Electronic Supplementary Information for Dalton Transactions

SUPPLEMENTARY INFORMATION

for

Heteroleptic binuclear palladium(II) and platinum(II) complexes containing 1,2-bis(diphenylphosphino)acetylene and 1,2-benzenedithiolates: syntheses, X-ray crystal structures, electrochemistry and photoluminescence properties

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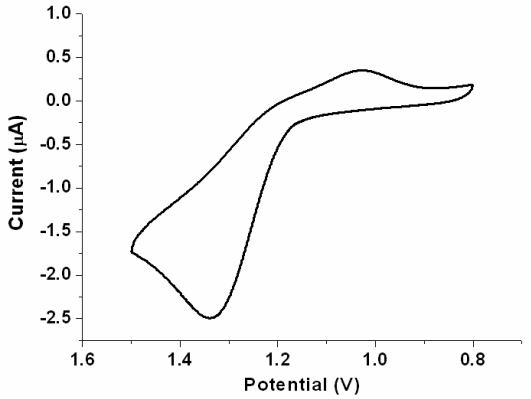


Fig. S1 The cyclic voltammogram of complex **2**.

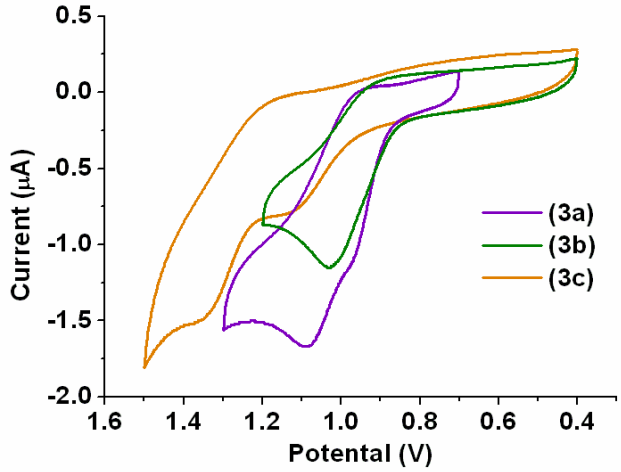


Fig. S2 The cyclic voltammograms of complexes **3a**, **3b** and **3c**.

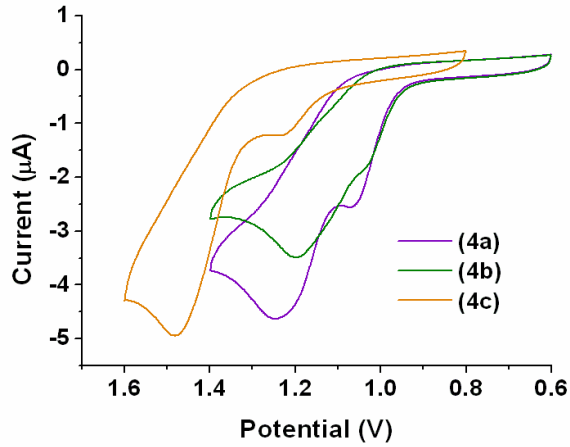


Fig. S3 The cyclic voltammograms of complexes **4a**, **4b** and **4c**.

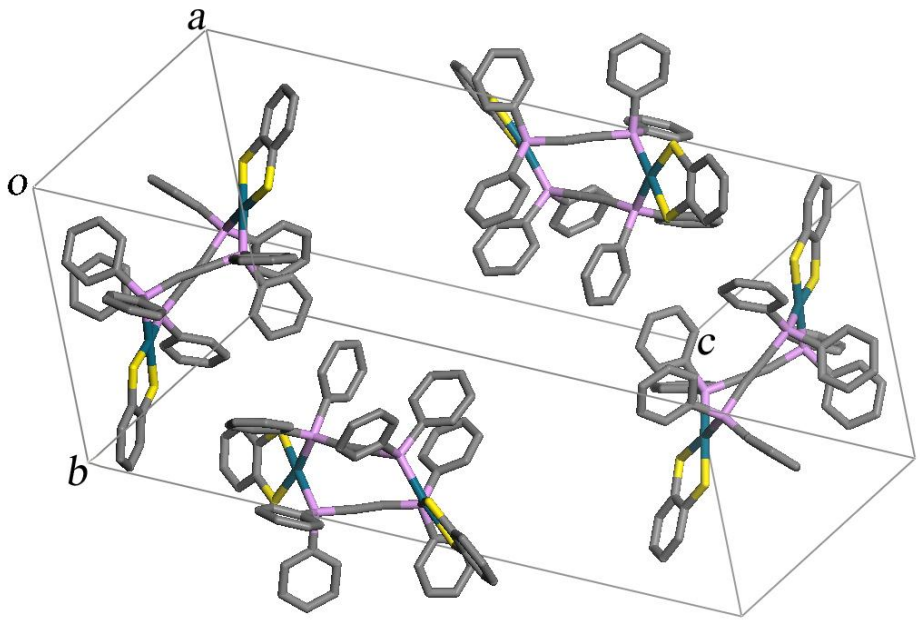


Fig. S4 Crystal packing diagram of $[Pd(bdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**3a**), showing the two sets of racemic isomers. Solvent molecules and hydrogen atoms are omitted for clarity.

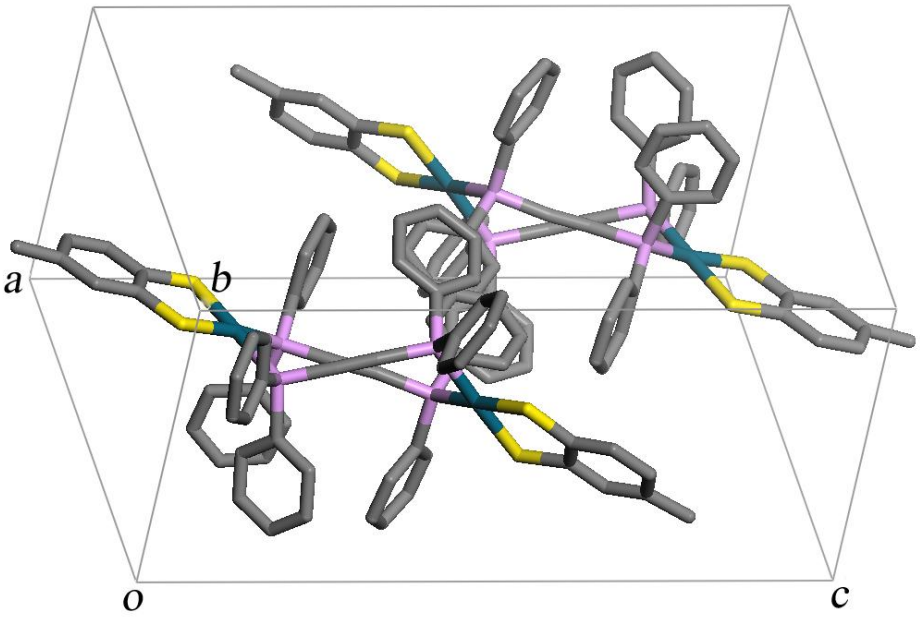


Fig. S5 Crystal packing diagram of $[Pd(tdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**3b**), showing the two racemic isomers. Hydrogen atoms are omitted for clarity.

