Electronic Supplementary Information for Dalton Transactions

Dinuclear Palladium (II) Compounds with Bridging Cyclometalated Phosphines. Crystal Structure and Electrochemical Study.

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Supporting Information

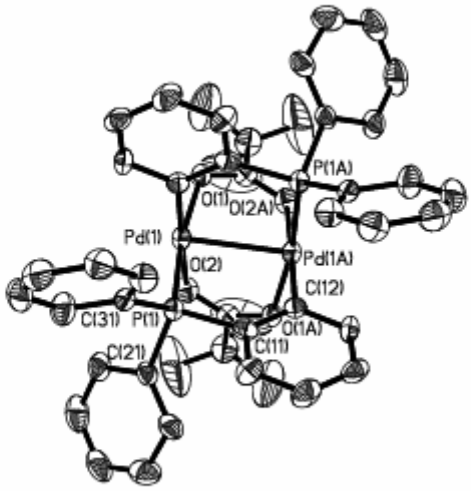

Fig.SI 1. ORTEP diagram for Compound **5**. Ellipsoids represented at 30% probability. Hydrogen atoms omitted for clarity.

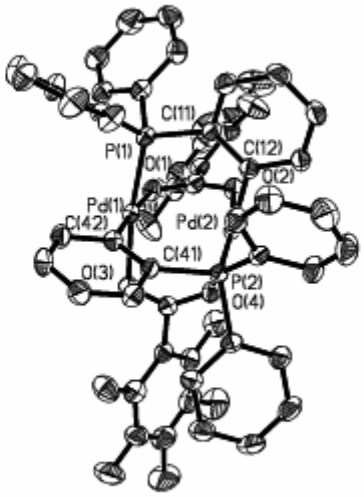

Fig.SI 2. ORTEP diagram for Compound **6**. Ellipsoids represented at 30% probability. Hydrogen atoms omitted for clarity.

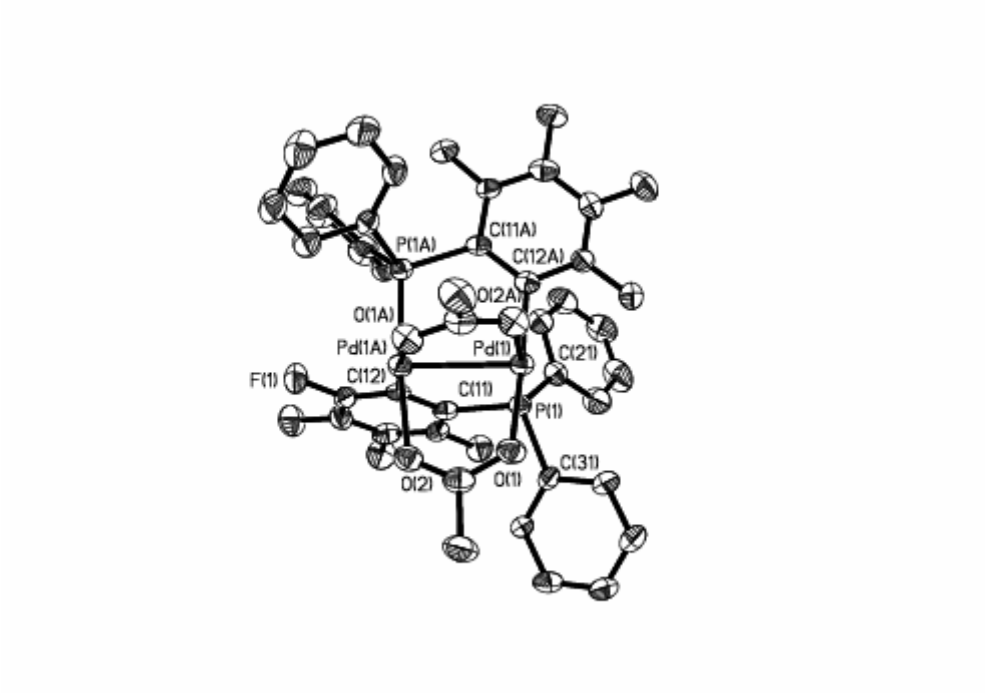

Fig.SI 3. C. ORTEP diagram for Compound **7**. Ellipsoids represented at 30% probability. Hydrogen atoms omitted for clarity.

