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IRMPD spectroscopy on mass-selected metal-ligand complex ions

Many studies are devoted to functionalized metallic nanoparticles, for many applications: in Physics, due to their localized surface plasmon resonances; in Chemistry, due to their specific catalytic properties; in Biology, due to their optical or magnetic properties coupled to their potential for targeting and vectorization of bioactive molecules within living cells. In solution, the characterization of the nanoparticle –ligand interface, is often performed with NMR or IR methods but data interpretations are somewhat difficult because of the relative lack of control of the stoichiometry of nanoparticles and of their ligand coverage [1].
In a bottom-up approach, we study not nanoparticles but sub-nanometer metallic complexes or nanoclusters (one to several metal atoms and few to several ligands) that allow for a size selection with mass spectrometry, for a precise spectroscopic characterization in the gas phase and for a possible direct comparison with reliable quantum chemistry calculations. Even if these functionalized nanoclusters do not display the same structural characteristics as the larger nanoparticles, their specific chemical/physical properties are very dependent from their size and structure and they are intermediate between those of the isolated metal –ligand and those of the nanoparticles in solution [2].
We will present IR MultiPhoton Dissociation (IRMPD) spectroscopy experiments on isolated mass-selected metal-ligand ions which will be compared to Quantum Chemistry (DFT) calculations and vibrational spectra computed either at the static harmonic, static anharmonic, or molecular dynamics levels. It is indeed interesting to have a fine knowledge of the structural properties and of the chemical stabilities of those species in order to build some benchmark experimental and theoretical results that could help for larger nanoparticles characterization.
Besides metal-acetylacetonate model systems [3], we also studied gold-phosphine, gold-thioglucose and silver-acid complexes or nanoclusters [4,5] from which we will present some selected results.

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