

Synthesis, Characterization, and Photophysical Properties of Mixed Ligand (η^3 -Allyl)palladium(II) Complexes with N,N' Aromatic Diimines

Antonia Garypidou ¹, Konstantinos Ypsilantis ¹, Evaggelia Sifnaiou ¹, Maria Manthou ¹, Dimitris Thomos ¹, John C. Plakatouras ^{1,2}, Theodoros Tsolis ¹ and Achilleas Garoufis ^{1,2,*}

¹ Department of Chemistry, University of Ioannina, GR-45110 Ioannina, Greece; a.garypidou@uoi.gr (A.G.); k_ypsilantis@yahoo.gr (K.Y.); e.sifnaiou@uoi.gr (E.S.); maria.manthou13@gmail.com (M.M.); d.thomos@uoi.gr (D.T.); iplakatu@uoi.gr (J.C.P.); t.tsolis@uoi.gr (T.T.)

² Institute of Materials Science and Computing, University Research Center of Ioannina (URCI), GR-45110 Ioannina, Greece

* Correspondence: agaroufi@uoi.gr

Table of contents

Figure S1: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)Cl]₂ in CDCl₃ at 298K.

Figure S2: ¹³C NMR spectrum of the complex [Pd(η^3 -allyl)Cl]₂ in CDCl₃ at 298K.

Figure S3: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(bphen)](PF₆) (**1**) in acetone-d₆ at 298K.

Figure S4: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(ncp)](PF₆) (**2**) in acetone-d₆ at 298K.

Figure S5: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(bcp)](PF₆) (**3**) in acetone-d₆ at 298K.

Figure S6: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(mphen)](PF₆) (**4**) in acetone-d₆ at 298K.

Figure S7: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(tmphen)](PF₆) (**5**) in acetone-d₆ at 298K.

Figure S8: ¹H NMR spectrum of the complex [Pd(η^3 -allyl)(pqx)](PF₆) (**6**) in acetone-d₆ (a) and [Pd(η^3 -allyl)(pqx)][Pd(η^3 -allyl)Cl₂] (**6a**) in MeOD (b) at 298K.

Figure S9: HR-ESI-MS of the complex [Pd(η^3 -allyl)(bphen)](PF₆) (**1**) in acetone.

Figure S10: HR-ESI-MS of the complex [Pd(η^3 -allyl)(ncp)](PF₆) (**2**) in acetone.

Figure S11: HR-ESI-MS of the complex [Pd(η^3 -allyl)(bcp)](PF₆) (**3**) in acetone.

Figure S12: HR-ESI-MS of the complex [Pd(η^3 -allyl)(mphen)](PF₆) (**4**) in acetone.

Figure S13: HR-ESI-MS of the complex [Pd(η^3 -allyl)(tmphen)](PF₆) (**5**) in acetone.

Figure S14: HR-ESI-MS of the complex [Pd(η^3 -allyl)(pqx)](PF₆) (**6**) in acetone.

Figure S15: ¹³C NMR spectrum of the complex [Pd(η^3 -allyl)(mphen)](PF₆) (**4**) in acetone-d₆ at 298K.

Figure S16: ¹³C NMR spectrum of the complex [Pd(η^3 -allyl)(tmphen)](PF₆) (**5**) in acetone-d₆ at 298K.

Figure S17: ¹³C NMR spectrum of the complex [Pd(η^3 -allyl)(pqx)][Pd(η^3 -allyl)Cl₂] (**6a**) in MeOD at 298K.

Figure S18: A packing diagram of compound $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})](\text{PF}_6)$ (**6**), down to the b axis of the unit cell. Hydrogen atoms of the allyl group have been omitted for clarity.

Figure S19: A packing diagram of compound $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})][\text{Pd}(\eta^3\text{-allyl})\text{Cl}_2]$ (**6a**), down to the a axis of the unit cell.

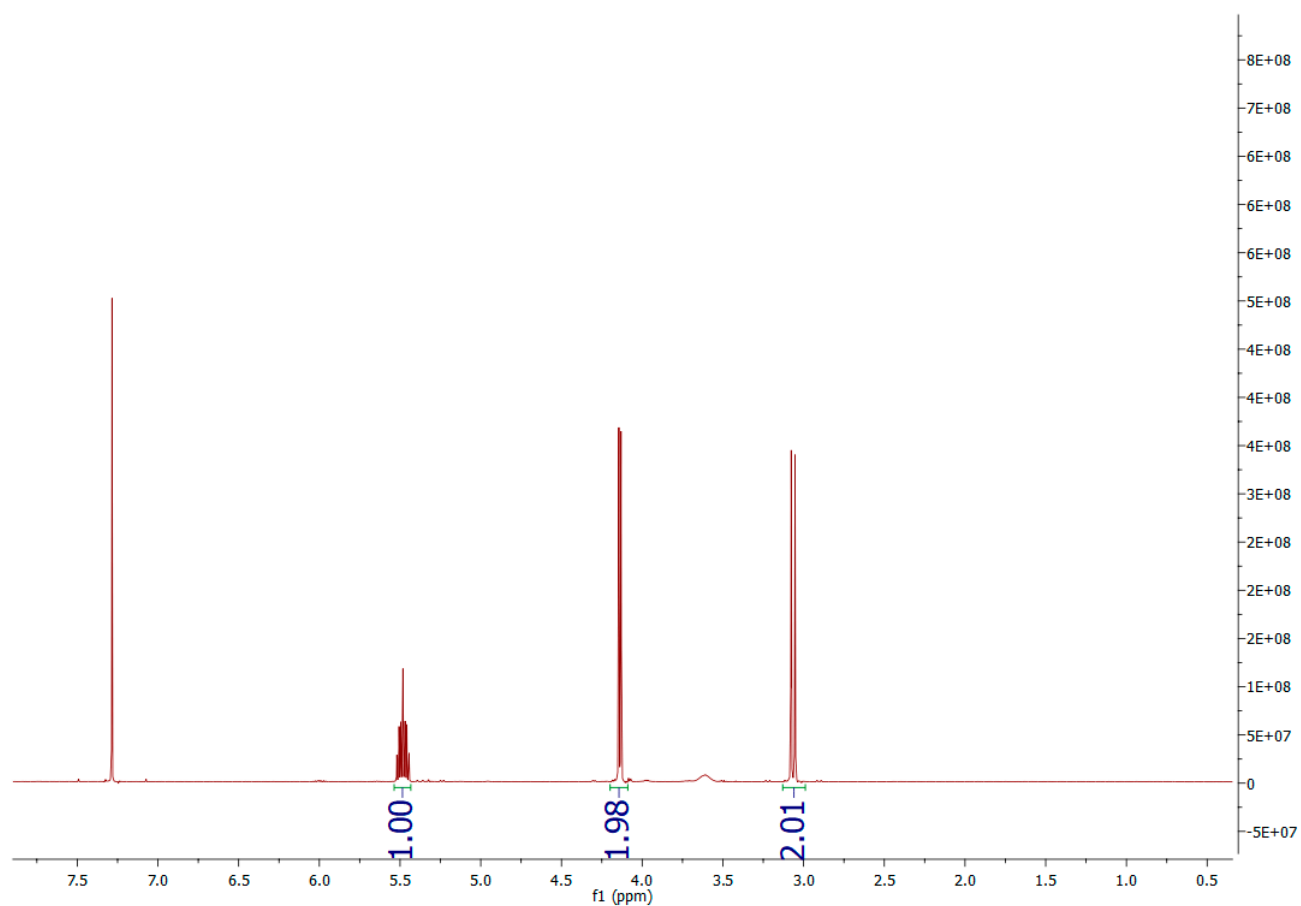


Figure S1: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})\text{Cl}]_2$ in CDCl_3 at 298K.