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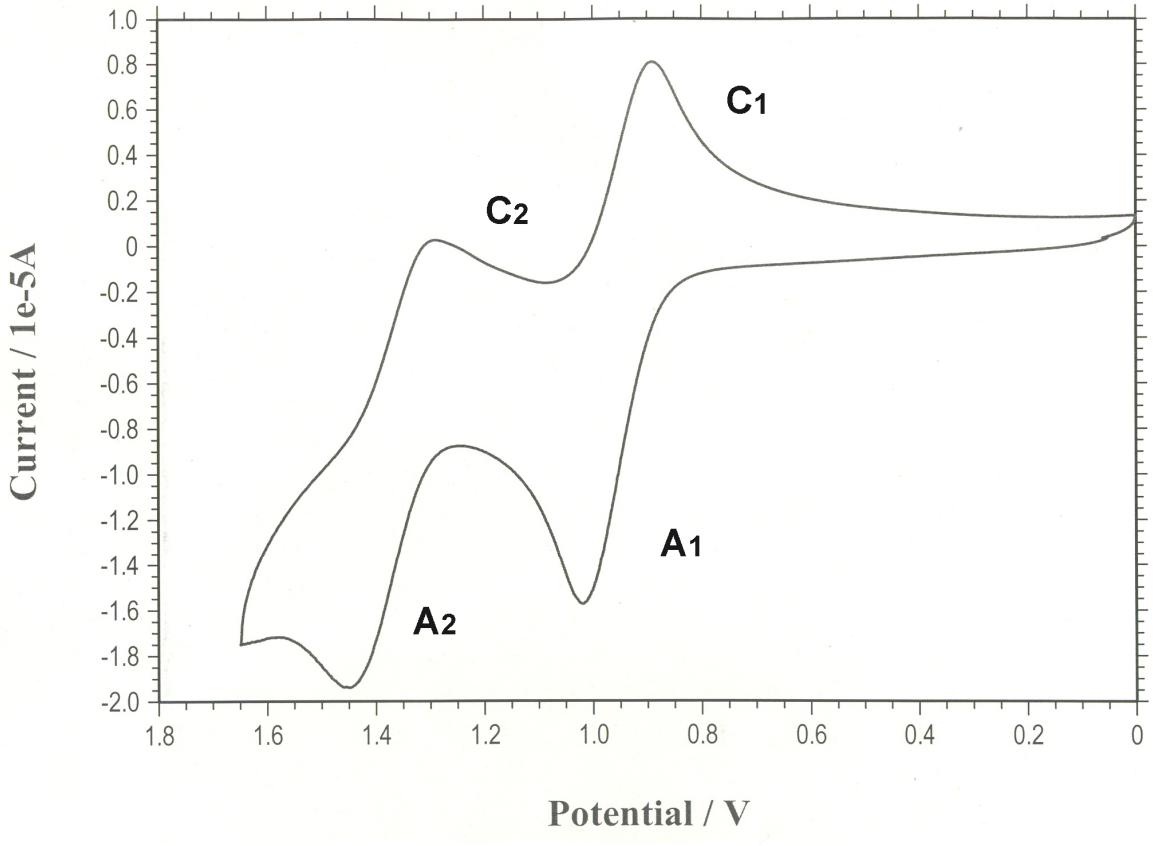


Fig. SI 4**.** CV at glassy carbon electrode for 1.0 mM solution of **3** in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

