Electronic Supplementary Material (ESI) for RSC Advances

ESI–MS Mechanistic Studies of the Wacker Oxidation of Alkenes: Dinuclear Species as Catalytic Active Intermediates

Dominique Harakat, Jacques Muzart, Jean Le Bras*

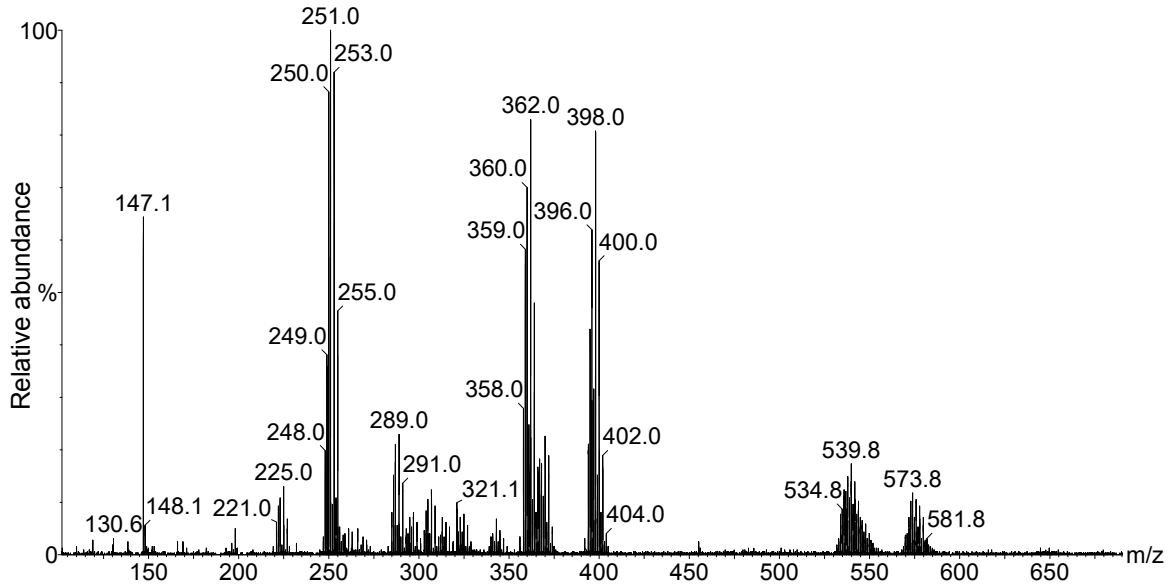
Institut de Chimie Moléculaire de Reims, UMR 7312, CNRS-Université de Reims Champagne-Ardenne, UFR des Sciences Exactes et Naturelles, BP 1039, 51687 REIMS Cedex 2, France

Fax: +33 3 26 91 31 66; E-mail: jean.lebras@univ-reims.fr

Supporting Information

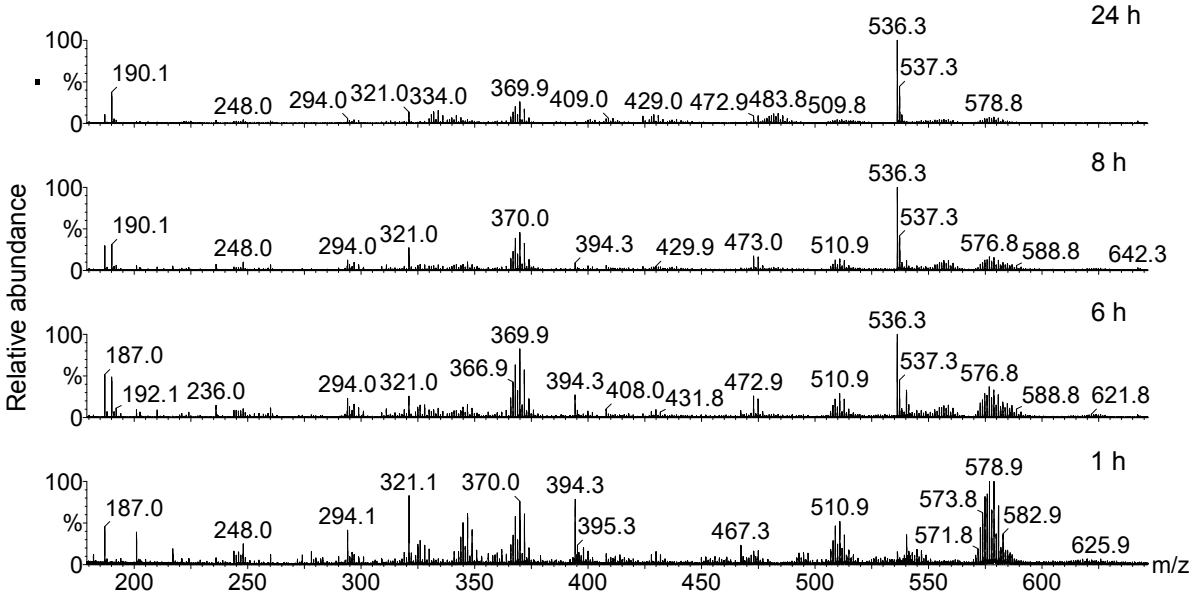
Table of Contents

Figure S1. ESI(+)-MS of a mixture of $PdCl_2$, BQ, DMF, and H_2O.[a]



[a] $PdCl_2$ (0.05 mmol), BQ (1.1 mmol), DMF (1.75 mL), H_2O (0.25 mL).