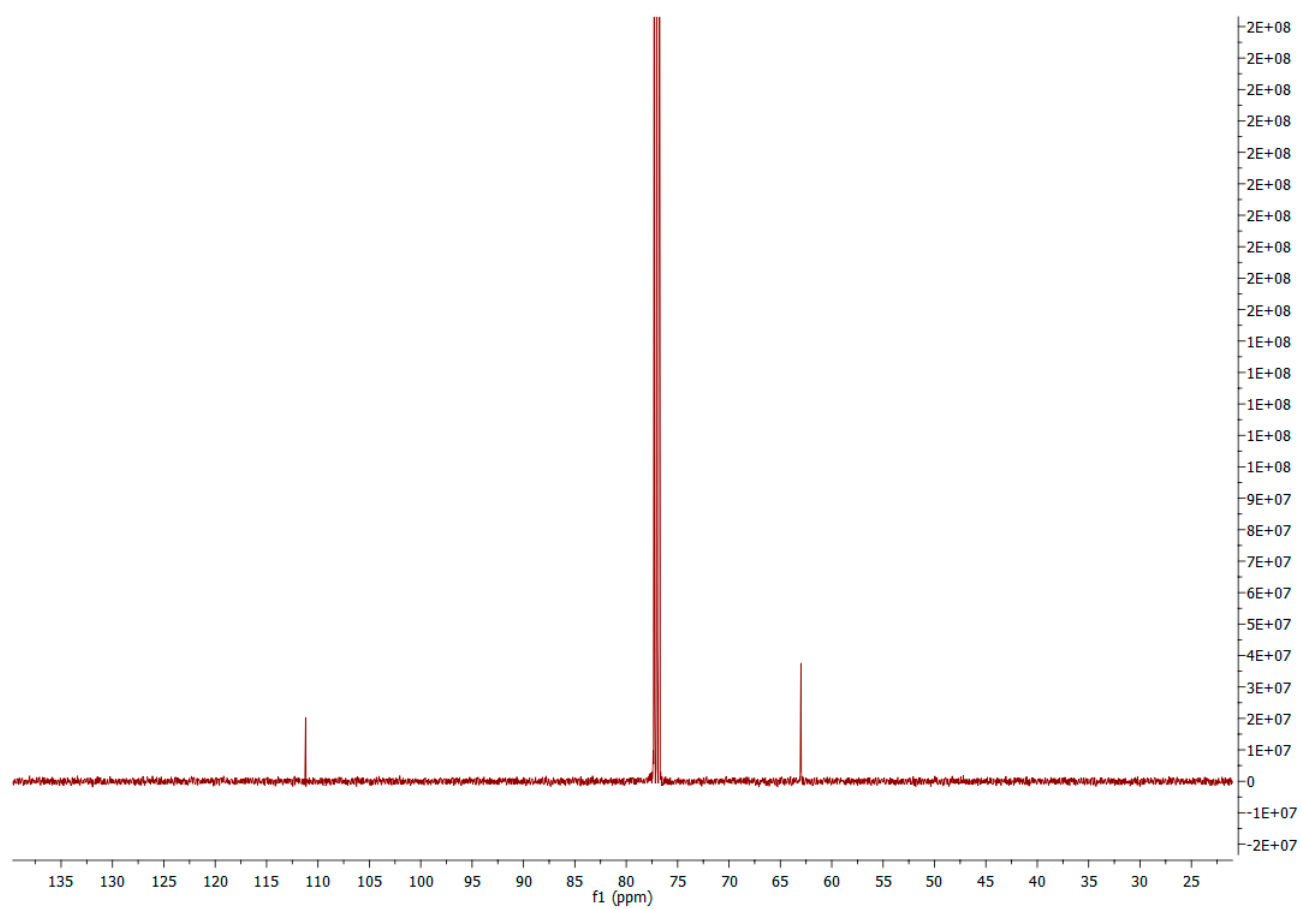


Figure S2: ^{13}C NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})\text{Cl}]_2$ in CDCl_3 at 298K.

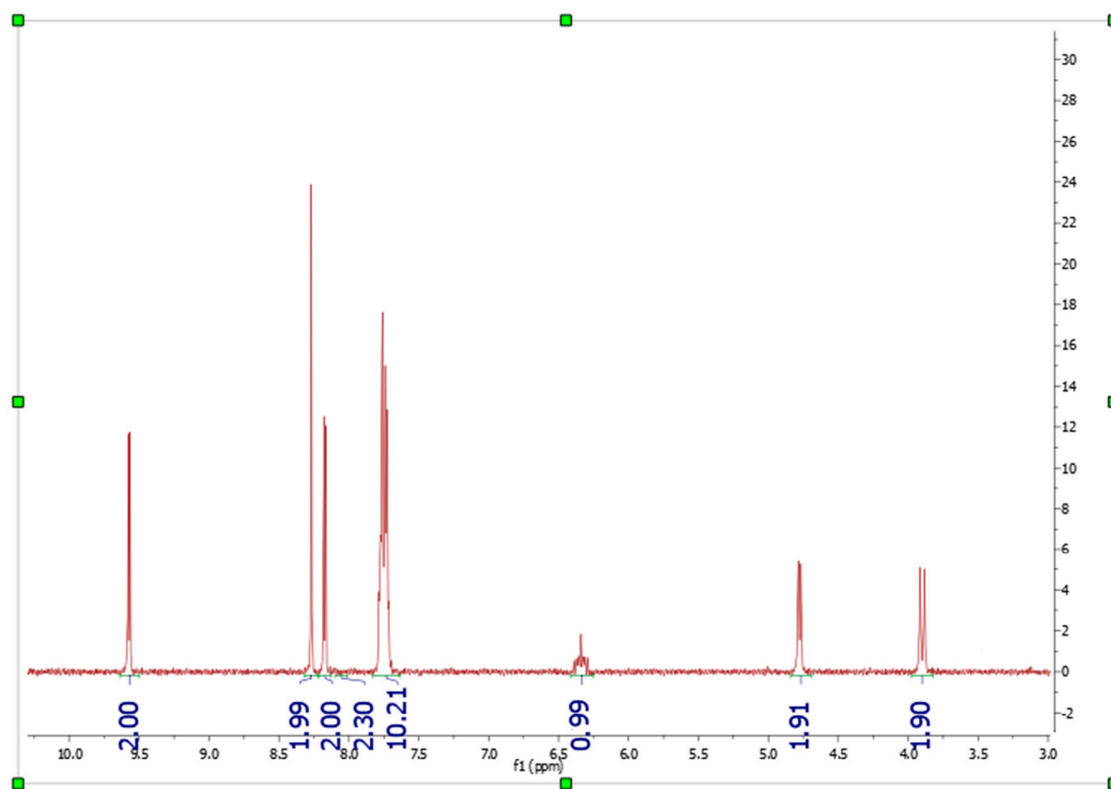


Figure S3: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{bphen})](\text{PF}_6)$ (1) in acetone- d_6 at 298K.