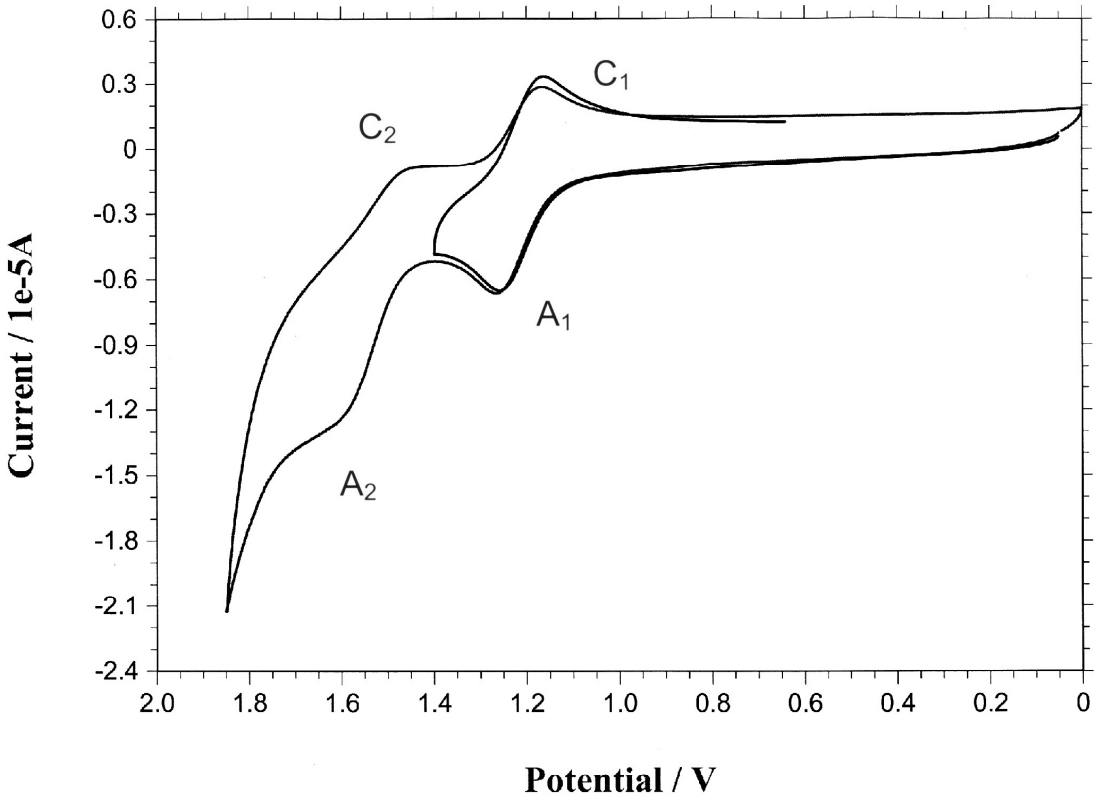


Fig. SI 5**.** CV at glassy carbon electrode for 1.0 mM solution of **4** in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