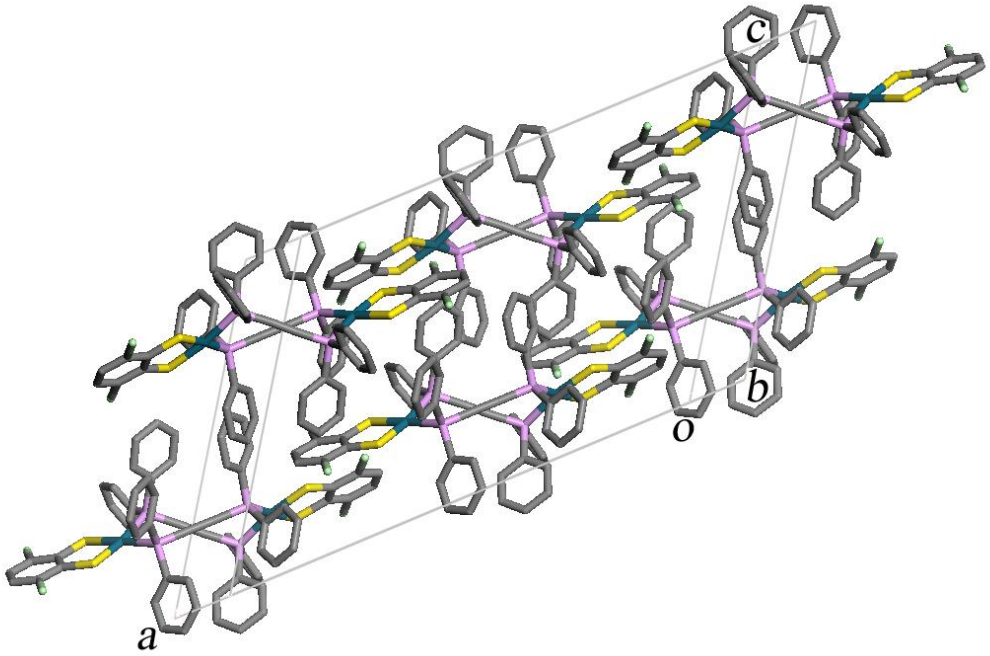


Fig. S6 Crystal packing diagram of $[Pd(Cl_2bdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**3c**), showing the two racemic isomers. Hydrogen atoms are omitted for clarity.

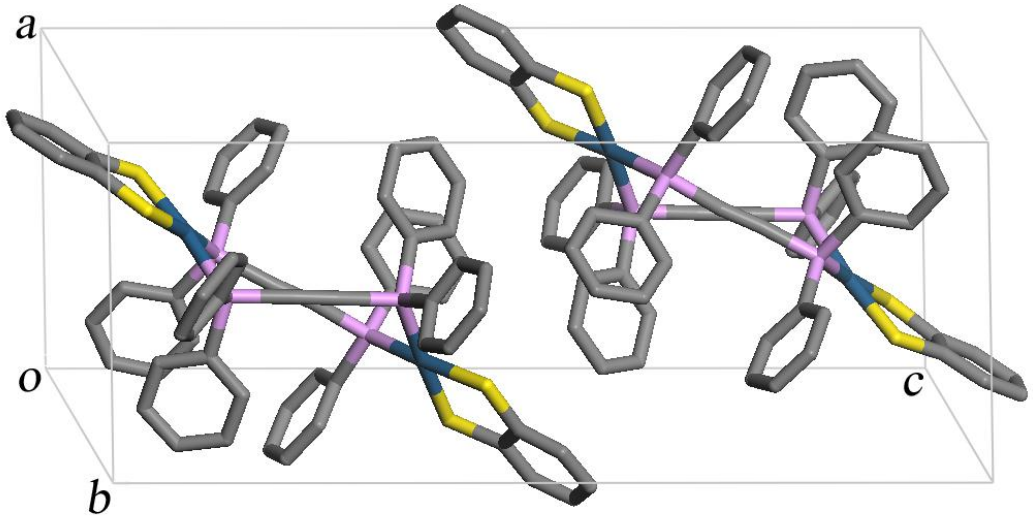


Fig. S7 Crystal packing diagram of $[Pt(bdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**4a**), showing the two racemic isomers. Solvent molecules and hydrogen atoms are omitted for clarity.

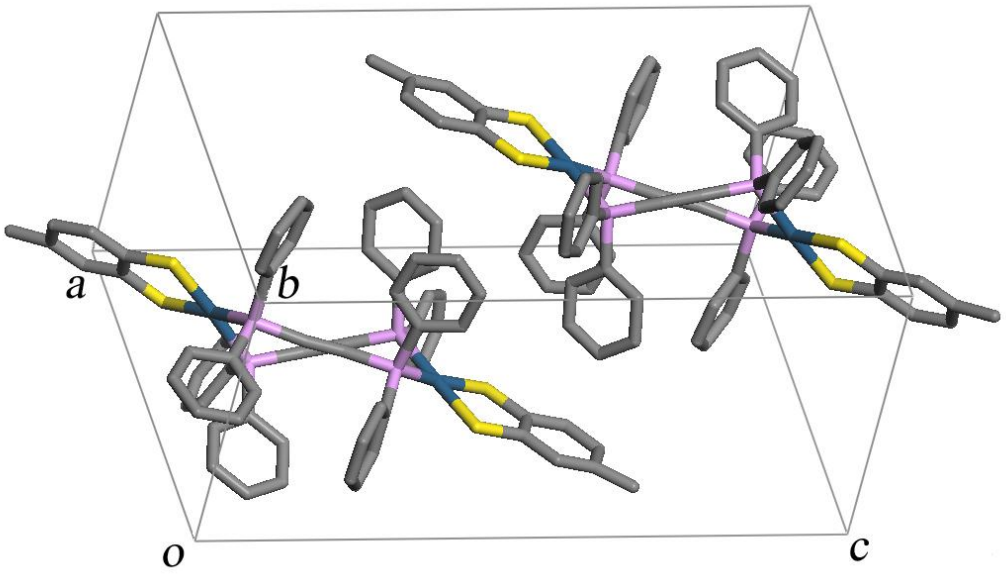


Fig. S8 Crystal packing diagram of $[Pt(tdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**4b**), showing the two racemic isomers. Solvent molecules and hydrogen atoms are omitted for clarity.