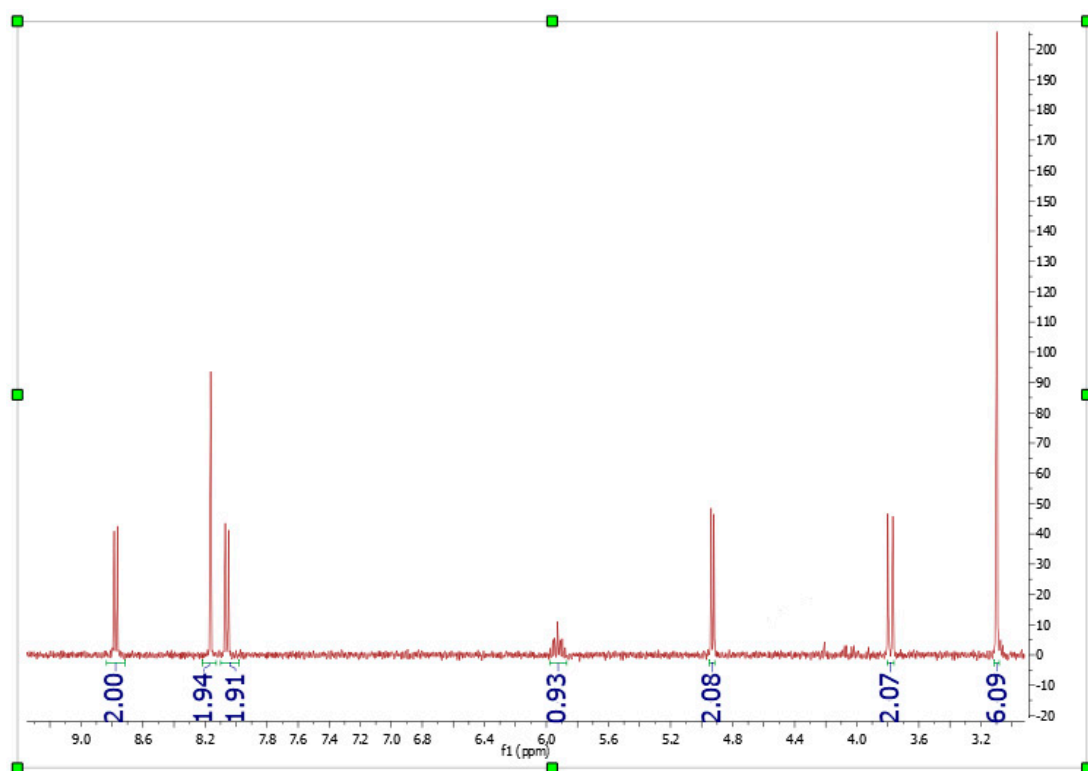


Figure S4: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{ncp})](\text{PF}_6)$ (**2**) in acetone- d_6 at 298K.

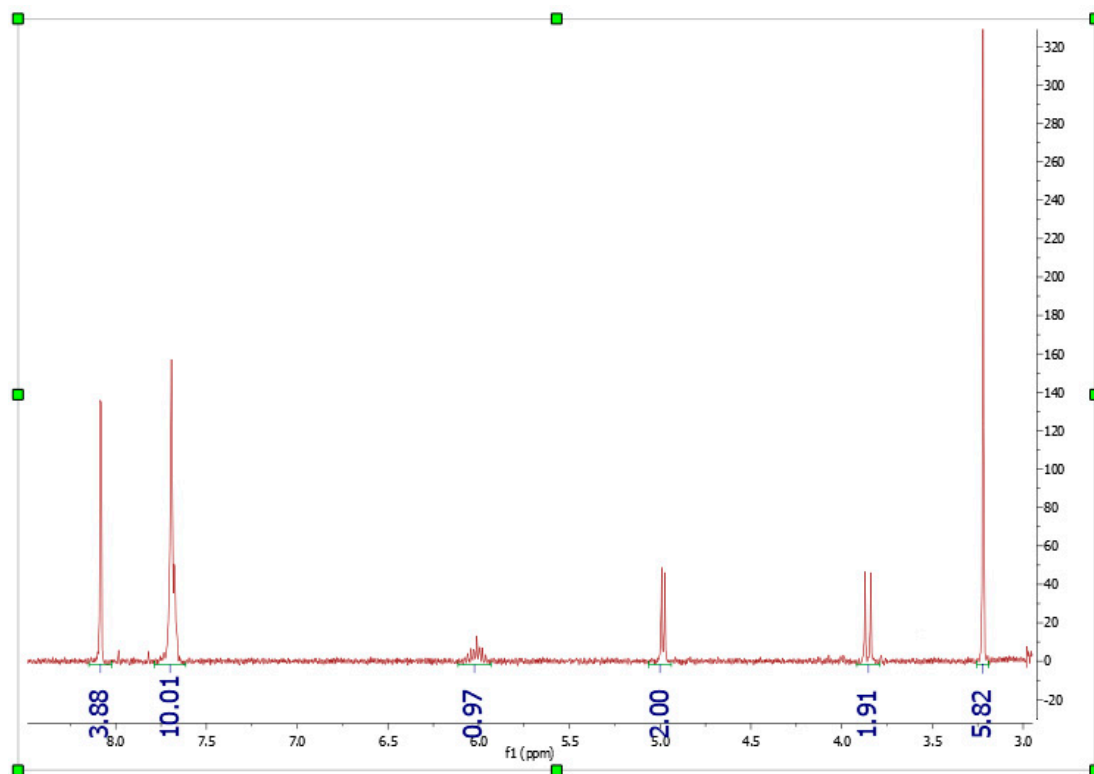


Figure S5: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{bcp})](\text{PF}_6)$ (**3**) in acetone- d_6 at 298K.

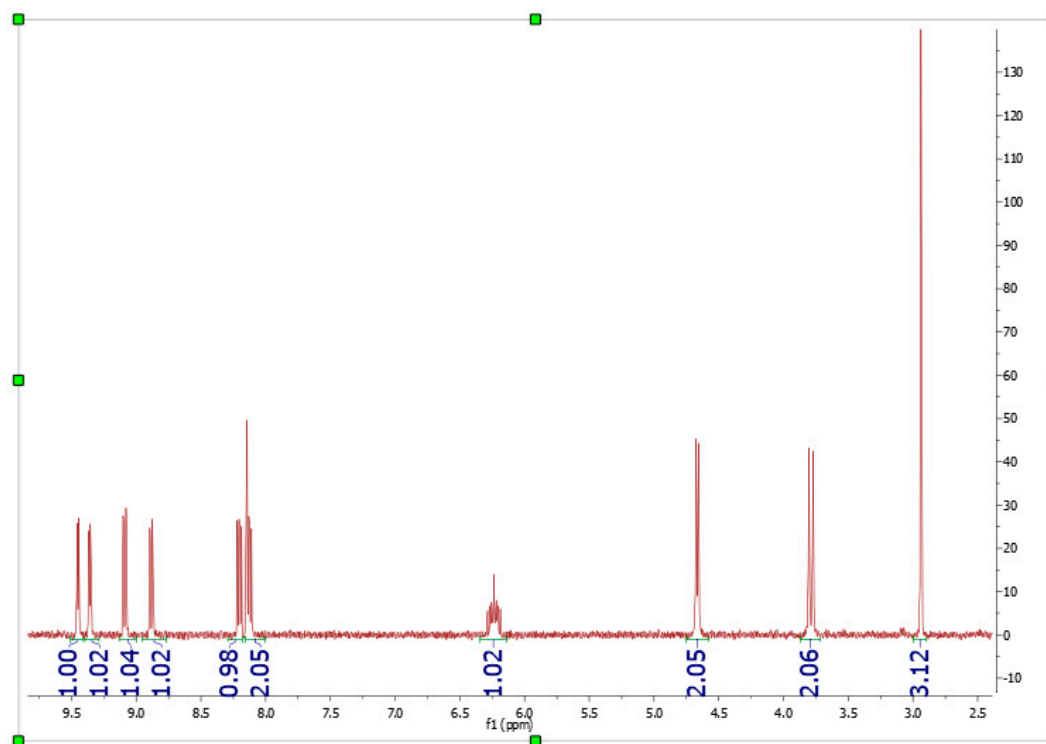


Figure S6: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{mphen})](\text{PF}_6)$ (**4**) in acetone- d_6 at 298K.

