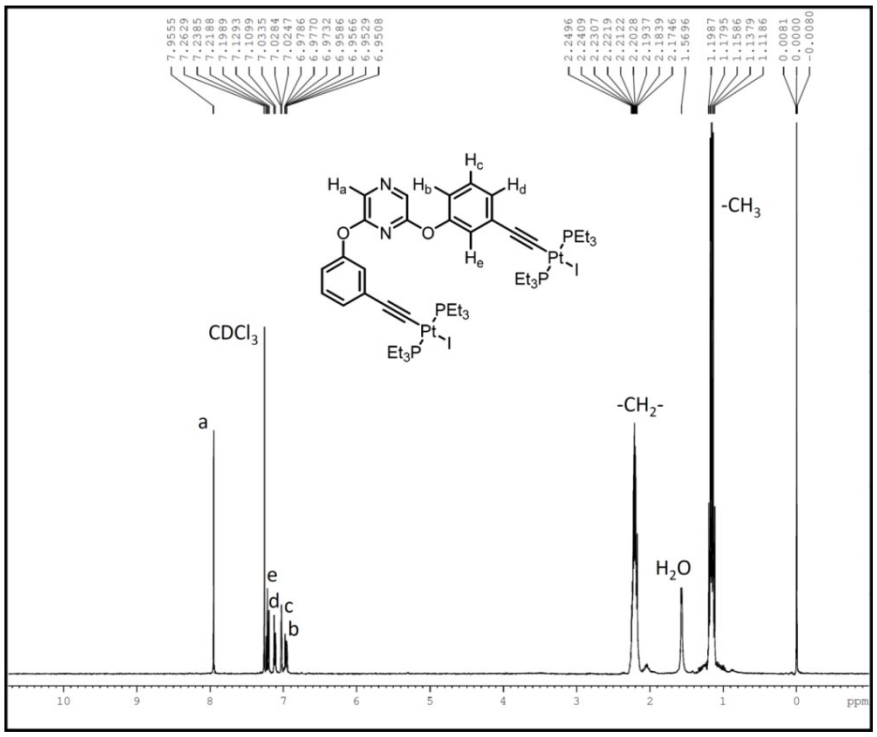
^{1}H NMR spectrum of 2 (2,6-bis(3-ethynylphenoxy)pyrazine):



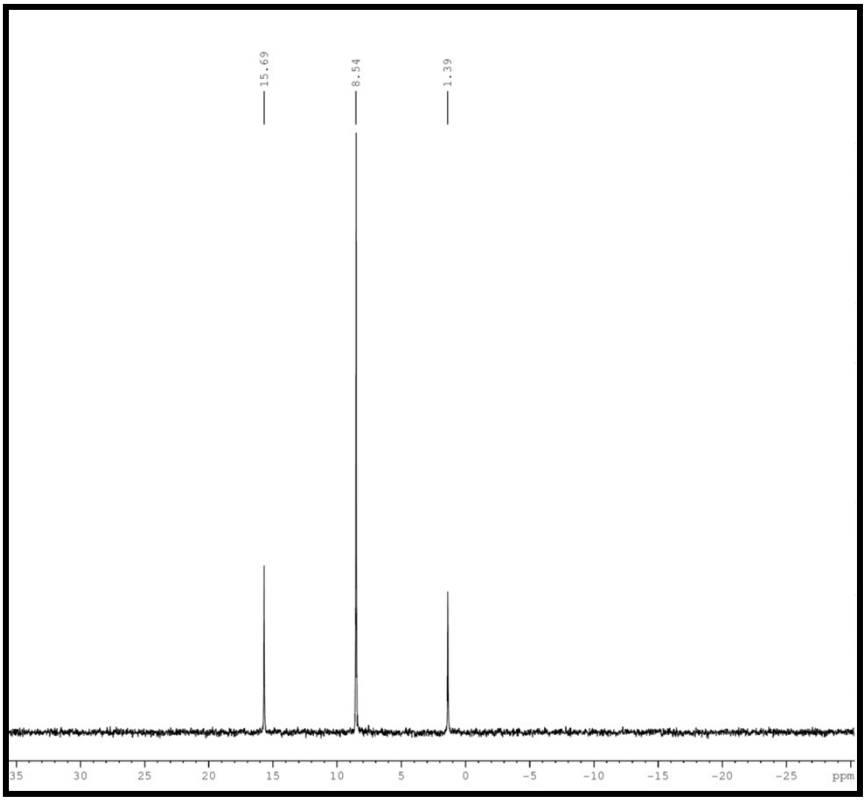
^{13}C NMR spectrum of 2 (2,6-bis(3-ethynylphenoxy)pyrazine):