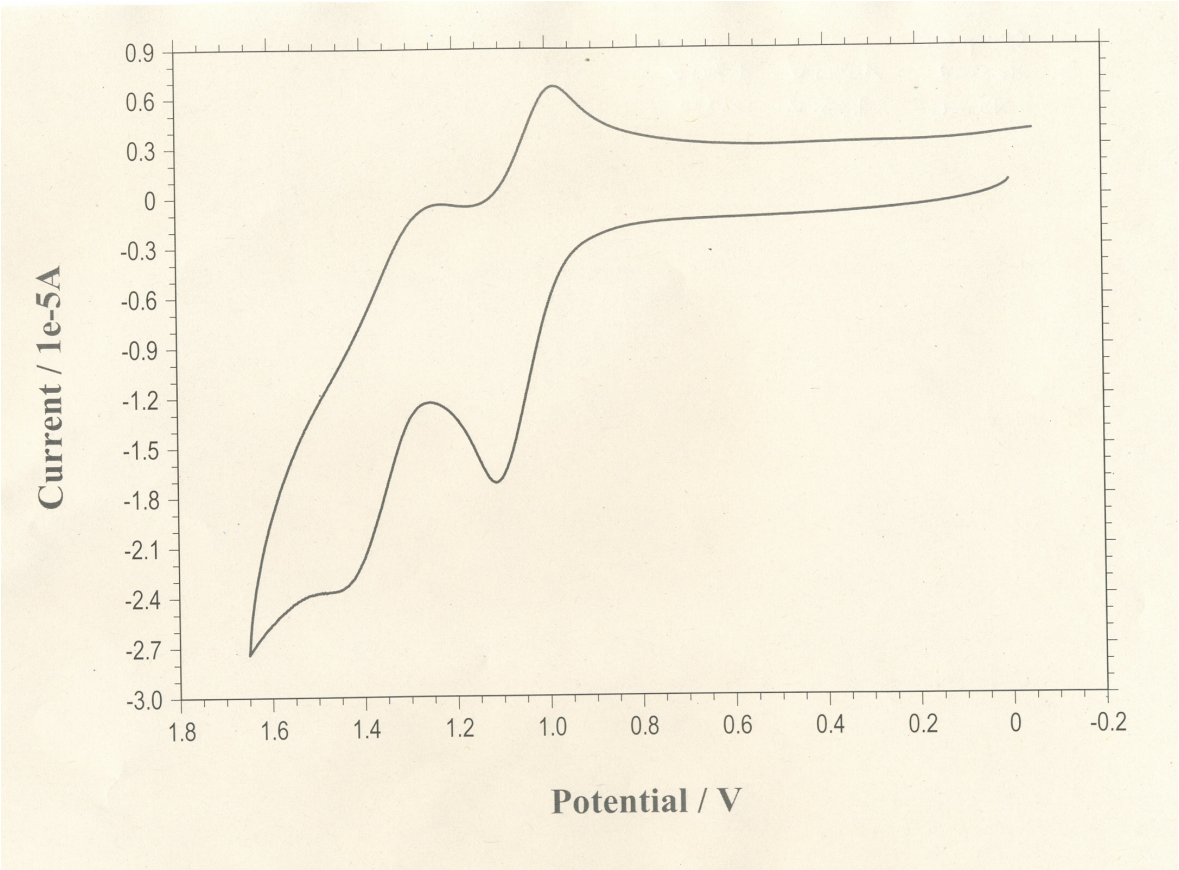


Fig. SI 6**.** CV at glassy carbon electrode for 1.0 mM solution of **6** in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

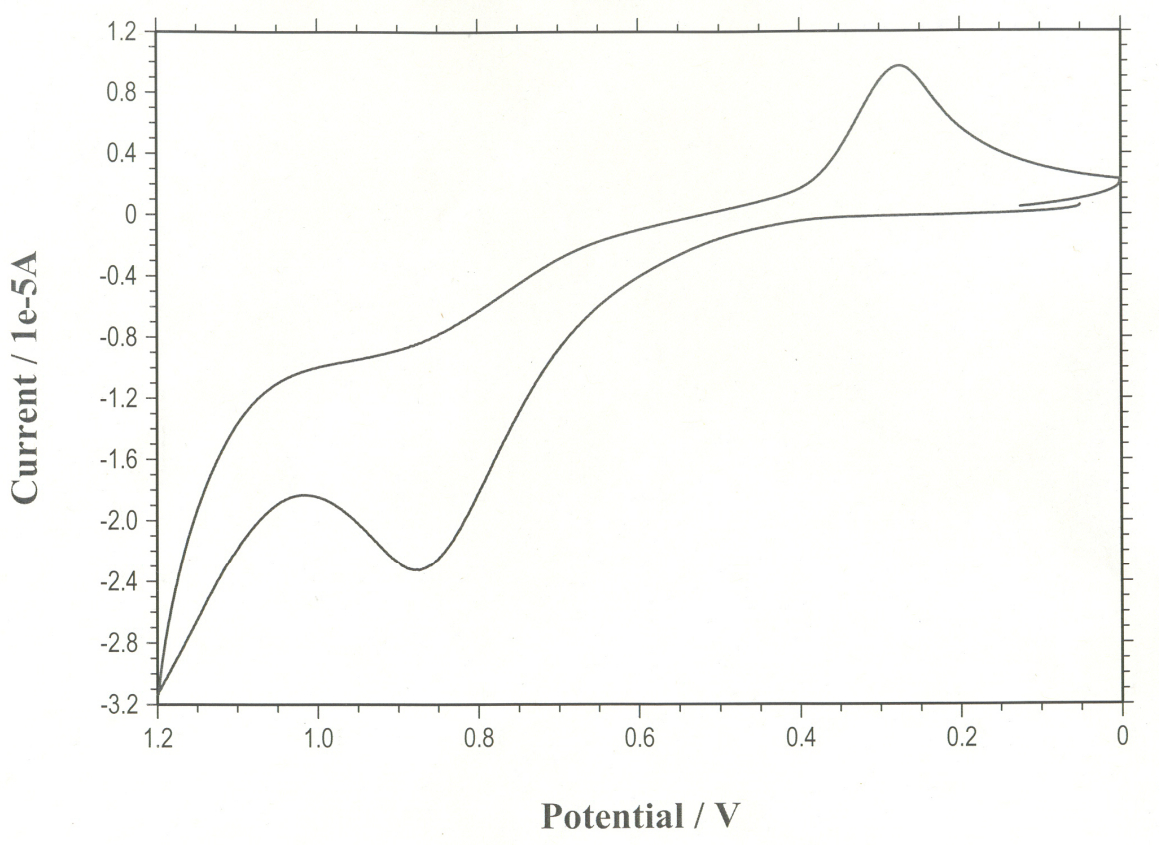


Fig. SI 7**.** CV at glassy carbon electrode for 1.0 mM solution of **3** and stoichiometric amount of $NEt_4^+ Cl^-$ in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