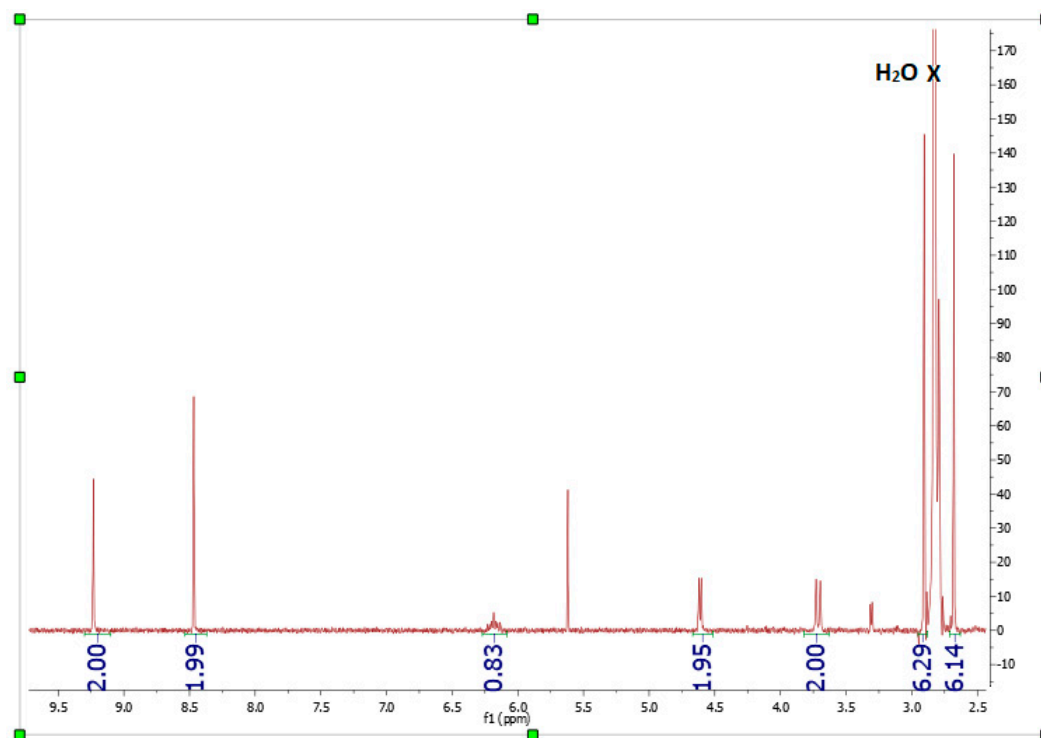
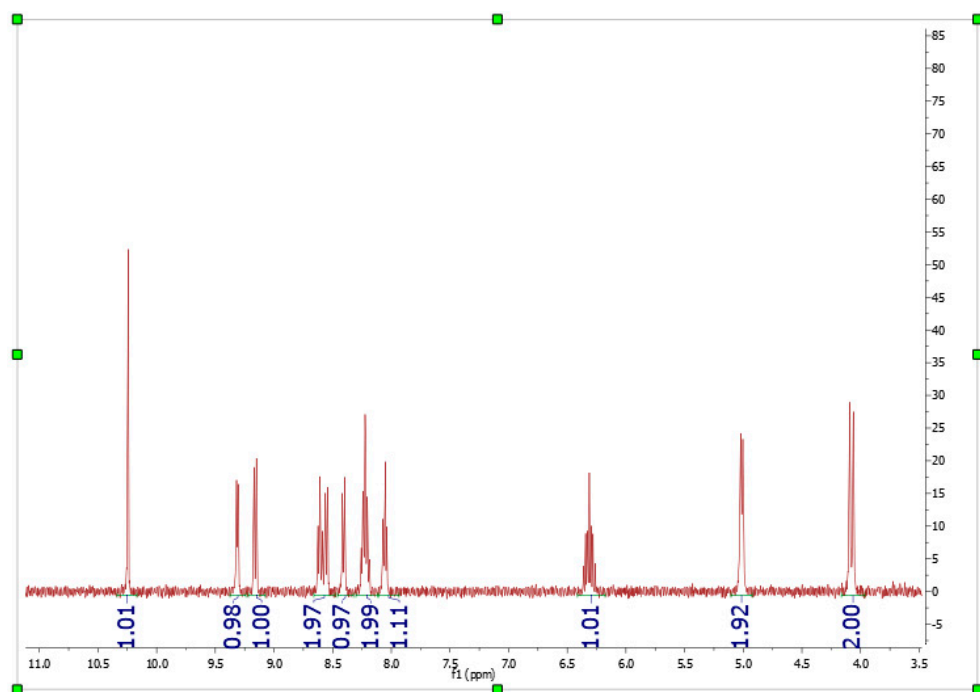
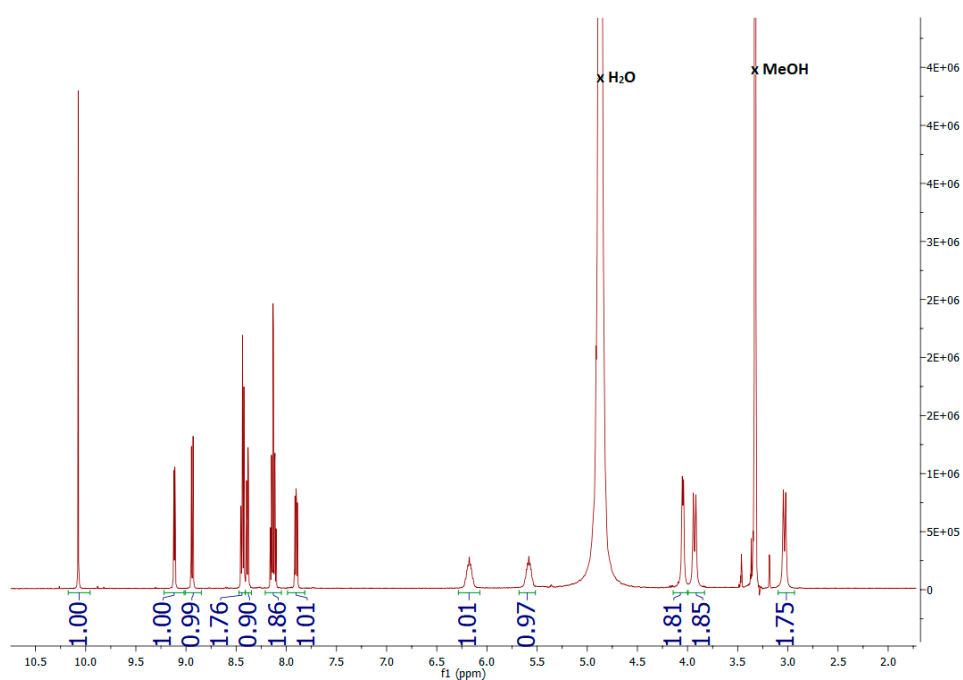


Figure S7: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{tmphen})](\text{PF}_6)$ (5) in acetone- d_6 at 298K.



(a)



(b)

Figure S8: ^1H NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})](\text{PF}_6)$ (**6**) in acetone- d_6 (a) and $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})][\text{Pd}(\eta^3\text{-allyl})\text{Cl}_2]$ (**6a**) in MeOD (b) at 298K.