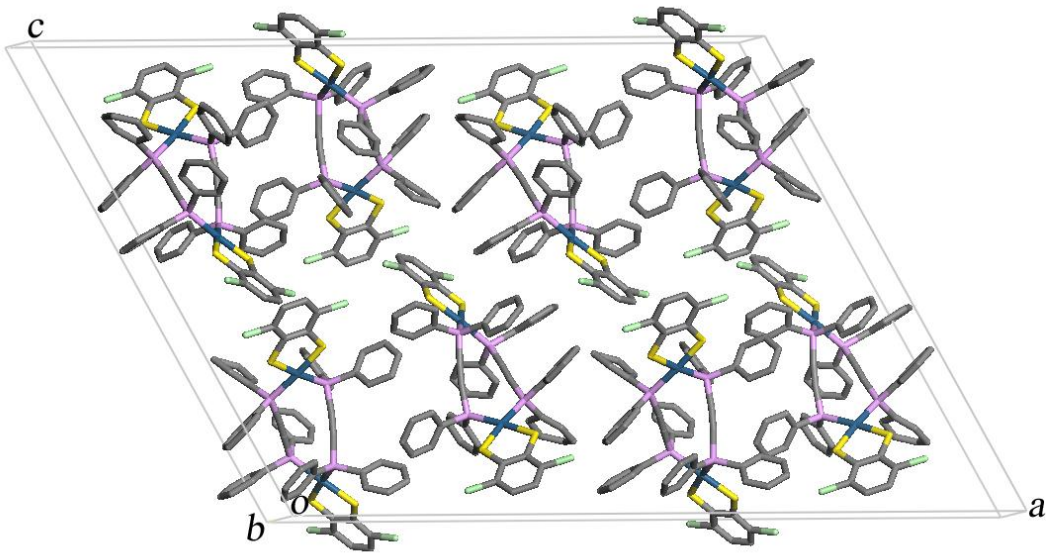


Fig. S9 Crystal packing diagram of $[Pt(Cl_2bdt)]_2(\mu\text{-}Ph_2PC{\equiv}CPPh_2)_2$ (**4c**), showing the two racemic isomers. Solvent molecules, hydrogen atoms and disordered phenyl groups are omitted for clarity.

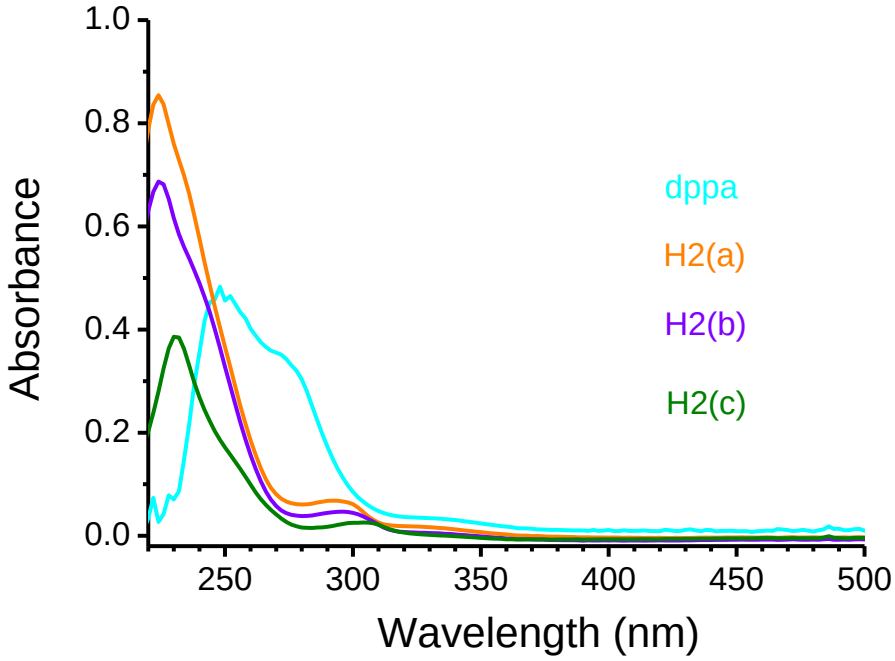


Fig. S10 UV-Vis spectra of ligands **dppa** (248, 270, 332 nm), **H_2(a)** (224, 292 nm), **H_2(b)** (224, 296 nm) and **H_2(c)** (230, 304 nm).

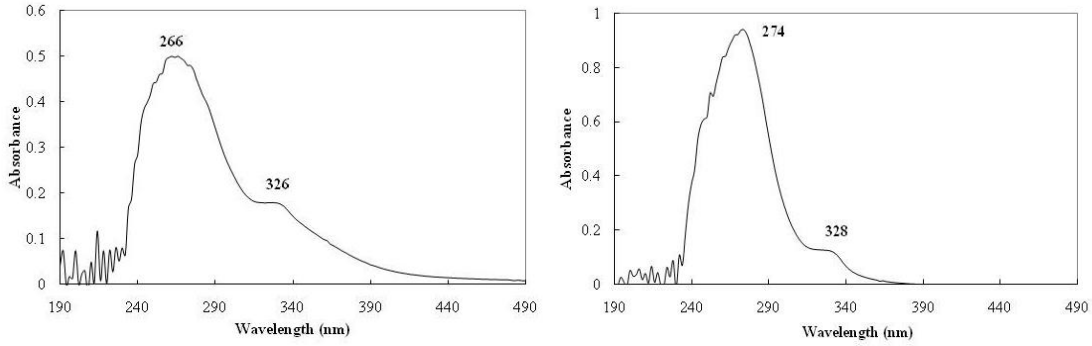


Fig. S11 UV-Vis spectra of complexes **1** (left: 266, 326 nm) and **2** (right: 274, 328 nm).

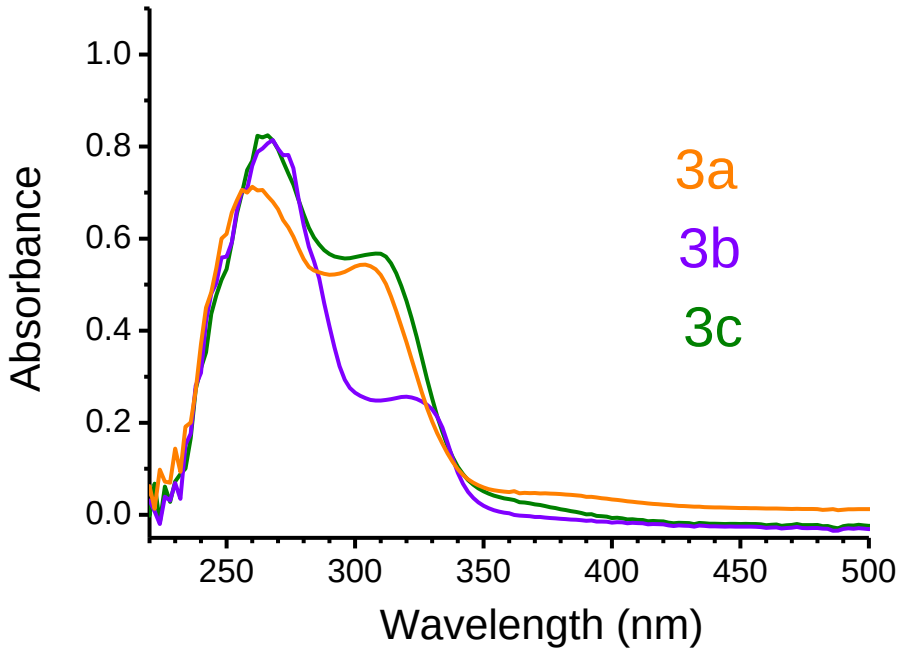


Fig. S12 UV-Vis spectra of complexes **3a** (260, 304 nm), **3b** (268, 320 nm) and **3c** (266, 308 nm).