Figure S2. ESI(+)-MS of the reaction solution of the oxydation of **1c** over 24h.[a]



[a] **1c** (1.0 mmol), $PdCl_2$ (0.05 mmol), BQ (1.1 mmol), DMF (1.75 mL), H_2O (0.25 mL).

Figure S3. ESI(-)-MS/MS (6-8 eV) of $[Pd_2Cl_5(\mathbf{1f})]^-$ and $[Pd_2Cl_5(\mathbf{2f})]^-$.

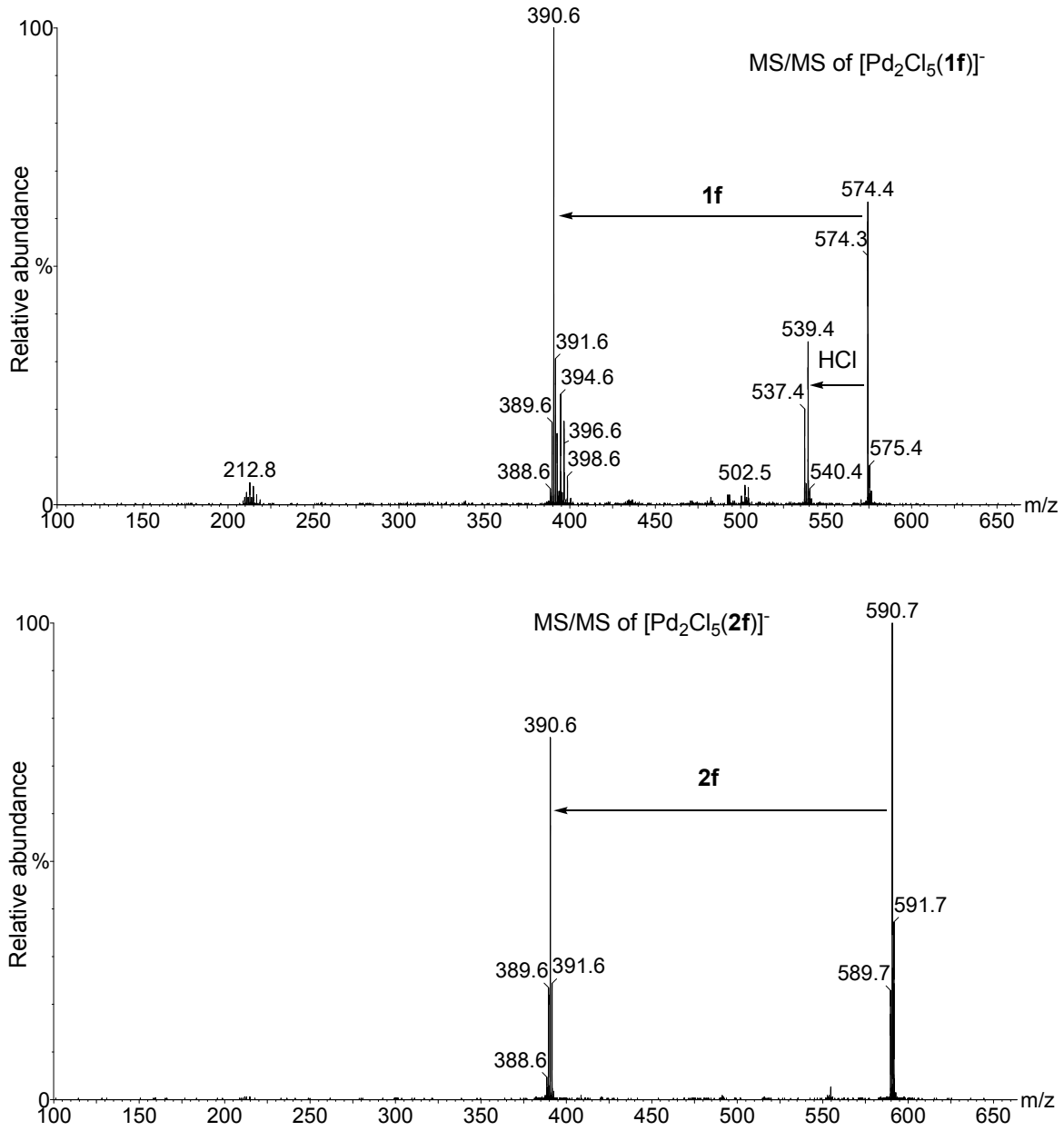


Figure S4. ESI(-)-MS/MS (6-8 eV) of $[Pd_2Cl_5(\mathbf{1e})]^-$ and $[Pd_2Cl_5(\mathbf{2e})]^-$ showing the loss of H_2O and HCl.