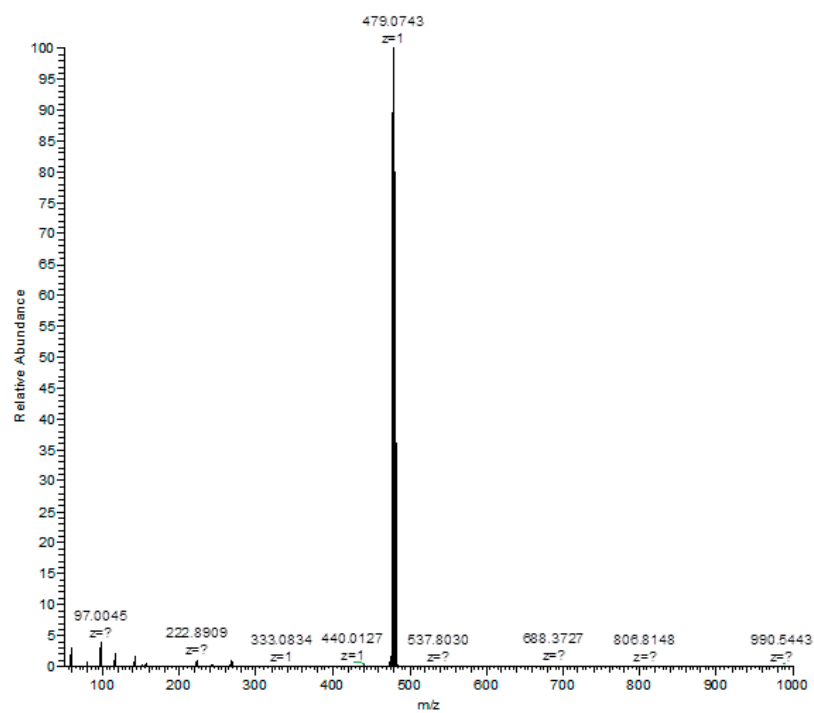


Figure S9: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{bphen})](\text{PF}_6)$ (**1**) in acetone.

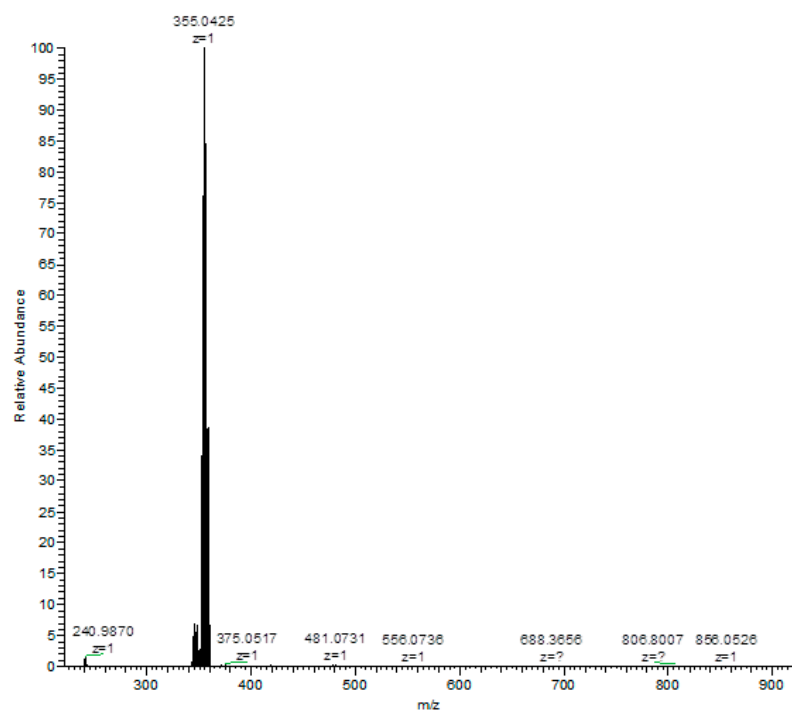


Figure S10: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{ncp})](\text{PF}_6)$ (**2**) in acetone.

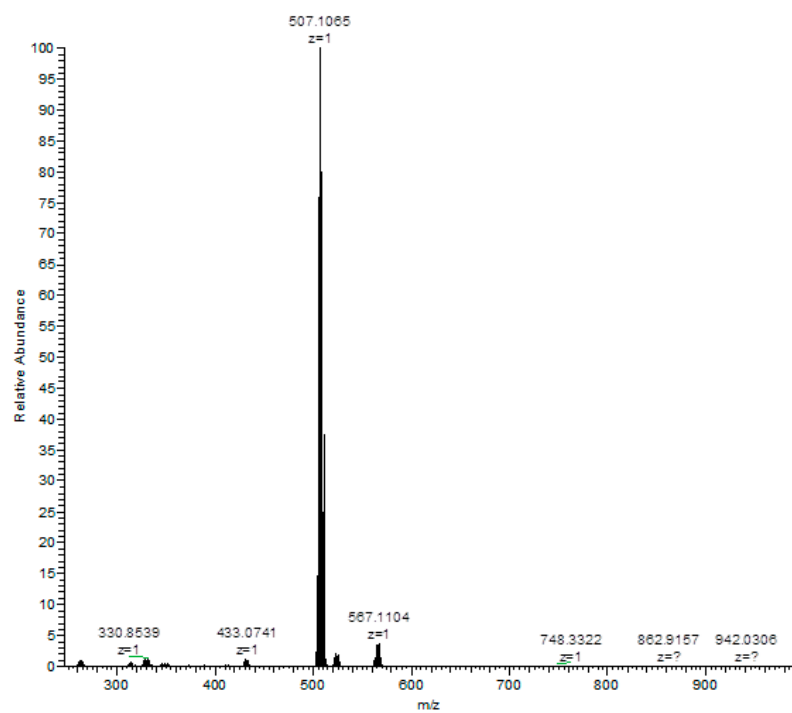


Figure S11: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{bcp})](\text{PF}_6)$ (**3**) in acetone.

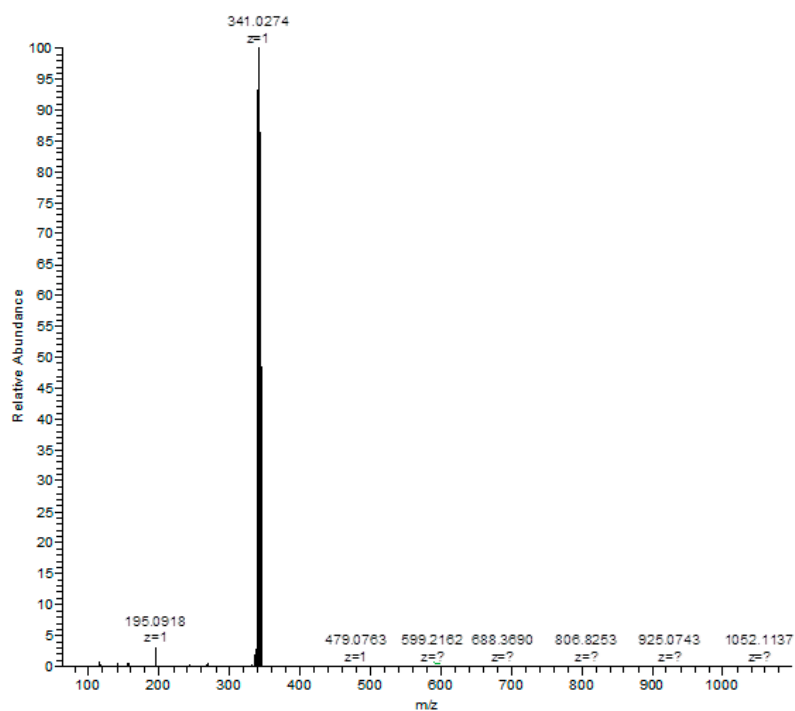


Figure S12: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{mphen})](\text{PF}_6)$ (**4**) in acetone.

