Energetics of the Ligand and Solvent Coordination of Catalytically Important Organometallic Complexes

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Photoelectron photoion coincidence (PEPICO) spectroscopy is a marriage of photoelectron spectroscopy and mass spectrometry. Electron / ion pairs are created by single photon ionization and the two charged species are measured in delayed coincidence with each other. Ions are selected in narrow range of internal energy by collecting only ions created in delayed coincidence with the photoelectrons. Using the newly constructed imaging Photoelectron Photoion Coincidence (iPEPICO) experiment of the new VUV beamline of the Swiss Light Source synchrotron, we have embarked on a project to determine highly accurate bond energies in the gas phase, especially of metal-ligand bonds. In the first phase of the experiments, we have perfected the experimental procedure and the data analysis and have published a number of papers on the PEPICO experiments of smaller molecules as well as organometallics and have published the PEPICO data analysis software.