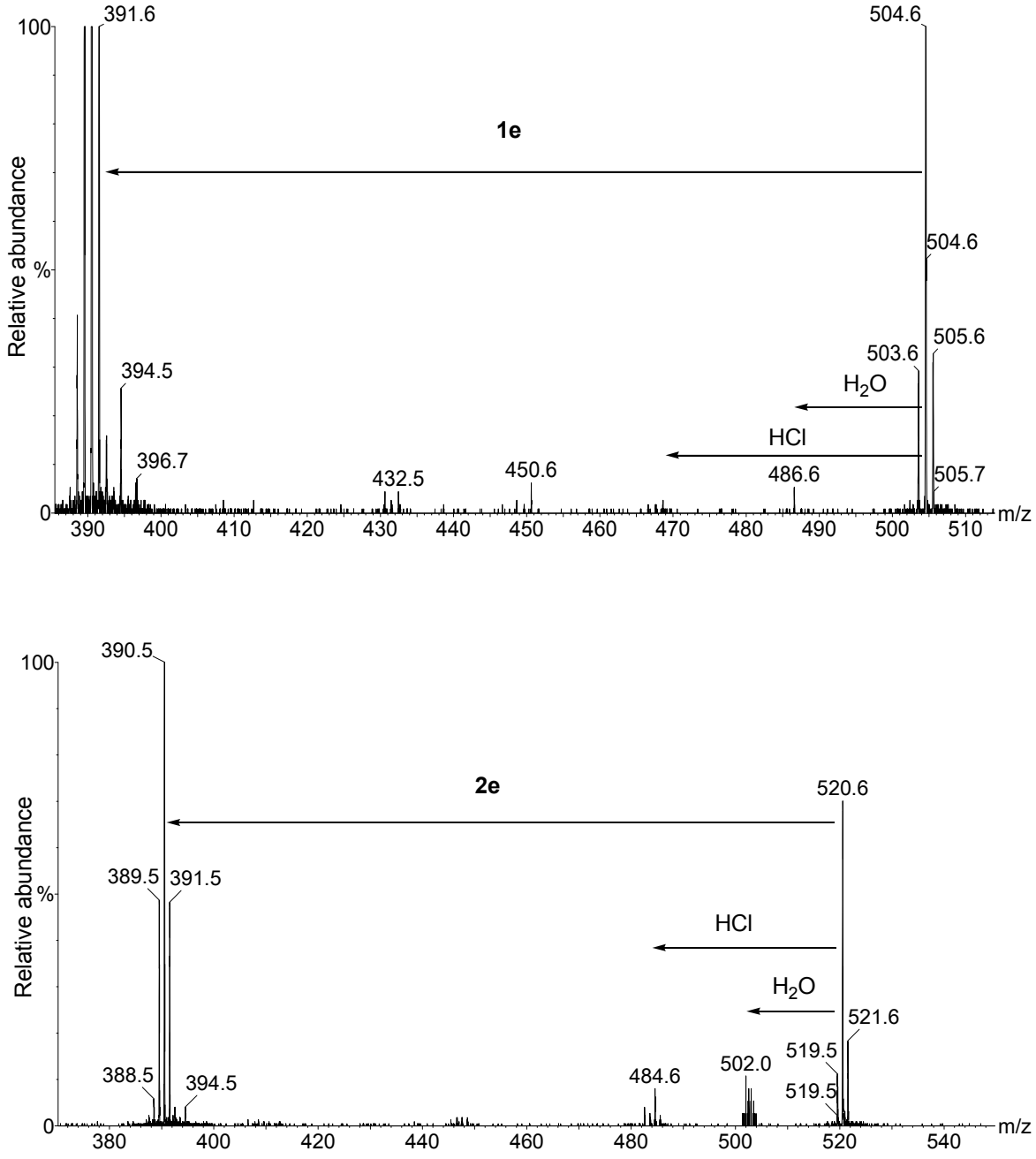


Figure S5. Isotopic distribution of $[Pd_2Cl_5(\mathbf{1e})]^-$, $[Pd_2Cl_4(H_2O)(OH)(\mathbf{1e})]^-$ and experimental spectra.