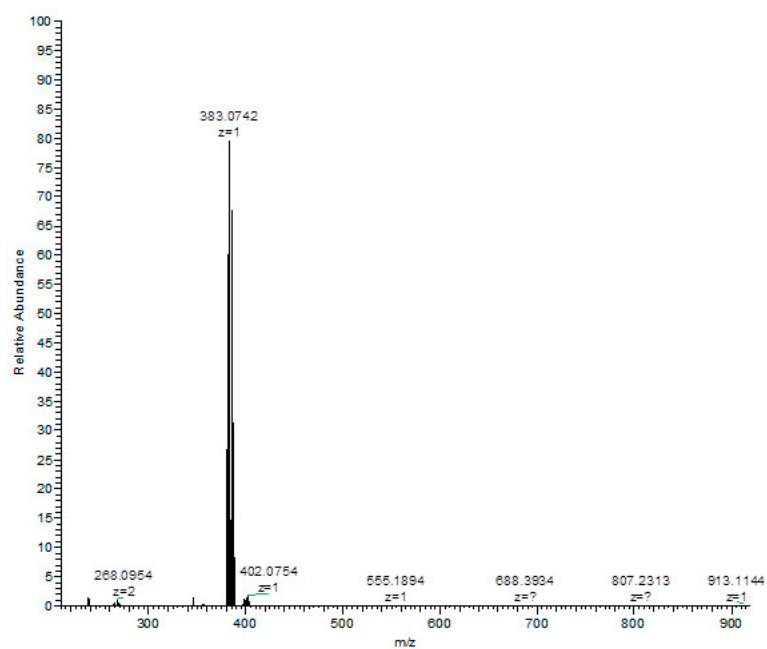


Figure S13: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{tmphen})](\text{PF}_6)$ (**5**) in acetone.

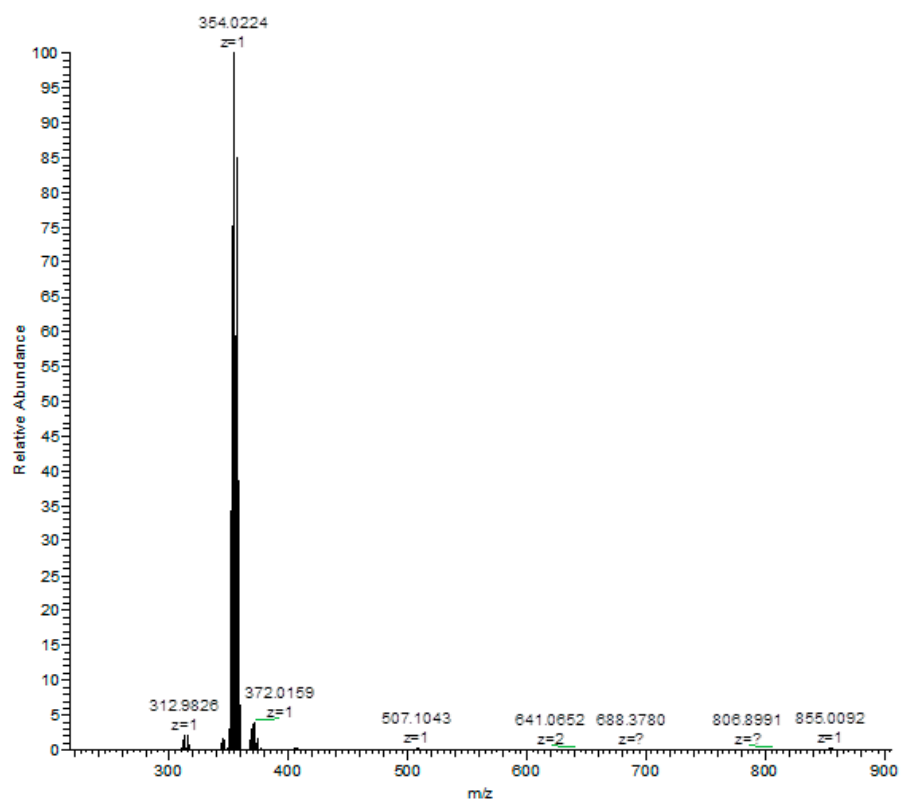


Figure S14: HR-ESI-MS of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})](\text{PF}_6)$ (**6**) in acetone.

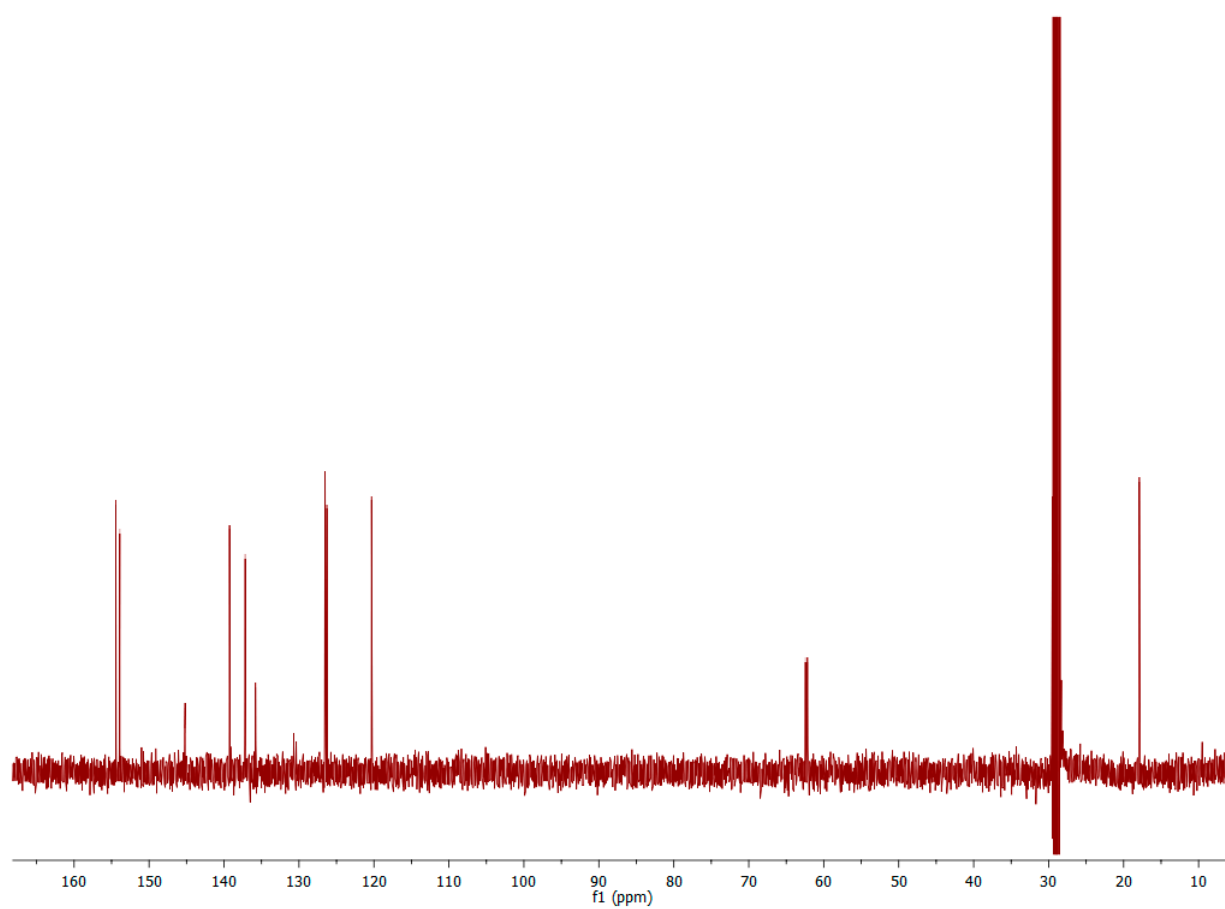


Figure S15: ^{13}C NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{mphen})](\text{PF}_6)$ (**4**) in acetone- d_6 at 298K.

