Synthesis and X-ray Diffraction of Cyclopalladated Compounds Derived from Imine Ligands †

Basma Al Janabi *, Juan M. Ortigueira and Jose Manuel Vila

Department of Inorganic Chemistry, Faculty of Chemistry, University of Santiago de Compostela, Avd. das Ciencias s/n, 15782 Santiago de compostela, Spain

* Correspondence: basma.raad@usc.es

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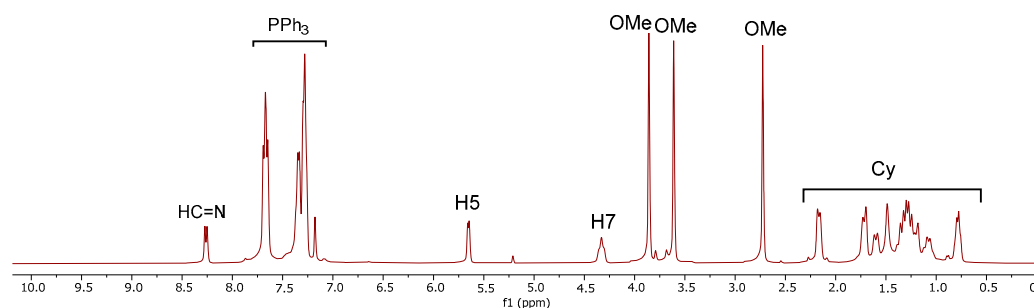
Figure S1. ^{1}H NMR of compound **1a** in CDCl$_3$.

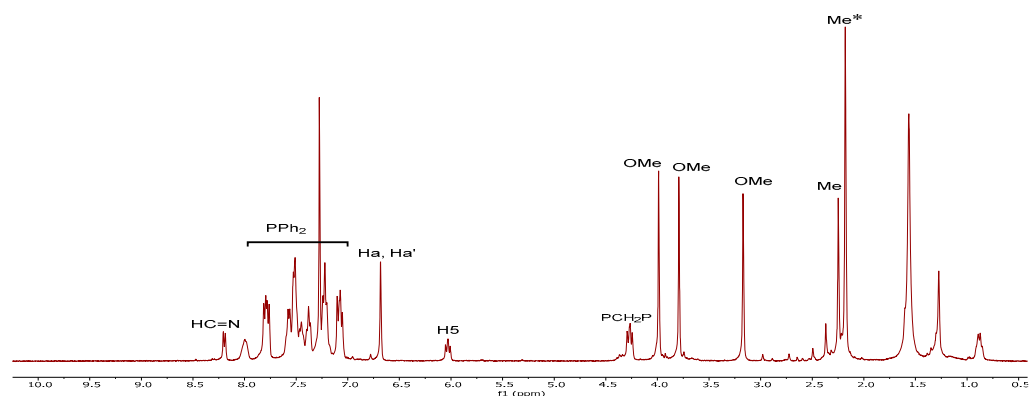**Figure S2.** ^{1}H NMR of compound **1b** in CDCl$_3$.

Table S1. Crystal data and structure refinement for compounds **1a** and **1b**.

Crystal Structure	1a	1b
Molecular formula	C$_{34}$H$_{37}$ClNO$_3$PPd	C$_{44}$H$_{44}$F$_6$NO$_3$P$_3$Pd
Formula weight	680.46	948.11
Temperature/K	100.00	100.00
Crystal system	Orthorhombic	monoclinic
Space group	P2$_1$/n	P2$_1$/n
a/Å	22.5430 (14)	14.2798 (8)
b/Å	9.7727 (5)	14.0263 (8)
c/Å	13.6276 (9)	21.2483 (11)
α/°	90	90

β/°	90	98.393 (2)
γ/°	90	90
Volume/Å^3	3002.2 (3)	4210.3 (4)
Z	4	4
ϱ_{calc}g/cm^3	1.505	1.496
μ/mm^{-1}	0.797	0.622
F (000)	1400.0	1936.0
Crystal size/mm^3	0.08 × 0.03 × 0.02	0.33 × 0.07 × 0.02
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
θ range for data collection/°	4.542 to 56.558	4.092 to 55.752
Index ranges	$-30 \leq h \leq 30$, $-13 \leq k \leq 13$, $-18 \leq l \leq 18$	$-18 \leq h \leq 18$, $-18 \leq k \leq 18$, $-27 \leq l \leq 25$
Reflections collected	120820	91837
Independent reflections	7453 [R_{int} = 0.0977, R_{sigma} = 0.0378]	10,043 [R_{int} = 0.0905, R_{sigma} = 0.0485]
Data/restraints/parameters	7453/1/373	10,043/0/530
Goodness-of-fit on F^2	1.047	1.038
Final R indexes [I $\geq$ 2σ (I)]	R_1 = 0.0383, wR_2 = 0.0714	R_1 = 0.0446, wR_2 = 0.0966
Final R indexes [all data]	R_1 = 0.0524, wR_2 = 0.0786	R_1 = 0.0641, wR_2 = 0.1068
Largest diff. peak/hole / e Å^{-3}	0.64/−0.91	1.54/−1.47
Flack parameter	0.487(11)	