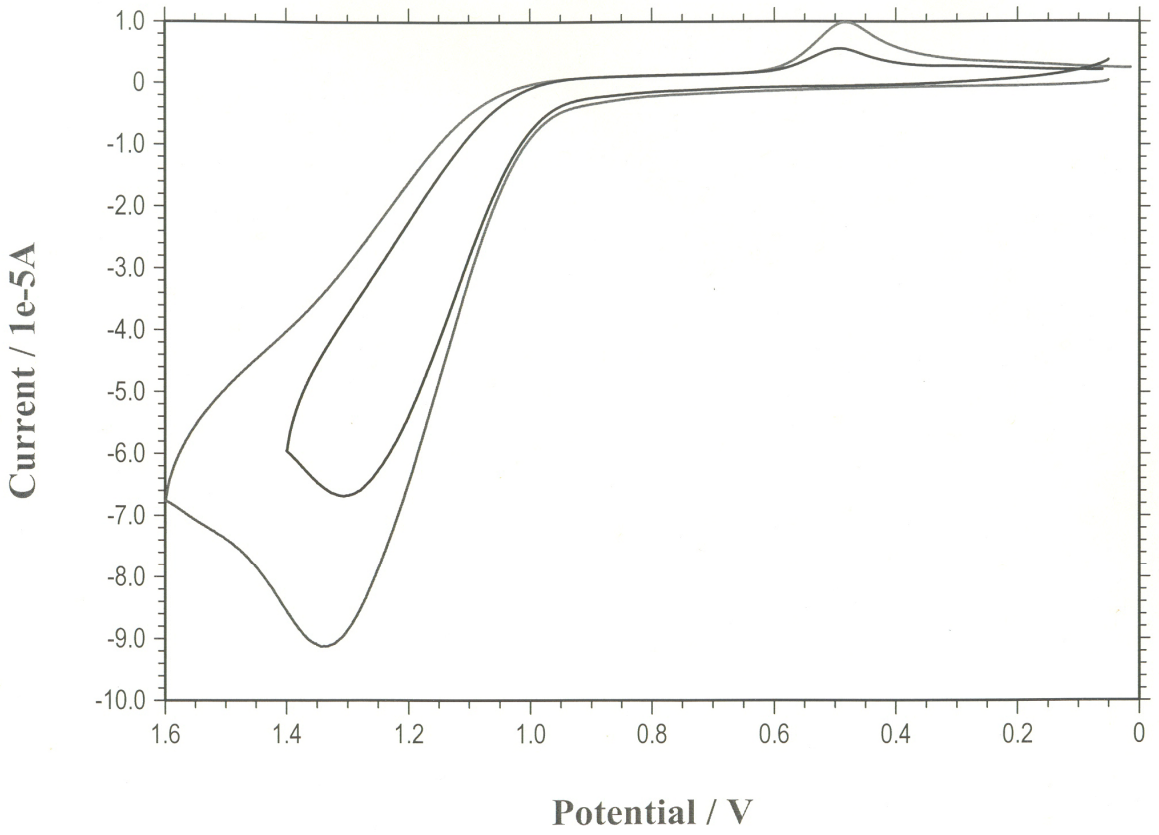


Fig. SI 8**.** CV at glassy carbon electrode for 1.0 mM solution of **4** and stoichiometric amount of $NEt_4^+ Cl^-$ in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