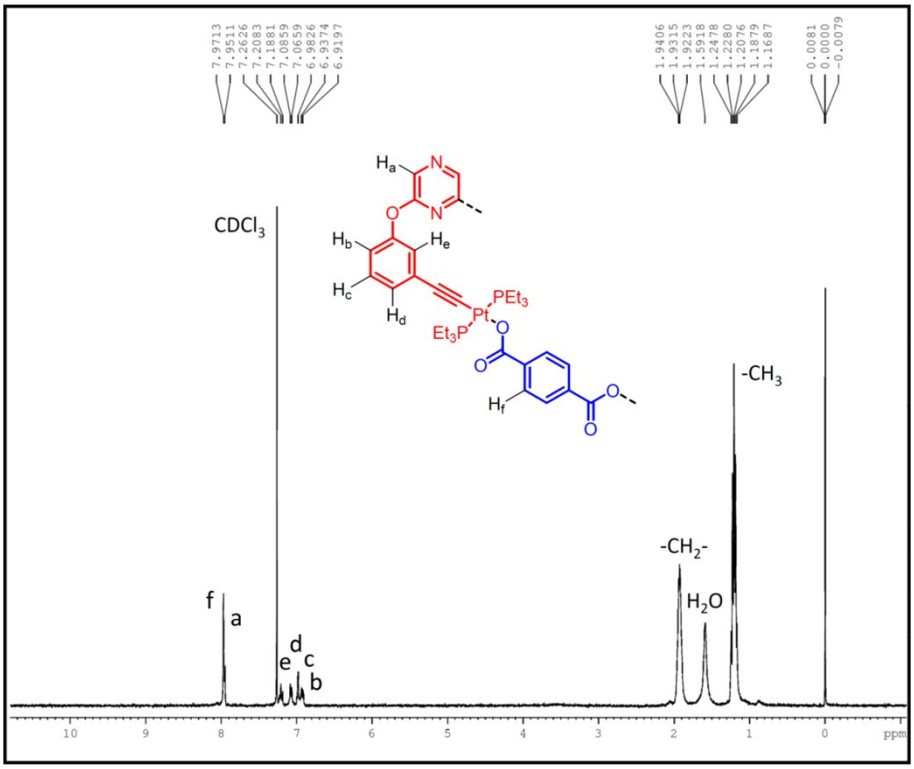
^{1}H NMR spectrum of 3:



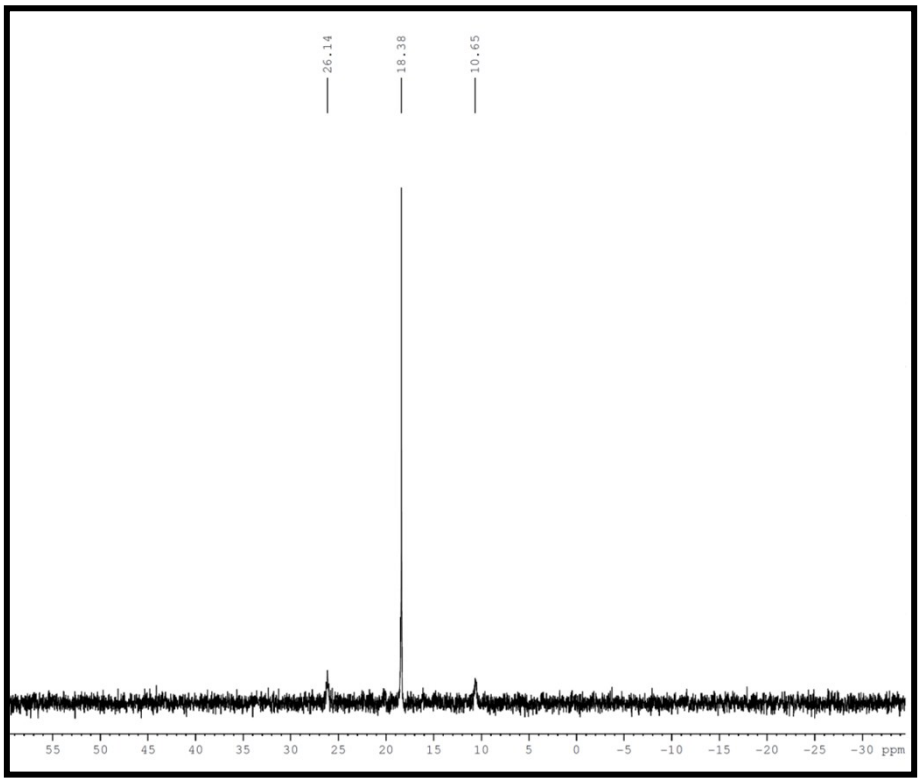
^{31}P NMR spectrum of 3:



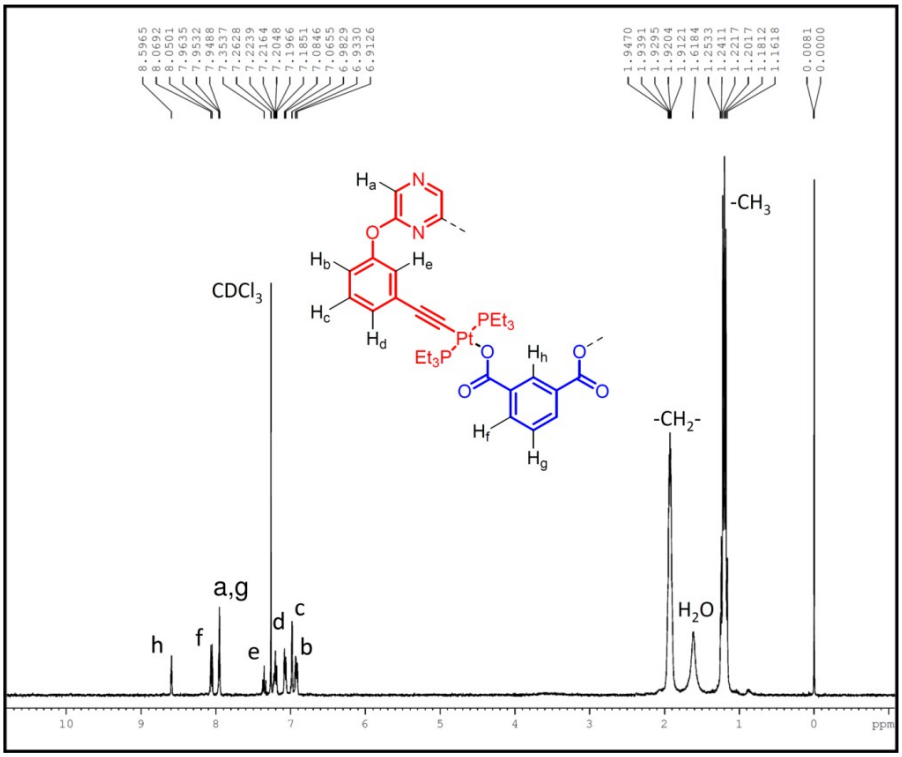
^{1}H NMR spectrum of M_1:



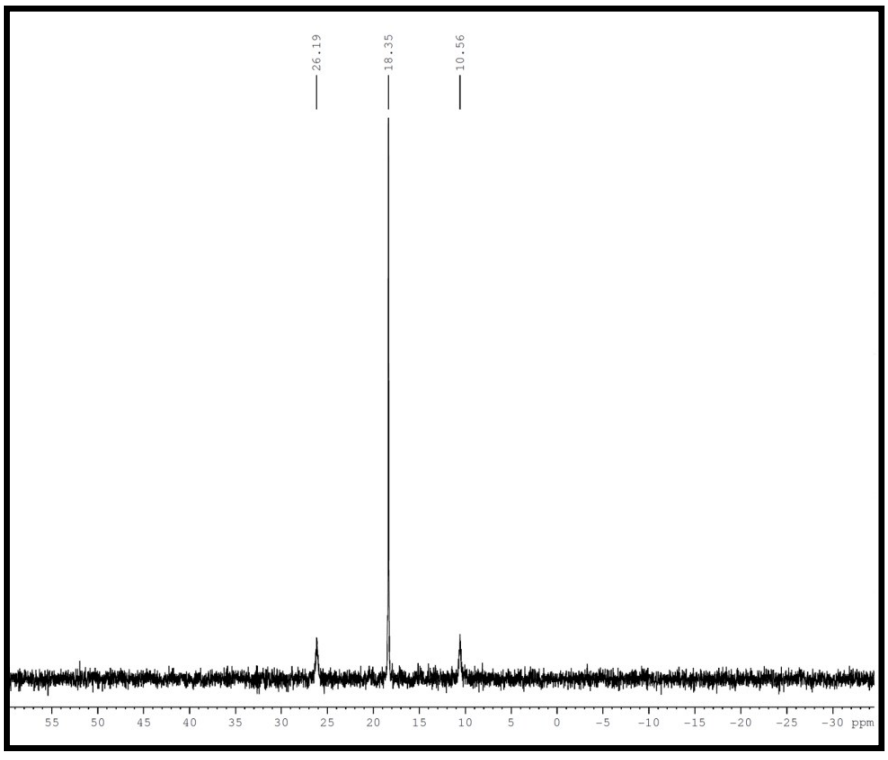
^{31}P NMR spectrum of M_1:



^{1}H NMR spectrum of M_2:



^{31}P NMR spectrum of M_2:



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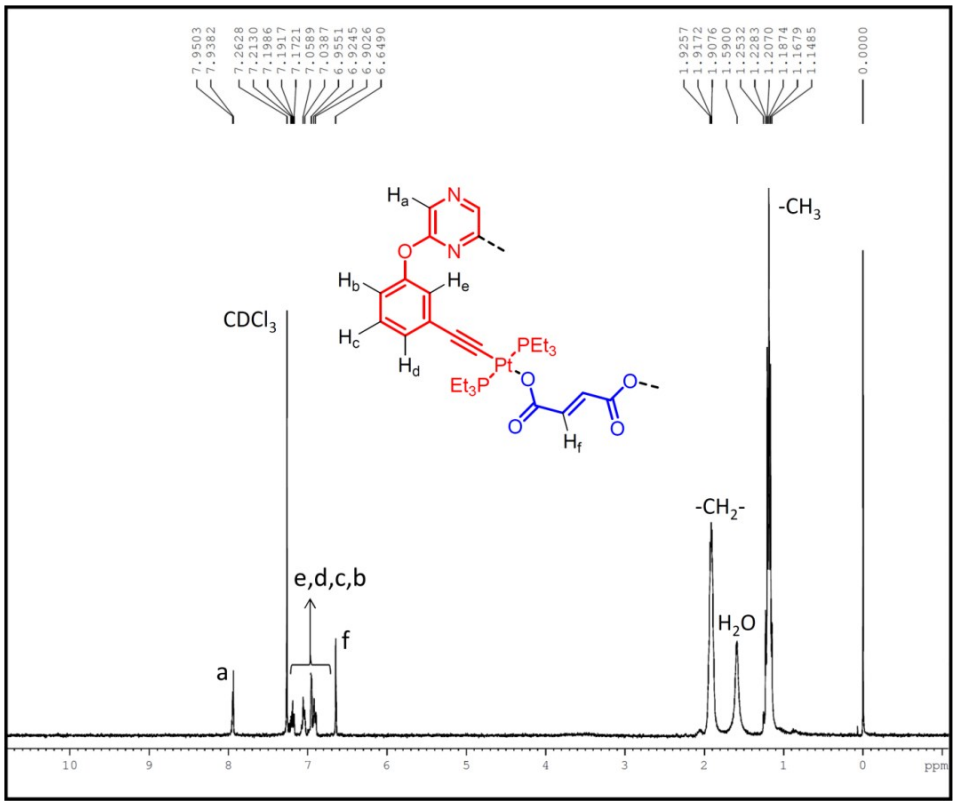