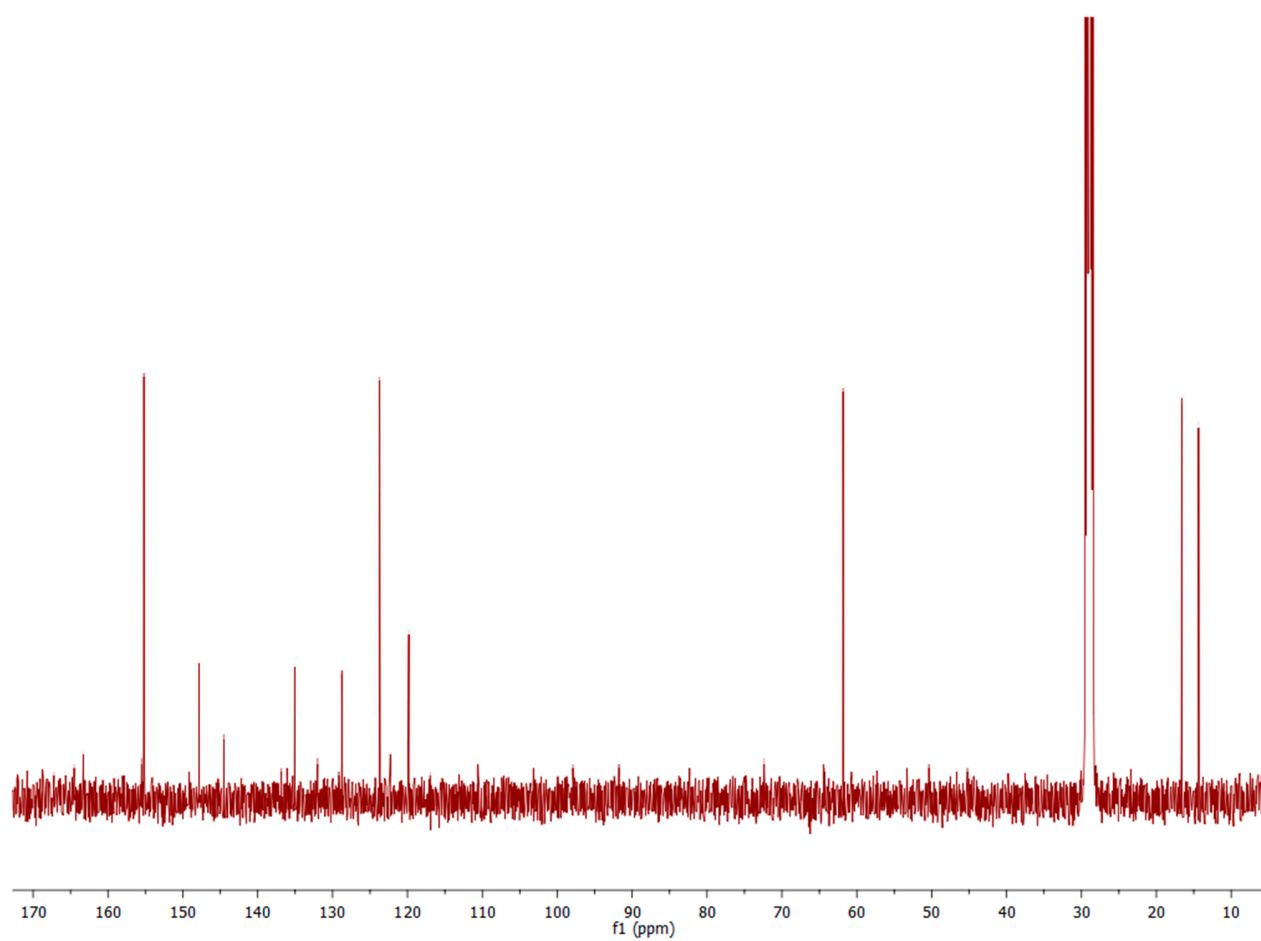


Figure S16: ^{13}C NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{tmphen})](\text{PF}_6)$ (**5**) in acetone- d_6 at 298K.

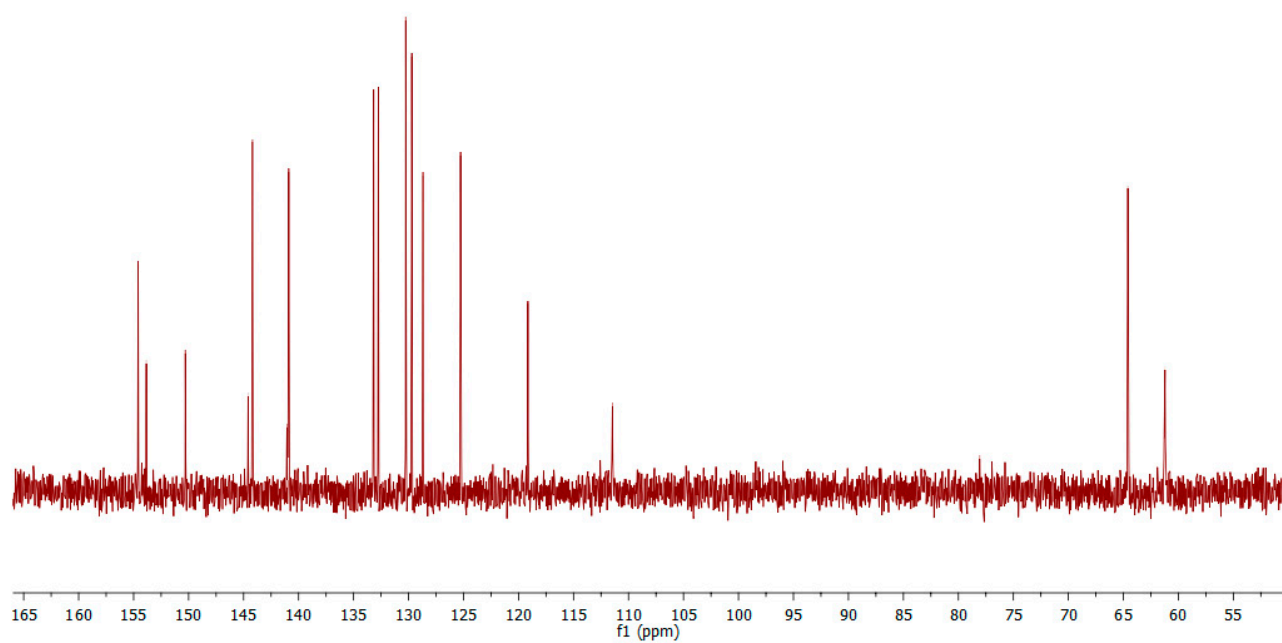


Figure S17: ^{13}C NMR spectrum of the complex $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})][\text{Pd}(\eta^3\text{-allyl})\text{Cl}_2]$ (6a) in MeOD at 298K.