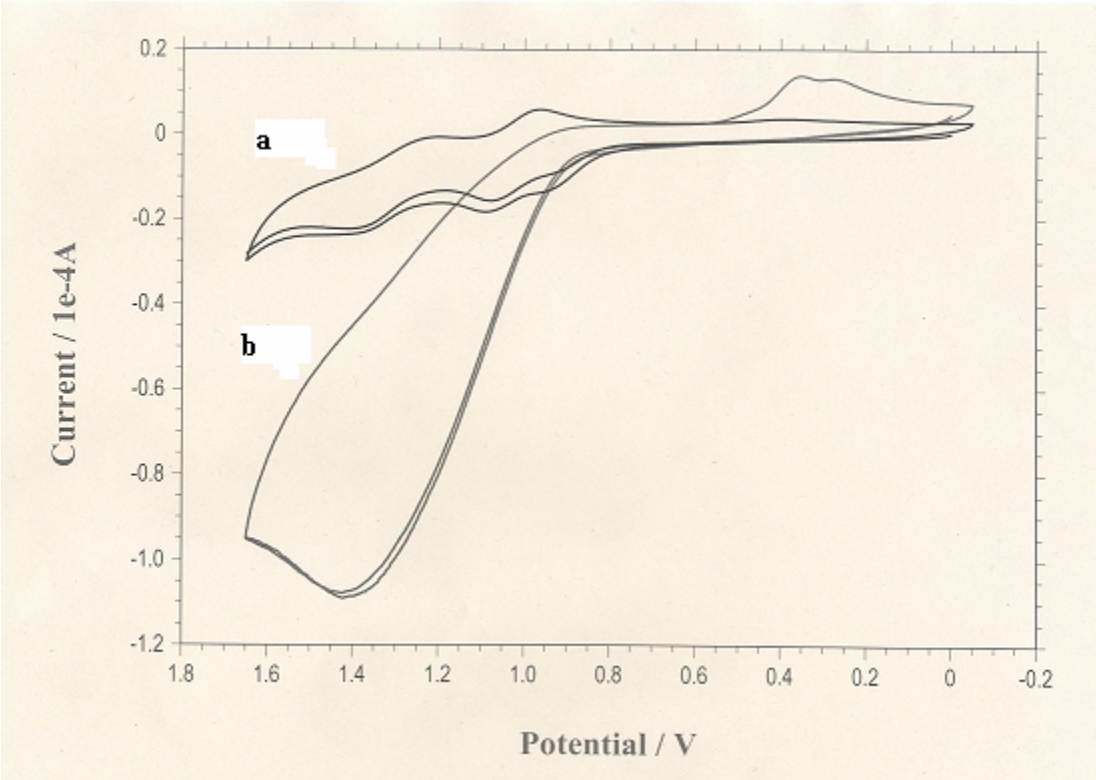


Fig. SI 9**.** CV at glassy carbon electrode for 1.0 mM solution of **6** and a) stoichiometric or b) excess amount of $NEt_4^+ Cl^-$ in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