^{31}P NMR spectrum of M_3:

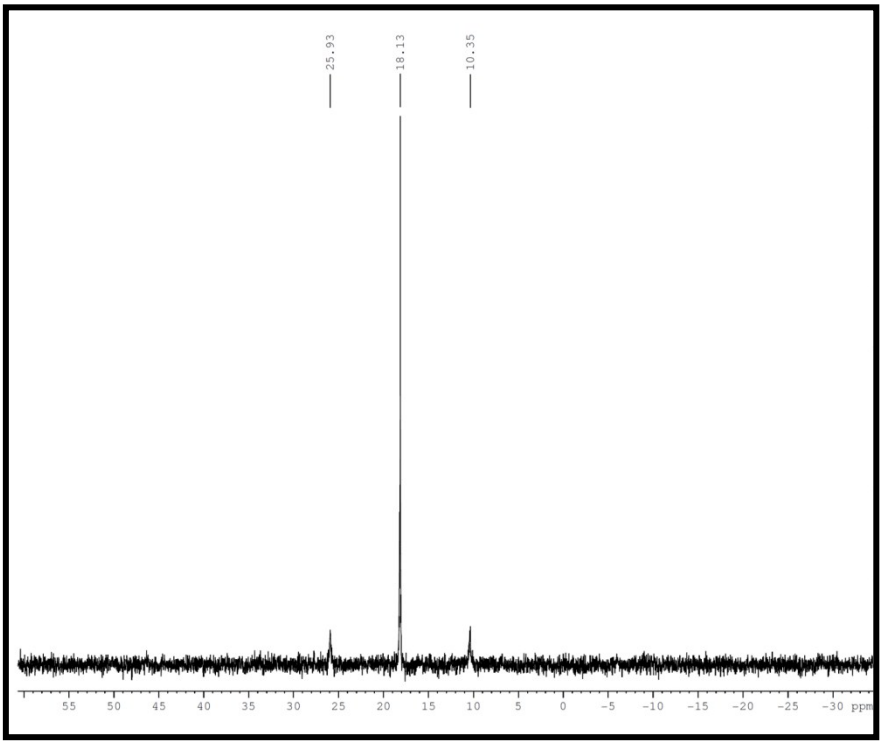
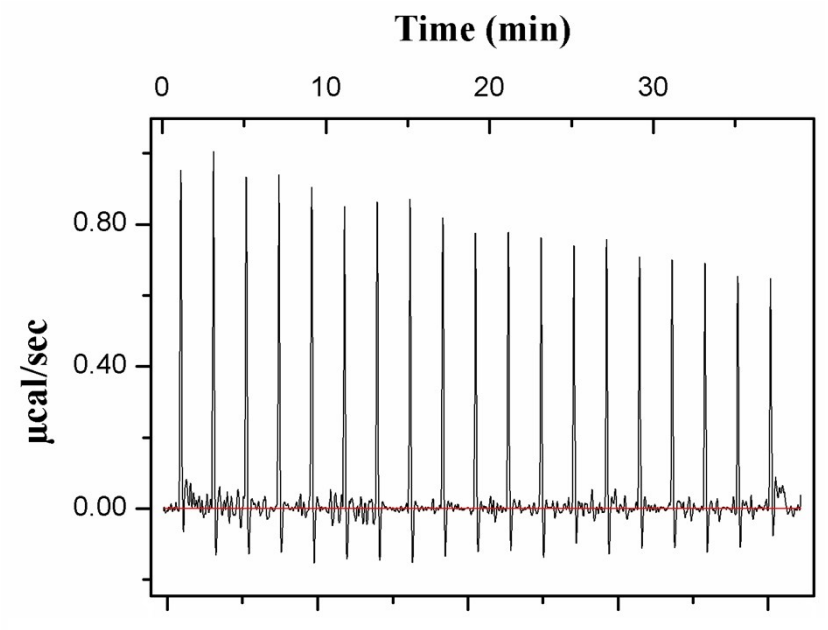


Table 1.Thermodynamic parameters for the binding interaction between 3 and picric acid (PA) as obtained by ITC.