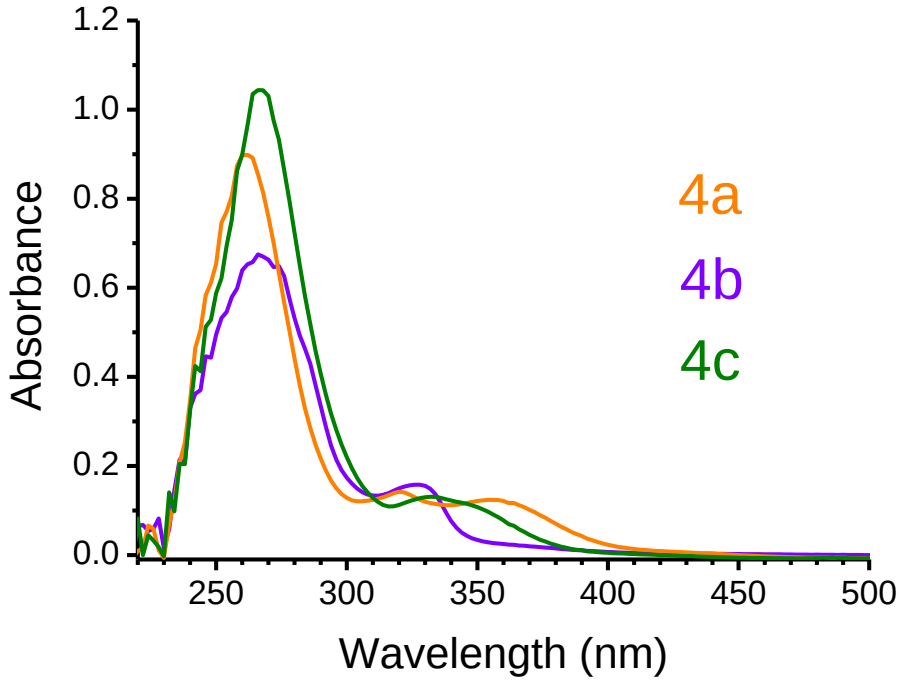
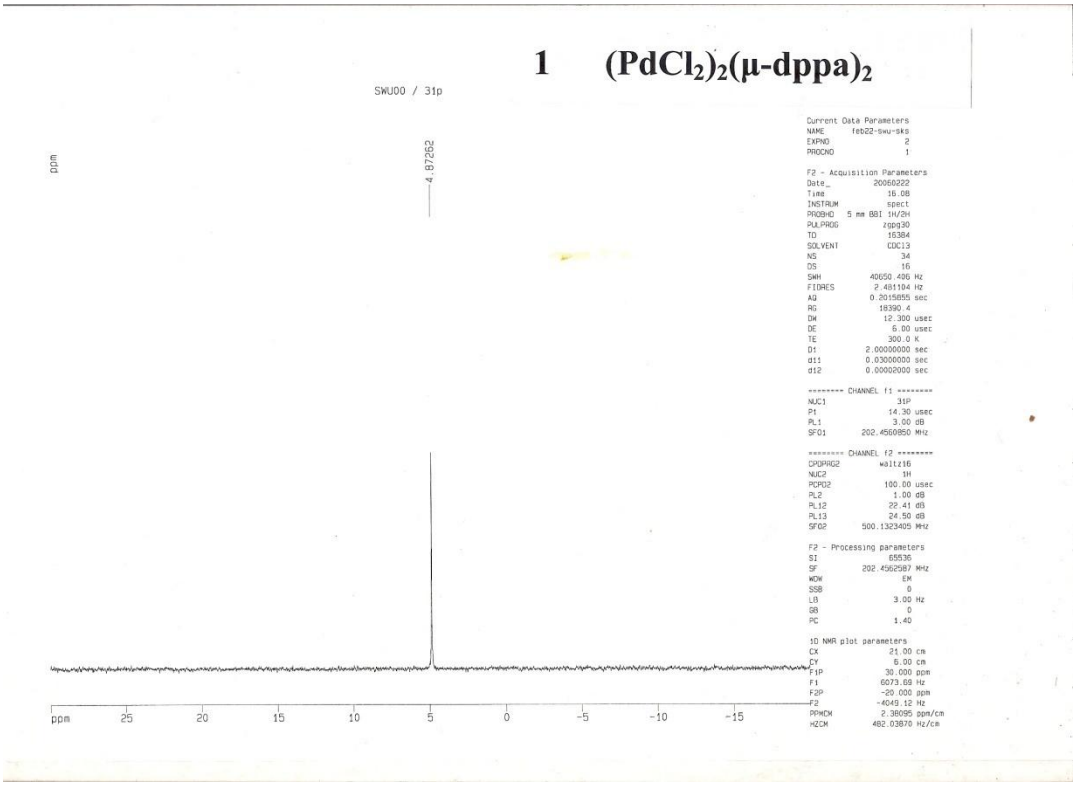
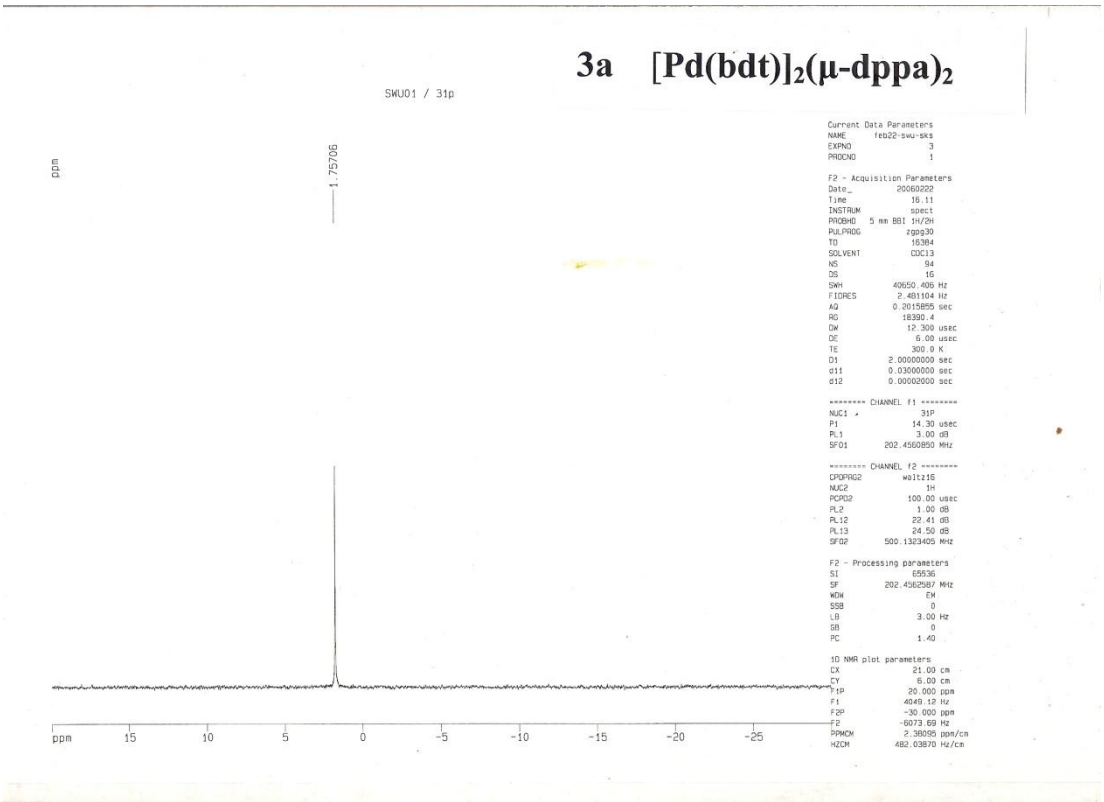