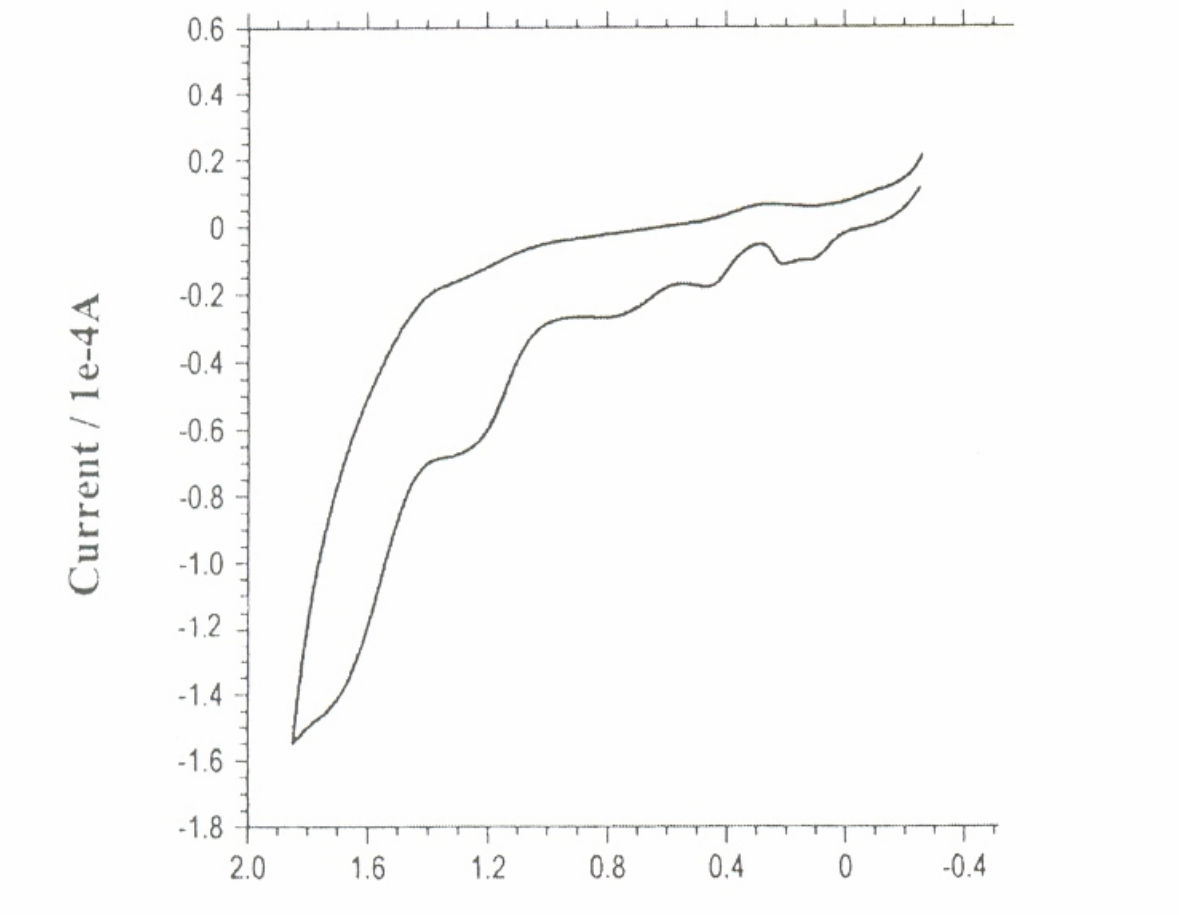


Fig. SI 10**.** CV at glassy carbon electrode for 1.0 mM solution of **7** in 0.10 M Bu_4NPF_6/CH_2Cl_2. Potential scan rate 0.050 V s^{-1}.

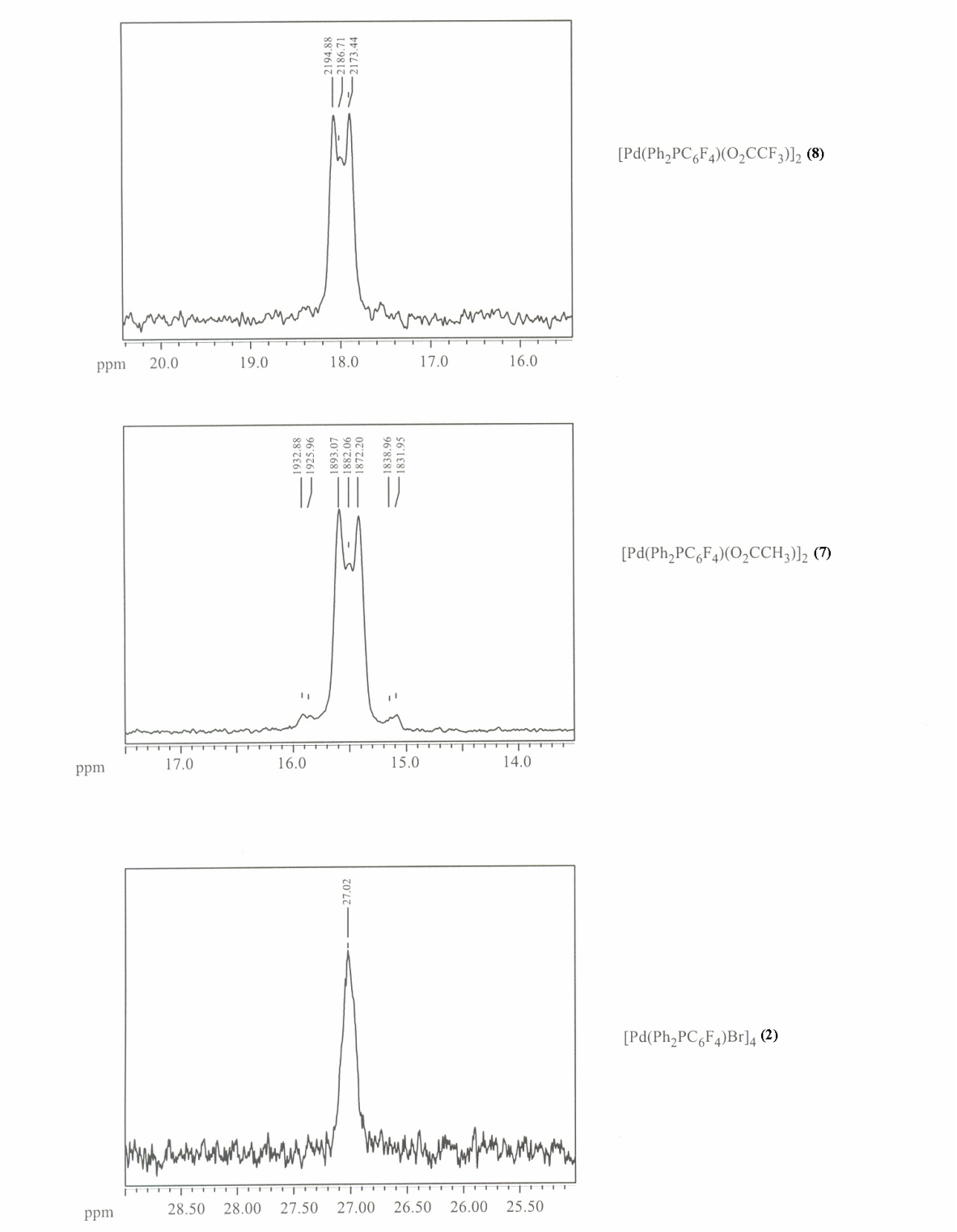
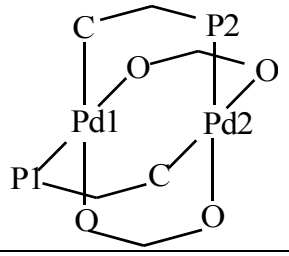