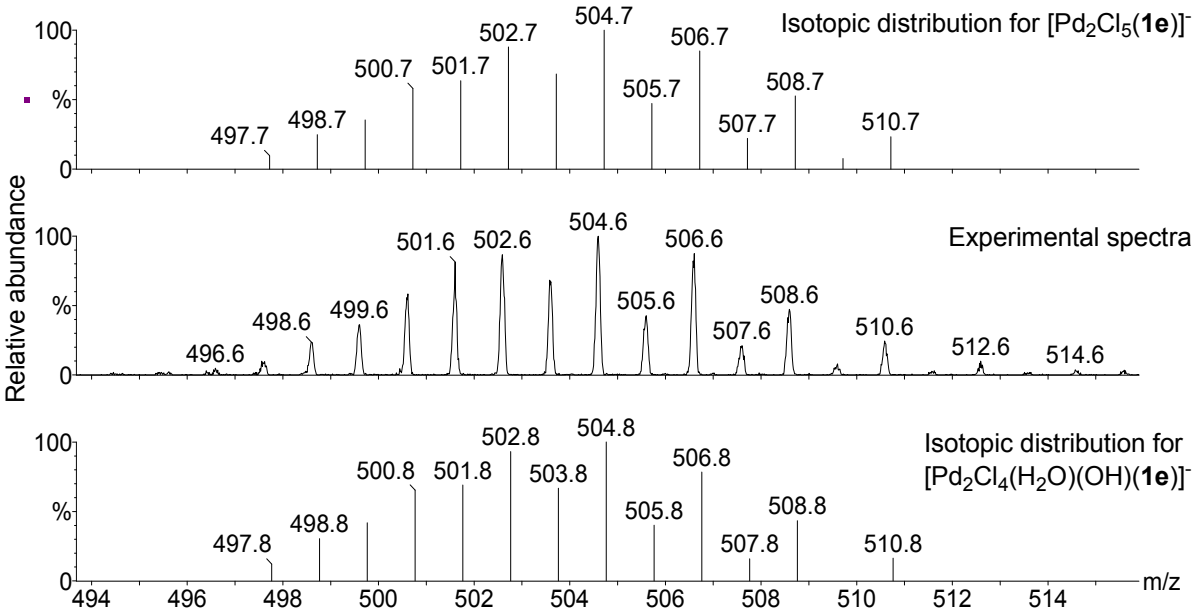
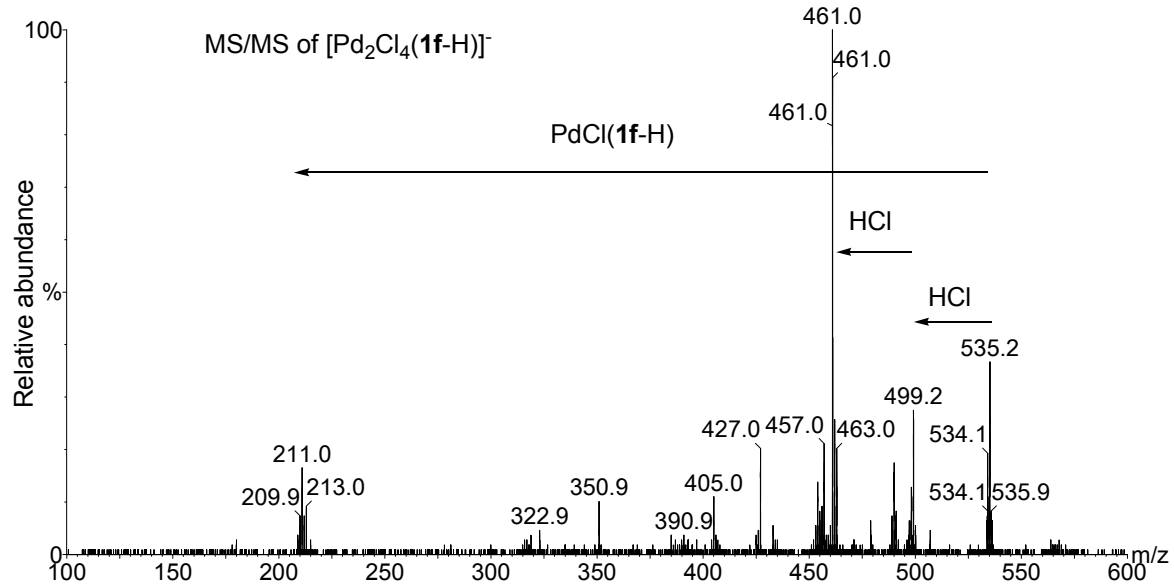


Figure S6. ESI(-)-MS/MS (15-20 eV) of $[Pd_2Cl_4(\mathbf{1f}\text{-H})]^-$ and $[Pd_2Cl_4(\mathbf{2f}\text{-H})]^-$.