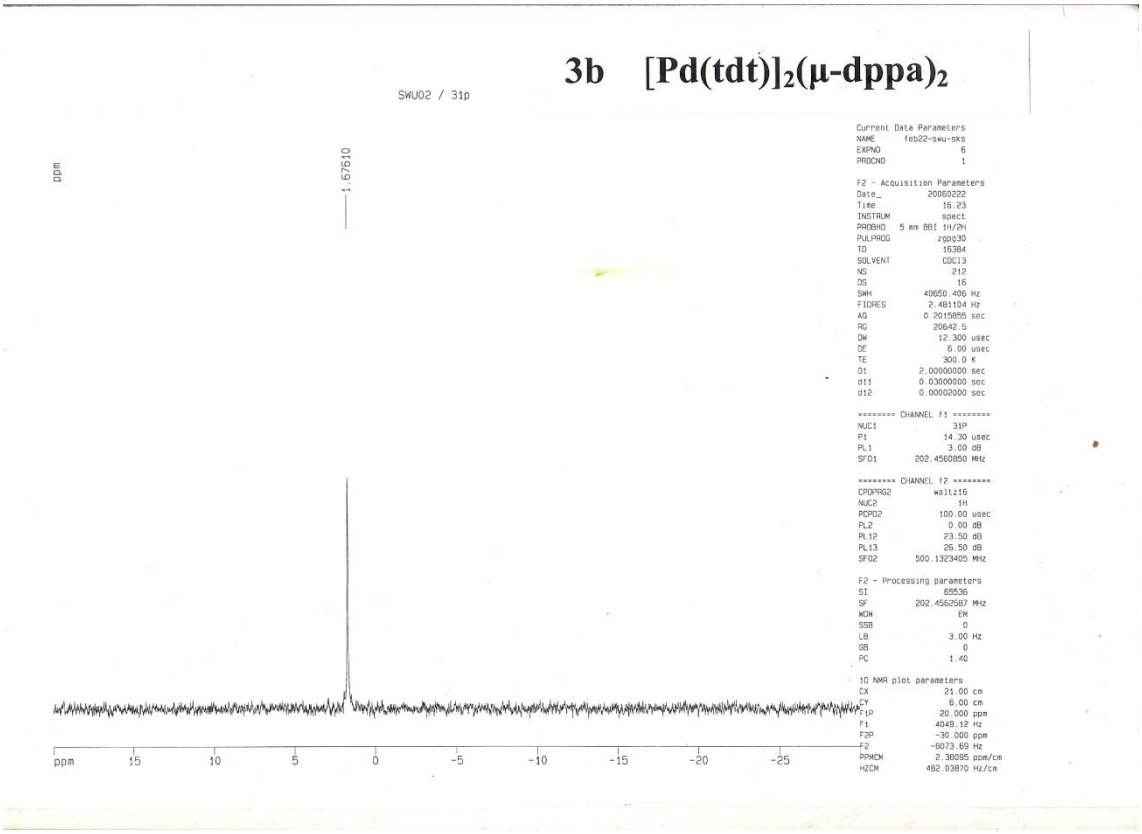
Fig. S13 UV-Vis spectra of complexes **4a** (262, 320, 356 nm), **4b** (266, 326, 358 nm) and **4c** (266, 322, 348 nm).

Fig. S14 ^{31}P NMR spectra of Pd(II) complexes (**1** and **3**).