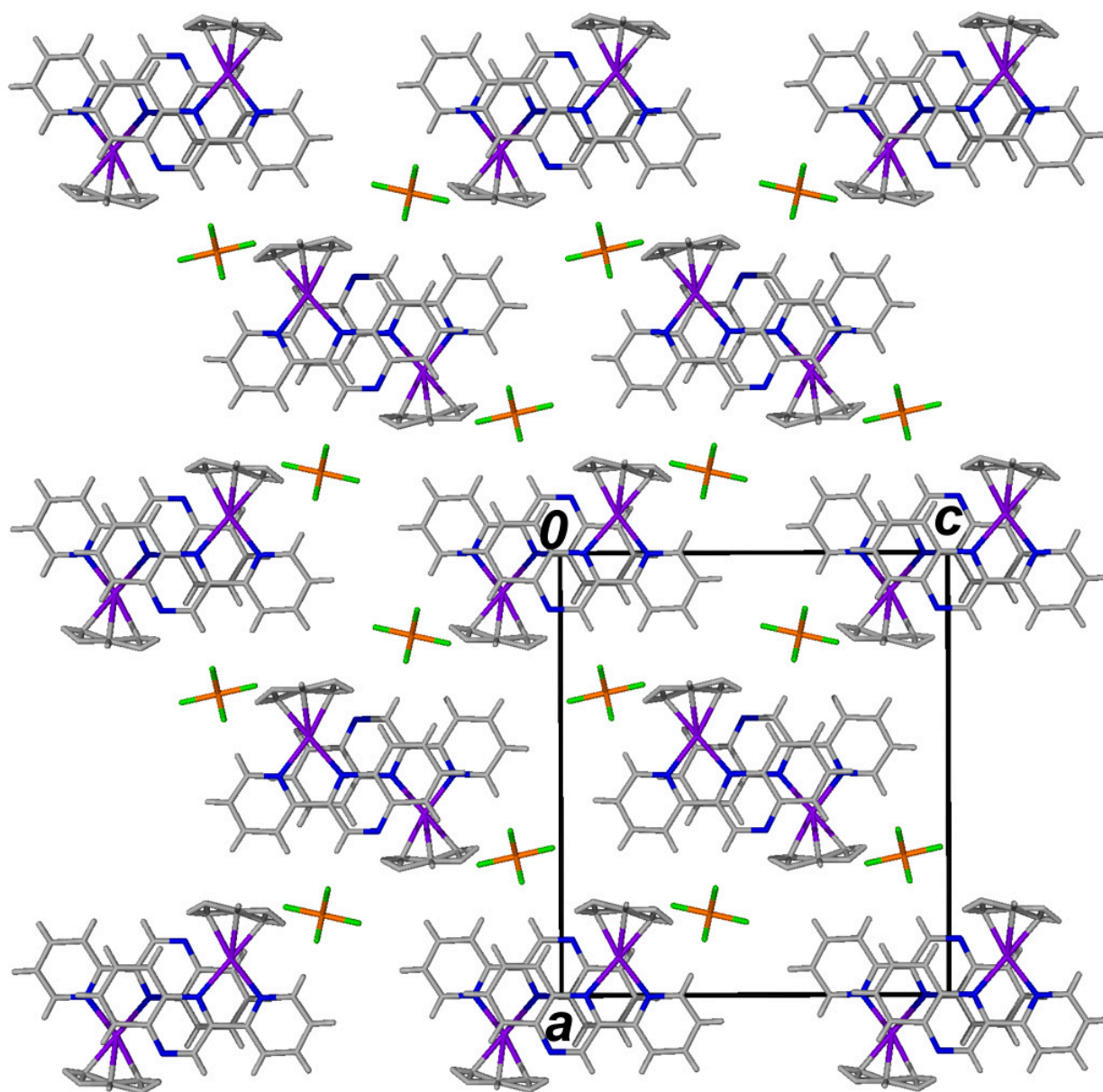


Figure S18: A packing diagram of compound $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})](\text{PF}_6)$ (**6**), down to the b axis of the unit cell. Hydrogen atoms of the allyl group have been omitted for clarity.

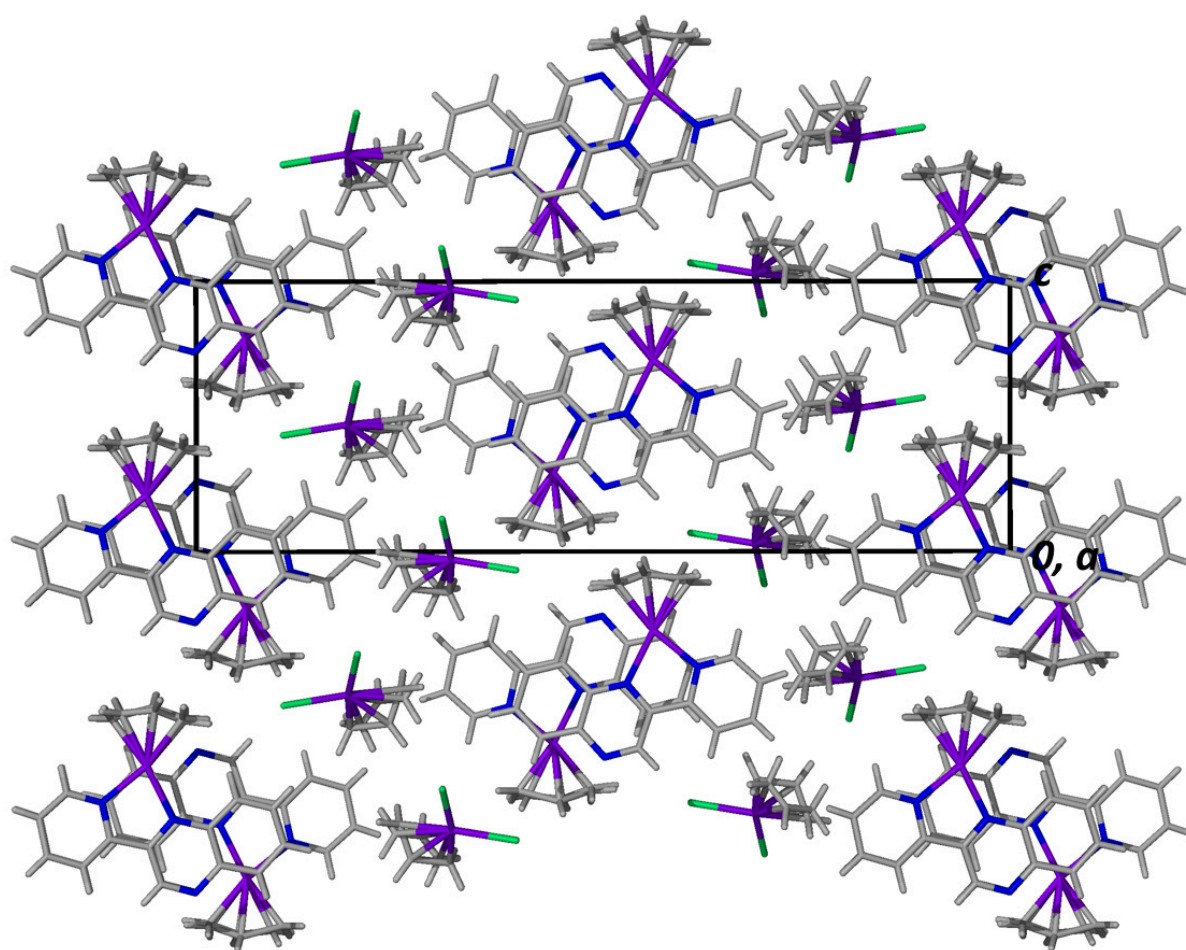


Figure S19: A packing diagram of compound $[\text{Pd}(\eta^3\text{-allyl})(\text{pqx})][\text{Pd}(\eta^3\text{-allyl})\text{Cl}_2]$ (**6a**), down to the a axis of the unit cell.