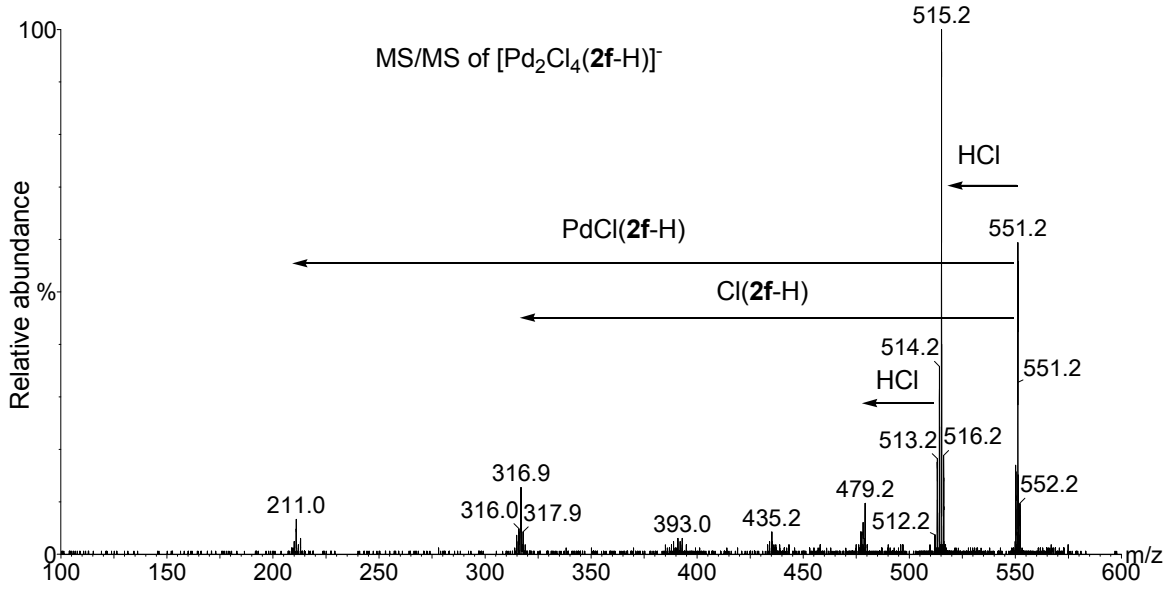
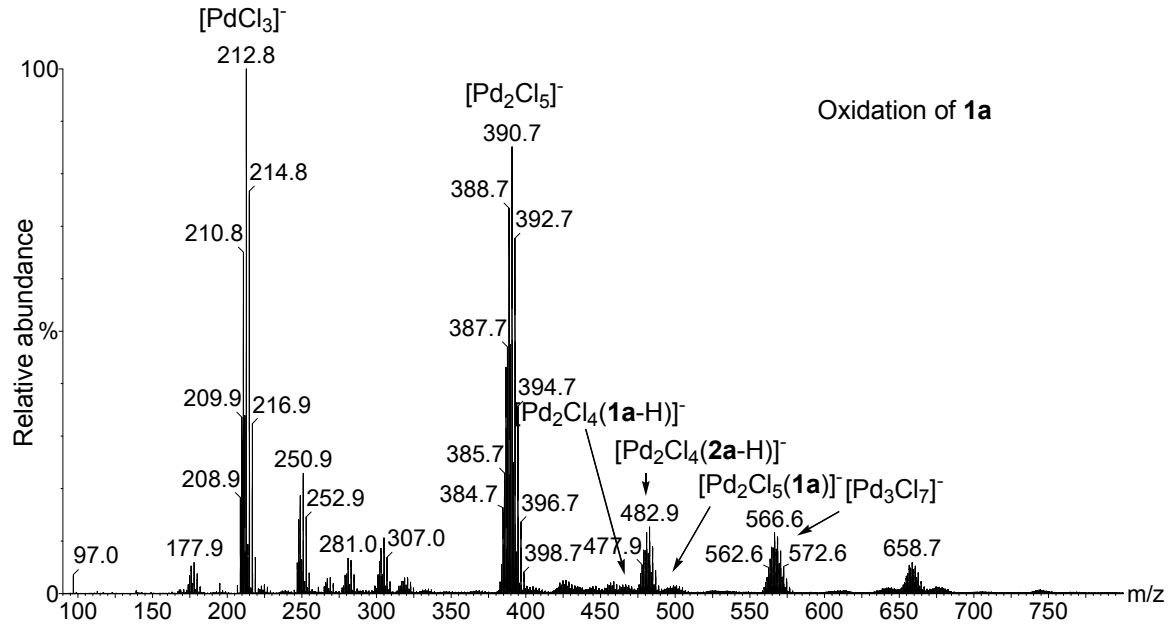
