IR CHARACTERIZATION OF METAL MEDIATED METHANE COUPLING

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Large amounts of methane are present in natural gas, but its great stability hinders wide-spread utilization. Conversion of methane requires a suitable, often transition metal-based catalyst. However, the reaction mechanism is often only poorly understood. To get insight in fundamental chemical interactions at the highest level of detail, we study the interaction between isolated metal ions and methane. For this, we generate metal ions using laser vaporization and react them with methane in a radio-frequency ion trap. After the reaction we analyze the formed products via a combination of mass spectrometry and IR spectroscopy using the Free Electron Laser for IntraCavity Experiments FELICE. We elucidate product structures and reconstruct the reaction pathway by comparison with Density Functional Theory calculations. In this contribution we focus on methane activation by Pt^+ and Ru^+ ions. Previously, it was shown that Pt^+ ions can activate methane to form $PtCH_2^+$. Here, we show how the subsequent reaction with more methane molecules leads to dehydrogenation and C–C coupling to form ethene on both Pt^+ and Ru^+ ions.