Supporting Information

Enabling LIFDI-MS measurements of highly air sensitive organometallic compounds: A combined MS/glovebox technique

Maximilian Muhr^{# a,b}, Patricia Heiß^{# a,b}, Max Schütz ^{a,b}, Raphael Bühler ^{a,b}, Christian Gemel ^{a,b},

Mathias H. Linden^c, H. Bernhard Linden^c, Roland A. Fischer* ^{a,b}

a) Chair of Inorganic and Metal-Organic Chemistry, Department of Chemistry, Technical University Munich, Lichtenbergstrasse 4, D-85748 Garching, Germany.

b) Catalysis Research Center, Technical University Munich, Ernst-Otto-Fischer Strasse 1, D 85748 Garching, Germany.

c) Linden CMS GmbH, Auf dem Berge 25, D-28844 Weyhe, Germany.

Email: roland.fischer@tum.de

[#]M.M. and P.H. equally contributed to this work





Figure S1: Full range LIFDI mass spectrum of [(Cp)₂TiCl₂] + Zn.



Figure S2: Molecular ion peak of $[((Cp)_2TiCl)_2ZnCl_2]^+$. The spectrum was recorded under inert conditions.



Figure S3: LIFDI mass spectrum of [(Cp)₂TiCl₂] + Zn, zoomed into m/z range of 150 – 250. Major peaks in increasing m/z order: 182.9680 [(Cp)TiCl(OH)(OH₂)]⁺, 200.9354 [(Cp)TiCl₂(OH₂)]⁺, 212.9936 [(Cp)₂TiCl]⁺, 231.0054 [(Cp)₂TiCl(OH₂)]⁺, 247.9632 [(Cp)₂TiCl₂]⁺.



Figure S4: LIFDI mass spectrum of $[(Cp)_2 TiCl_2] + Zn$, zoomed into m/z range of 250 - 350.



Figure S5: LIFDI mass spectrum of $[(Cp)_2 TiCl_2] + Zn$, zoomed into m/z range of 350 - 450. Major peaks in increasing m/z order: 376.9465 $[(Cp)_3 Ti_2 Cl_2 O]^+$, 407.0148 $[(Cp)_4 Ti_2 ClO]^+$.



Figure S6: LIFDI mass spectrum of $[(Cp)_2 TiCl_2] + Zn$, zoomed into m/z range of 400 - 600. Major peaks in increasing m/z order: 542.8914 $[(Cp)_4 Ti_3 ClO_2]^+$, 570.9646 $[(Cp)_5 Ti_3 Cl_2 O_2]^+$.



Figure 7: LIFDI mass spectrum of $[(Cp)_2TiCl_2] + Zn$, zoomed into m/z range of 600 - 800.

Full range spectra of [CuMes] + AlCp*



Figure 8: Full range LIFDI mass spectrum with peak labels of [CuMes] + 3.6 eq. of AlCp*.