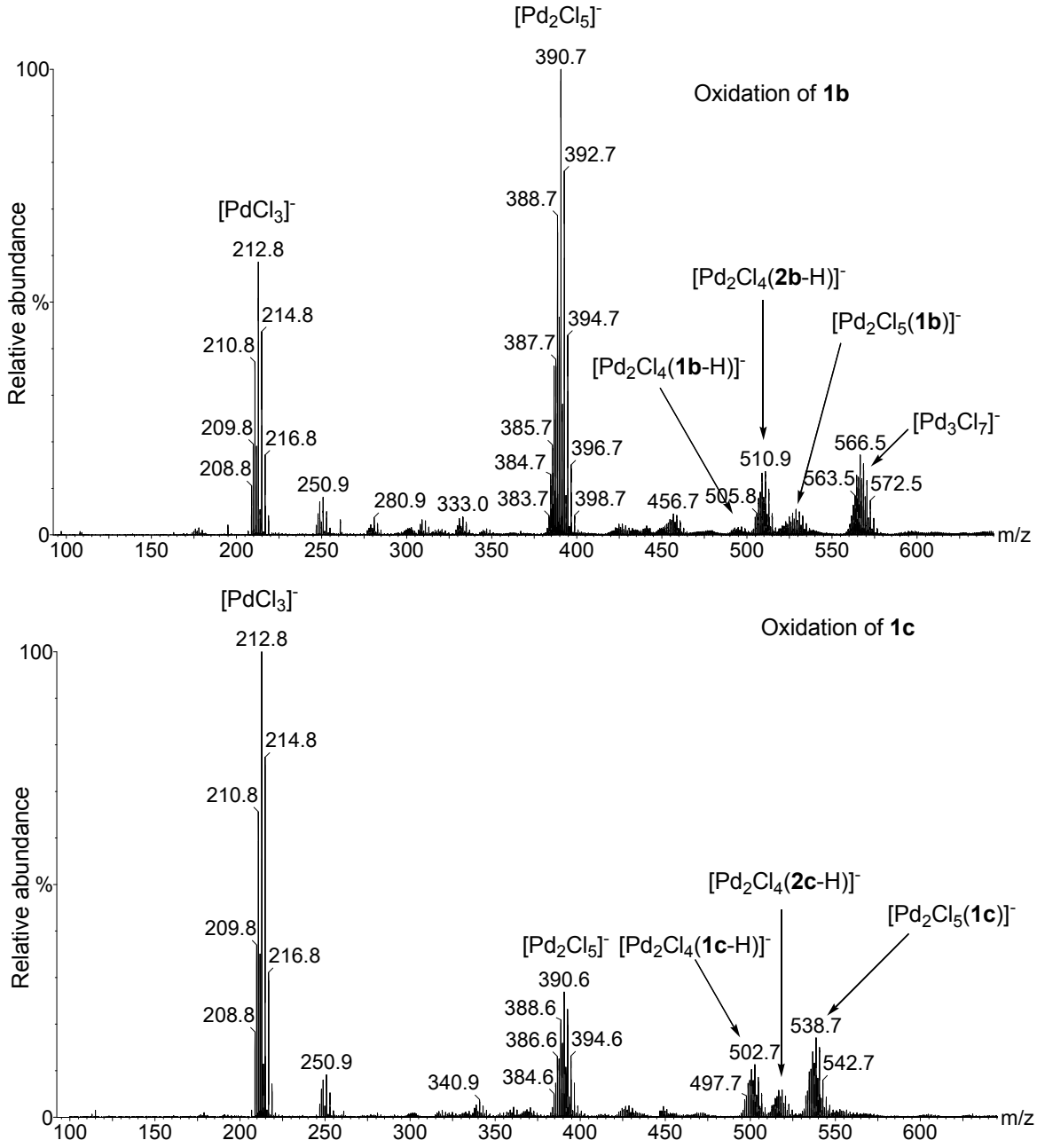