3b $[Pd(tdt)]_2(\mu\text{-dppa})_2$



3c $[Pd(Cl_2bdt)]_2(\mu\text{-dppa})_2$

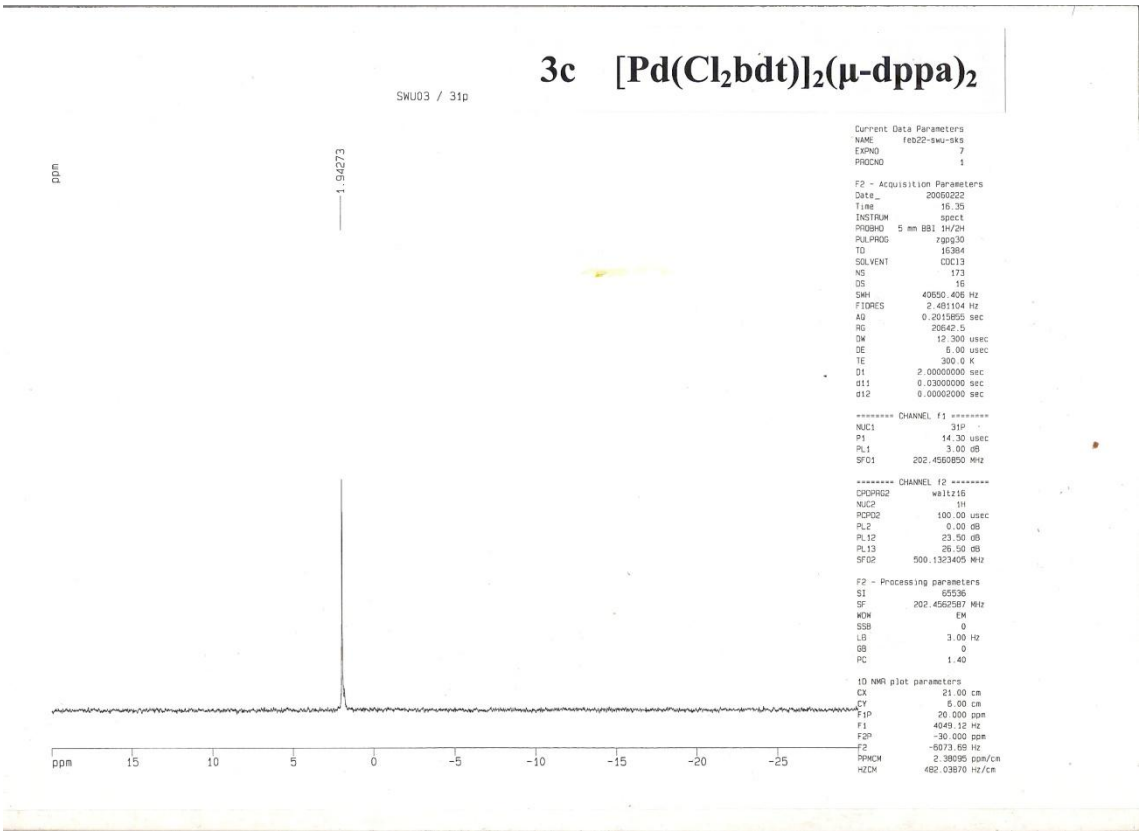
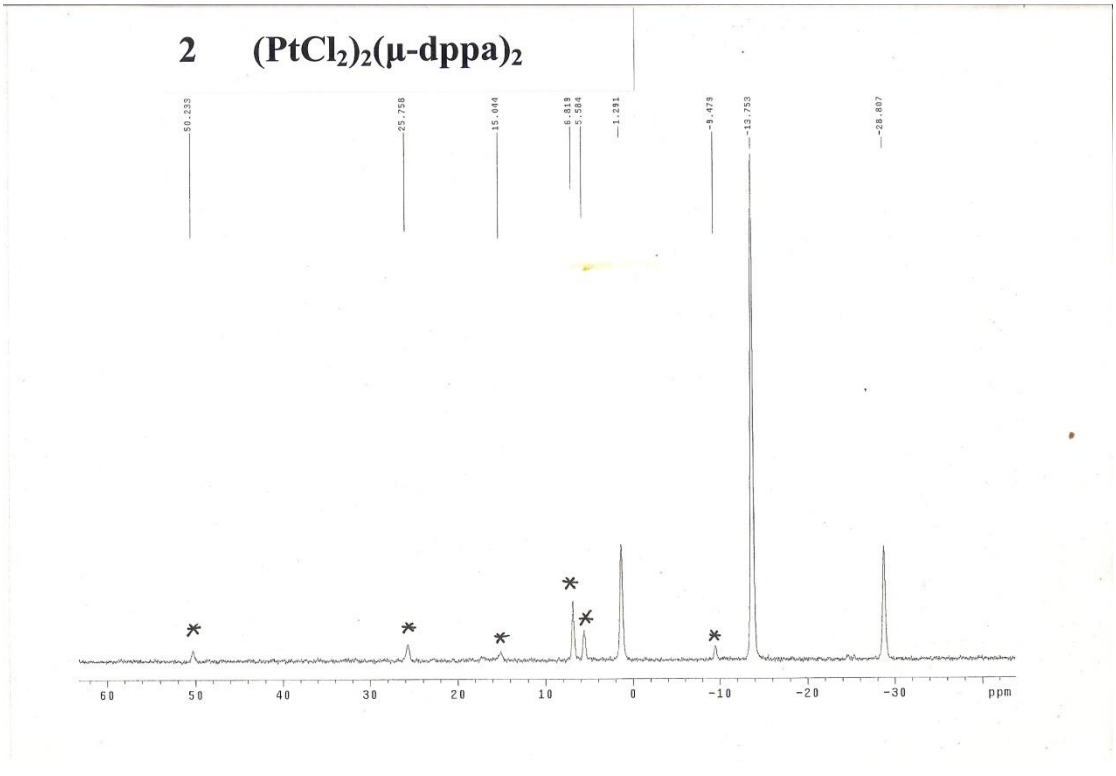
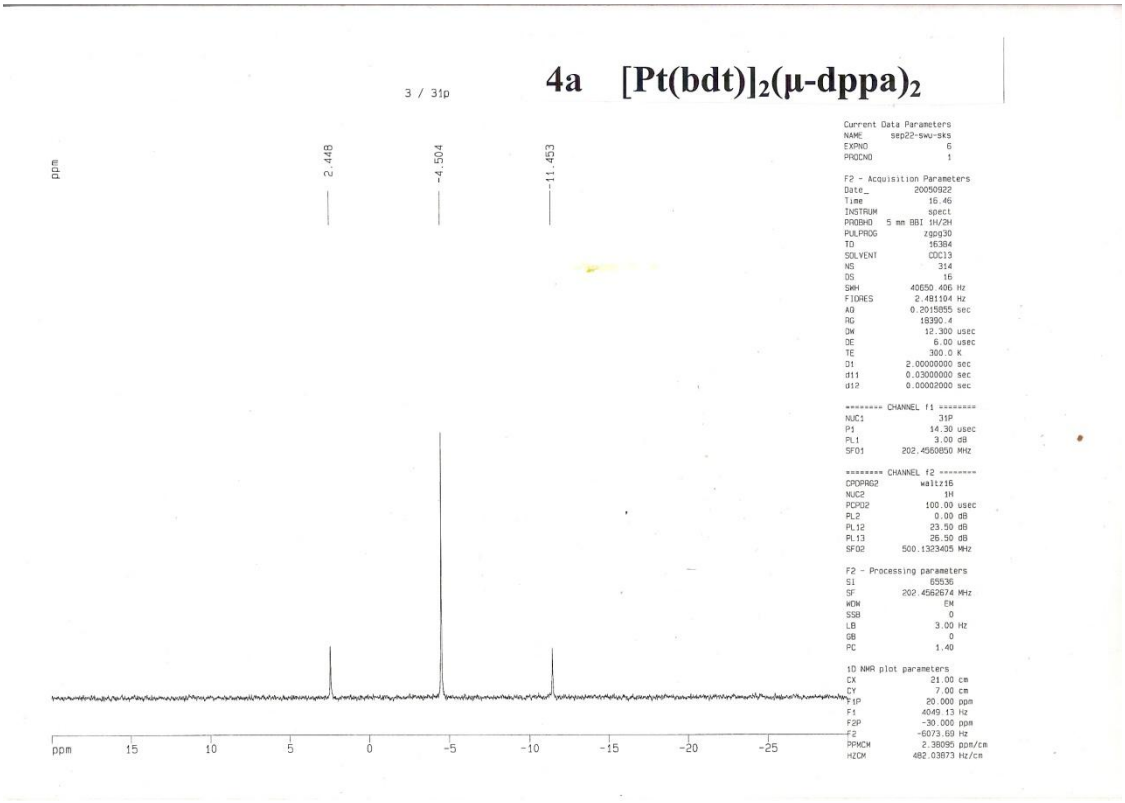
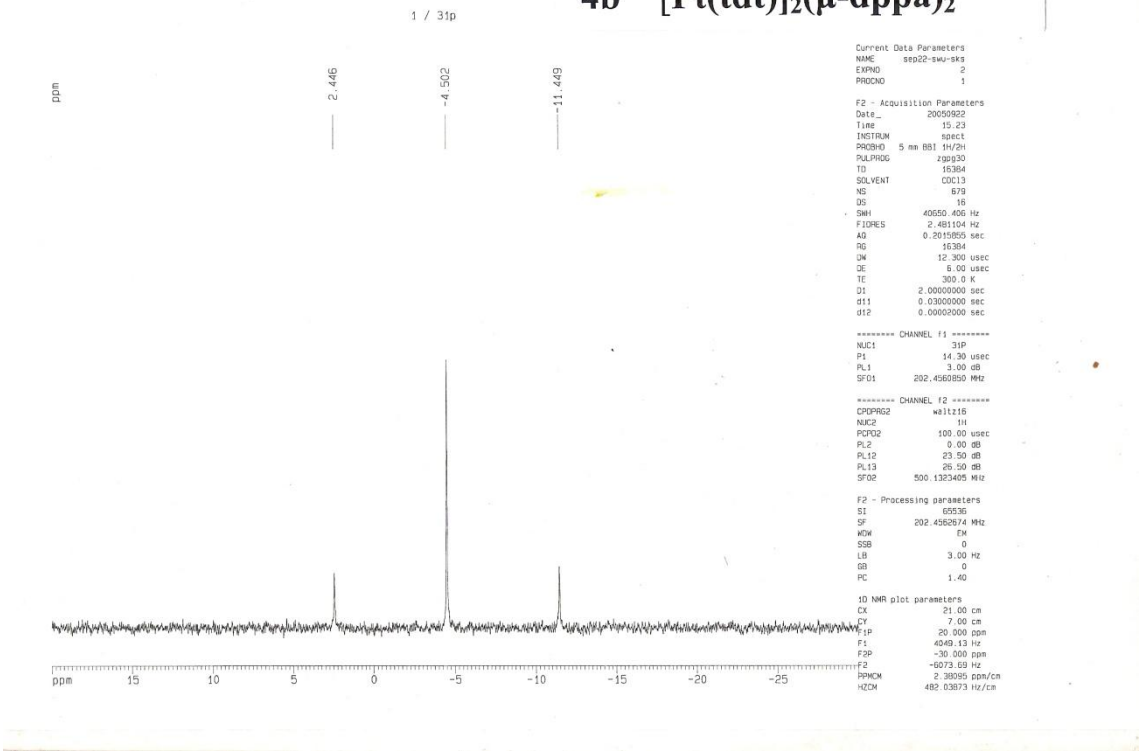