System	K_1 (M^{-1})	ΔG_1 *kcal/mol*	K_2 (M^{-1})	ΔG_2 *kcal/mol*
3 + picric acid	$2.63(\pm0.4) \times 10^4$	-6.02	$4.67(\pm0.7) \times 10^5$	-7.72

ITC isotherm for the injection of 5 mM solution of 3in 0.5 mM picric acid solution at 298 K.



ORTEP presentation of 3 (30% thermal ellipsoids) (green, Pt; violet, I; orange, P; blue, N; red, O; grey, C). Hydrogen atoms are omitted for the sake of clarity.

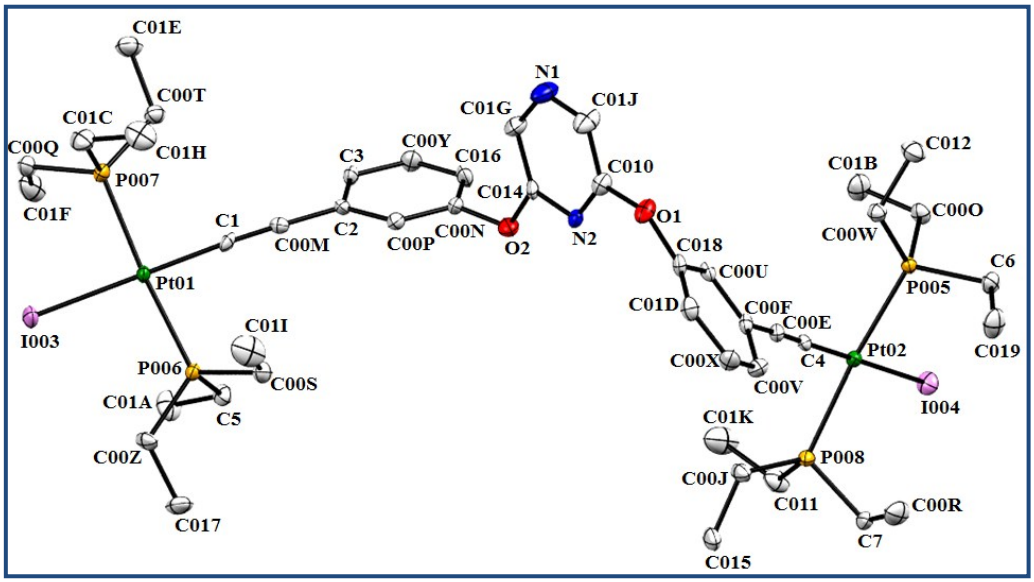


Table 2. Bond distances (Å) and bond angles (°) around Pt^{2+}centres found in complex 3.

Bond lengths (Å)			
Pt01—C1	1.968(10)	Pt02—C4	1.956(11)
Pt01—P007	2.304(8)	Pt02—P005	2.307(11)
Pt01—P006	2.306(7)	Pt02—P008	2.314(12)
Pt01—I003	2.643(8)	Pt02—I004	2.645(9)
Bond angles (°)			
C1—Pt01—P007	90.42(27)	C4—Pt02—P005	89.30(25)
C1—Pt01—P006	84.92(27)	C4—Pt02—P008	90.22(25)
P007—Pt01—P006	175.33(9)	P005—Pt02—P008	173.71(8)
C1—Pt01—I003	179.93(24)	C4—Pt02—I004	176.14(26)
P007—Pt01—I003	89.56(6)	P005—Pt02—I004	89.76(6)
P006—Pt01—I003	95.11(6)	P008—Pt02—I004	90.31(6)

Illustration of Planes Showing the Distance between the Pt (II) Centers and the Dihedral Angle between the planes.