Figure S7. ESI(-)-MS of the reaction solution of the oxydation of **1a-1d** after 10 min.





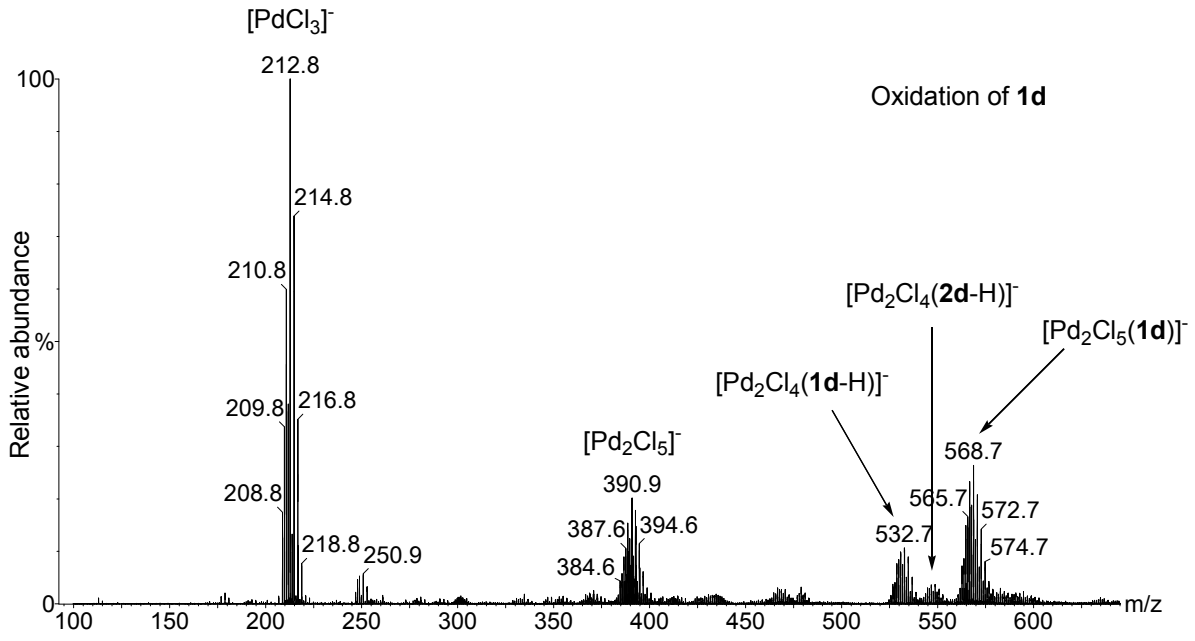
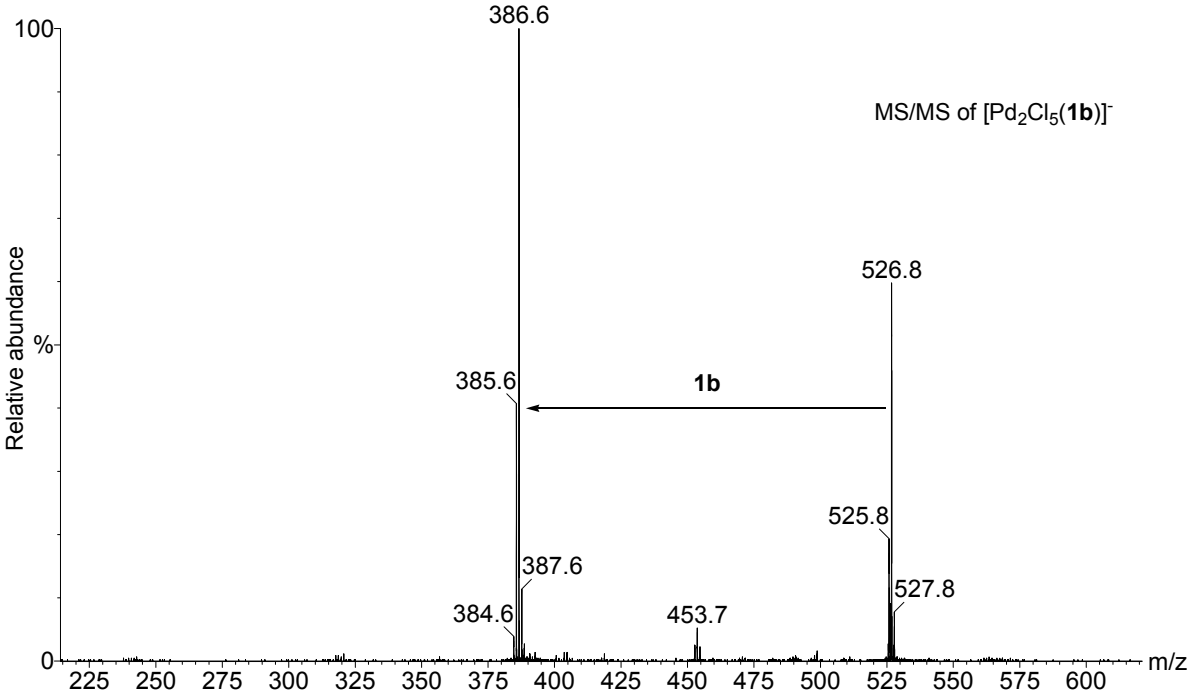
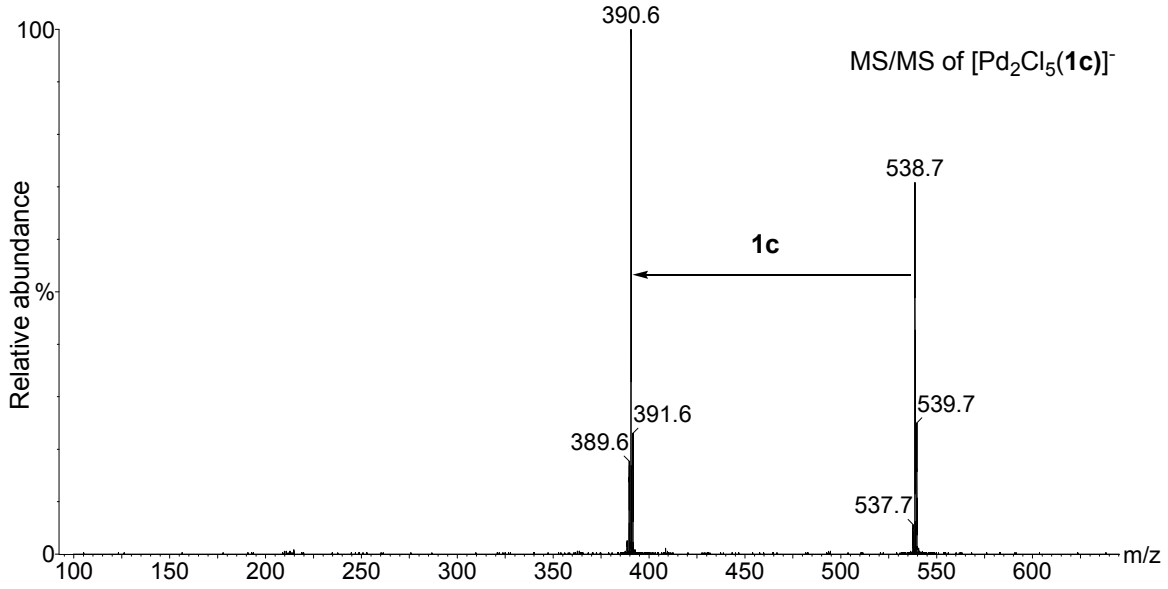