Fig. S15 ^{31}P NMR spectra of Pt(II) complexes (**2** and **4**).





4b $[Pt(tdt)]_2(\mu\text{-dppa})_2$



4c $[Pt(Cl_2bdt)]_2(\mu\text{-dppa})_2$

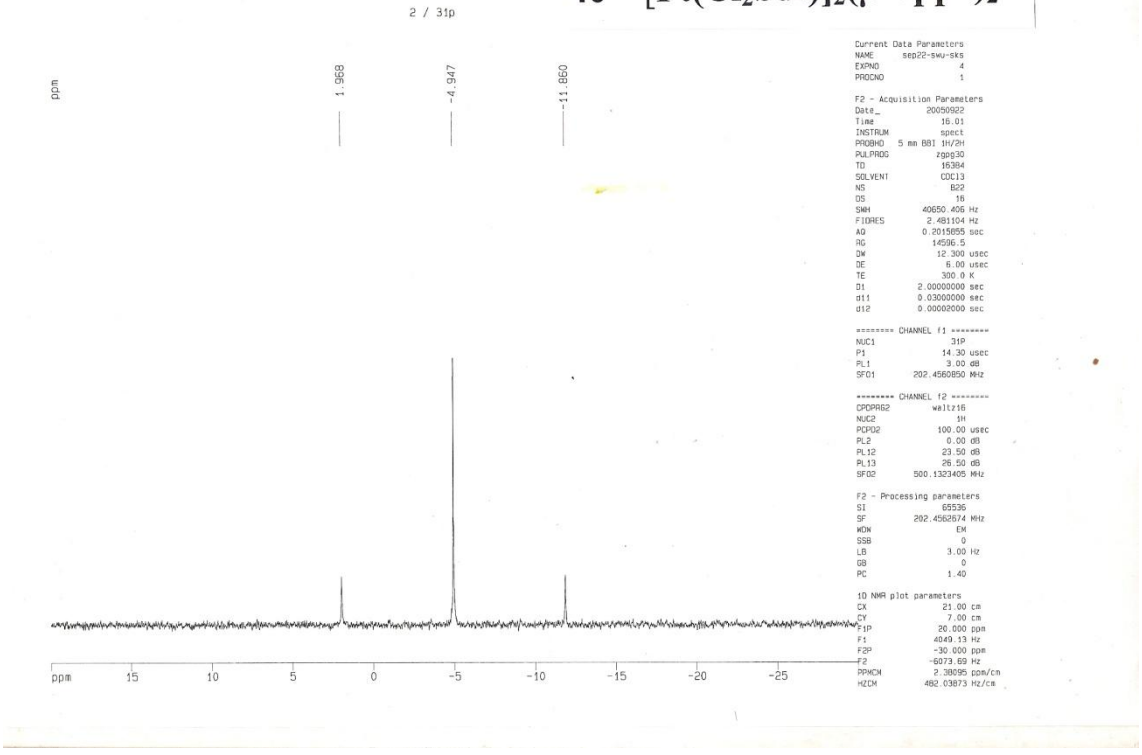
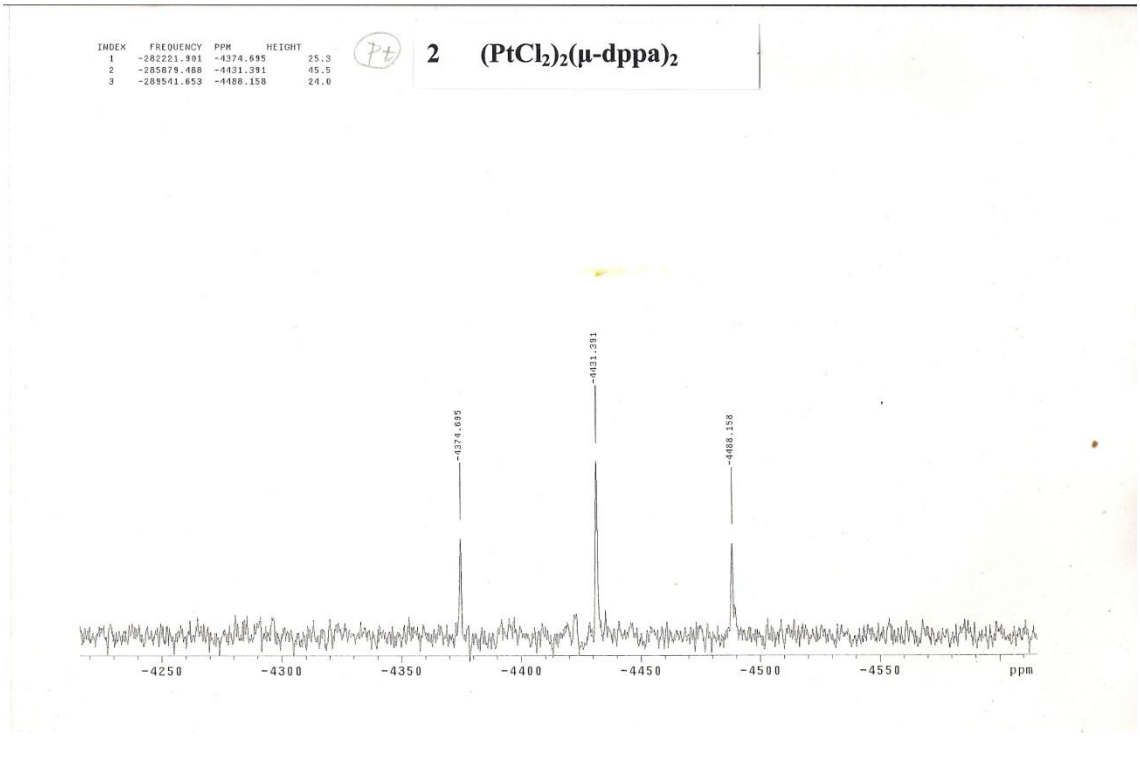
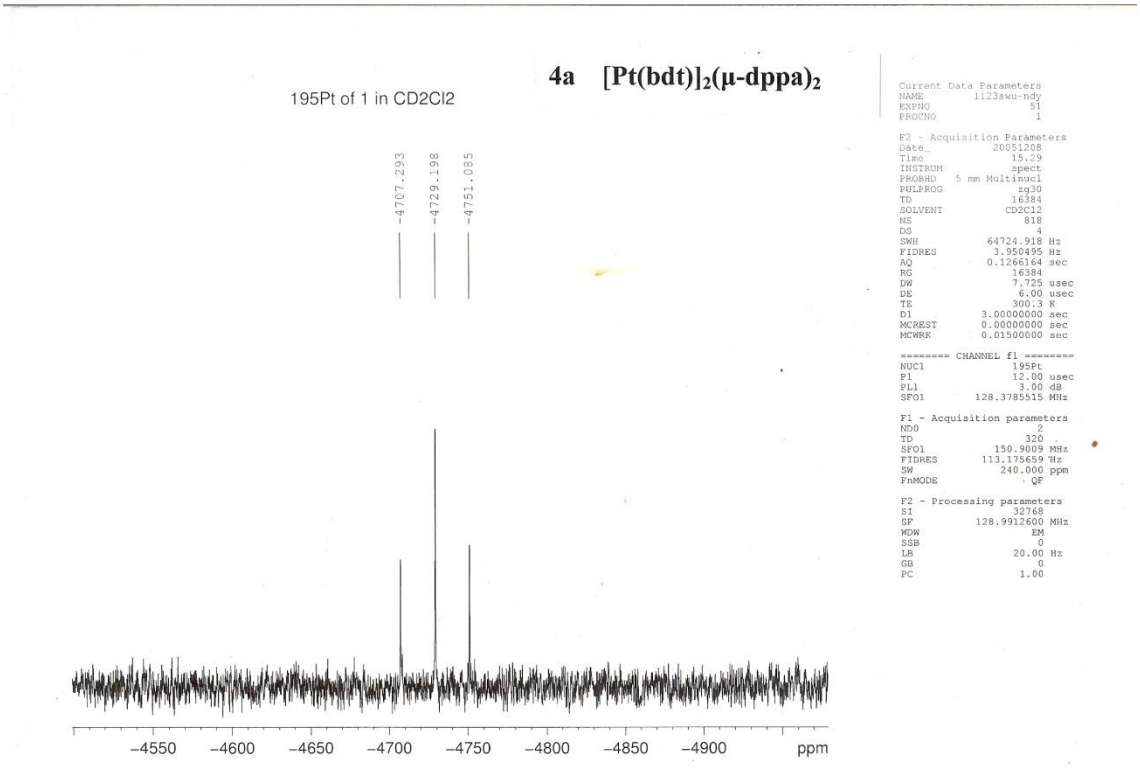


