SIZE SELECTIVE FAR-INFRARED SPECTROSCOPY OF TRANSITION METAL CLUSTERS IN A MOLECULAR BEAM

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Transition metal clusters are frequently used as model systems for low coordinated sites of extended surfaces and their study can provide valuable insights into the mechanisms of heterogeneous catalytic reactions. In many cases, however, there is still a lack of information on their structures and the relationship between structure and chemical behavior.

Size selective spectra of neutral and charged clusters in the gas-phase can be obtained by combining resonant photodissociation with mass spectrometric detection. This principle is used here in the far-infrared using the Free Electron Laser for Infrared eXperiments (FELIX) as an intense and widely tunable radiation source to induce multiple photon dissociation (MPD) of weakly bound complexes between the metal clusters and rare gas atoms. The far-IR spectra obtained are unique for each cluster size and are true fingerprints of the cluster's structure. The comparison with IR spectra calculated using density functional theory allows determination of their structures and to obtain insights into the growth mechanism. The capabilities of structure determination via far-IR MPD spectroscopy are demonstrated for cationic rhodium and neutral gold clusters.