Figure S8. ESI(-)-MS/MS (6-8 eV) of $[Pd_2Cl_5(\mathbf{1b})]^-$, $[Pd_2Cl_5(\mathbf{1c})]^-$, and $[Pd_2Cl_5(\mathbf{1d})]^-$.





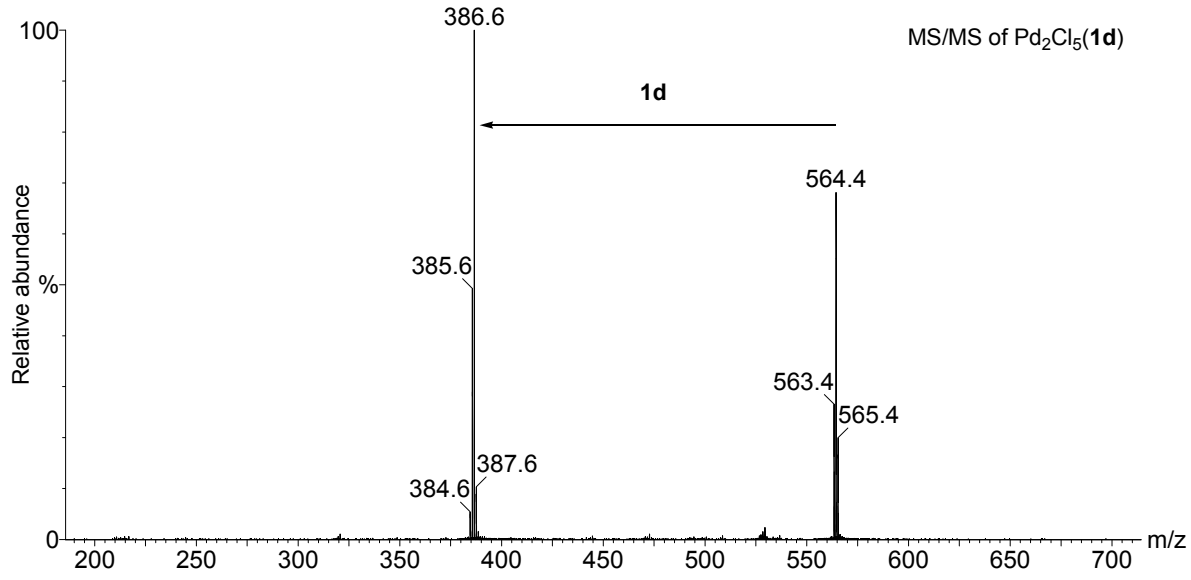


Figure S9. ESI(-)-MS/MS (15-20 eV) of $[Pd_2Cl_4(\mathbf{1a}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{1b}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{1c}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{1d}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{2a}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{2b}\text{-H})]^-$, $[Pd_2Cl_4(\mathbf{2c}\text{-H})]^-$ and $[Pd_2Cl_4(\mathbf{2d}\text{-H})]^-$.