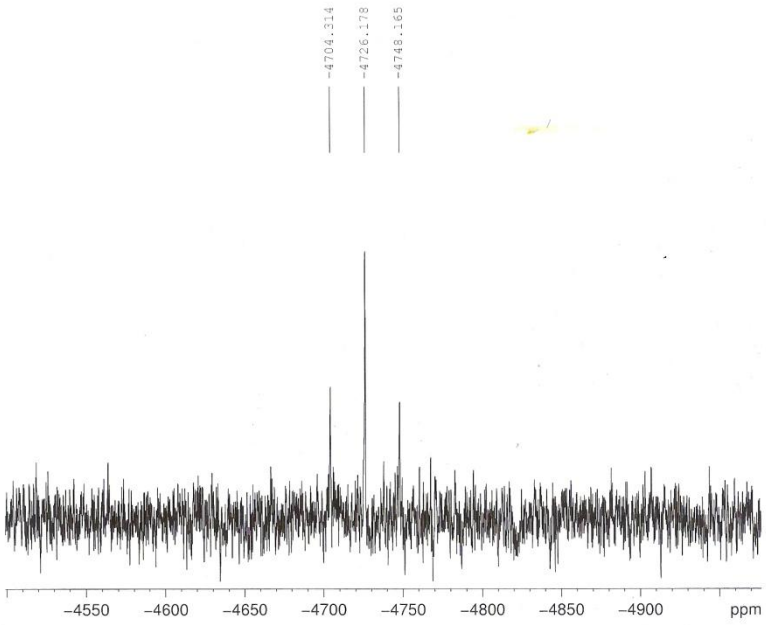
Fig. S16 ^{195}Pt NMR spectra of Pt(II) complexes (**2** and **4**).





4b $[Pt(tdt)]_2(\mu\text{-dppa})_2$

195Pt of 2 in CD2Cl2

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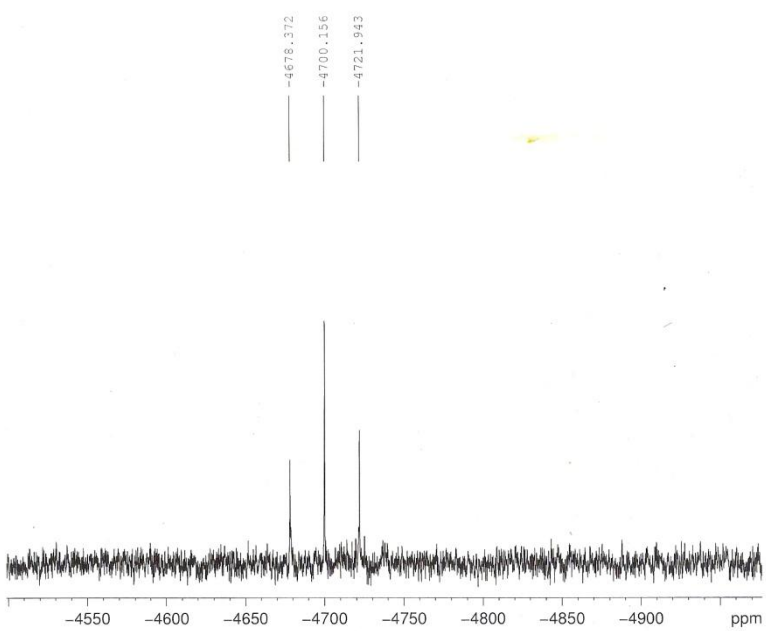
4c $[Pt(Cl_2bdt)]_2(\mu\text{-dppa})_2$

195Pt of 3 in CD2Cl2

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