Fig. SI 11. ^{31}P NMR of compounds **8**, **7** and **2**.

Table SI 1. Important bond distances and angles.



Compound	4	5	6	7	8
Bond lengths, (Å)					
Pd1-Pd2	2.7229(8)	2.6779(15)	2.7078(6)	2.6749(14)	2.7054(6)
Pd1-P1	2.2273(12)	2.226(3)	2.2303(17)	2.243(3)	2.2294(11)
Pd2-P2	2.2269(12)		2.2241(16)		
Pd1-O_{transP}	2.170(3)	2.132(7)	2.148(4)	2.094(7)	2.148(3)
Pd1-O_{transC}	2.158(3)	2.124(7)	2.141(4)	2.074(7)	2.116(3)
Pd1-C	1.982(4)	1.974(10)	1.992(6)	1.993(9)	1.987(4)
Pd2-O_{transP}	2.164(3)		2.158(5)		
Pd2-O_{transC}	2.163(3)		2.148(4)		
Pd2-C	1.980(4)		1.991(6)		
Torsion angles, (o)					
P1-Pd1-Pd2-P2	94.3(1)	96.3(1)	96.8(1)	98.9(1)	91.2(1)
P1-Pd1-Pd2-C	7.8(1)	8.4(1)	10.1(2)	7.0(1)	4.5(1)
P2-Pd2-Pd1-C	8.4(1)		8.4(2)		
O_{transP}-Pd1-Pd2-O_{transC}	11.7(1)	13.3(1)	11.4(2)	9.5(1)	7.0(1)
O_{transC}-Pd1-Pd2-O_{transP}	11.5(1)		11.7(2)		
Angles around Pd-Pd, (o)					
Pd1-Pd2-C	95.14(11)	95.7(3)	95.29(18)	94.4(3)	93.22(11)
C-Pd2-Pd1	95.12(11)		95.93(18)		
O_{transP}-Pd1-Pd2	82.90(8)	83.3(2)	85.45(12)	82.6(2)	84.56(8)
O_{transC}-Pd1-Pd2	83.64(8)	83.4(2)	82.25(12)	84.8(2)	83.33(8)
Pd1-Pd2-O_{transP}	82.93(8)		81.56(12)		
O_{transC}-Pd2-Pd1	83.70(8)		84.73(12)		
Pd1-Pd2-P2	87.35(3)	87.83(6)	87.74(4)	89.41(7)	89.89(3)

P1-Pd1-Pd2	87.50(3)	86.85(4)