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Stability of Phosphine-Ligated Gold Cluster Ions toward Dissociation: Effect of Ligand and Cluster Size[1]

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Precise control of the composition of phosphine-ligated gold clusters is of interest to their applications in catalysis, sensing, and drug delivery. Reduction synthesis in solution typically generates a distribution of ligated clusters containing different number of gold atoms and capping ligands. Ligand binding energy is an important factor determining the kinetics of cluster nucleation and growth in solution and hence the resulting cluster distribution. Phosphines are popular capping ligands with tunable electronic and steric properties that affect their binding to the gold core. We examined the effect of the number of gold atoms in the cluster and the properties of the phosphine ligand on the ligand binding energy to the gold core using surface-induced dissociation (SID) of mass selected cluster cations produced through electrospray ionization. SID of vibrationally excited ions is ideally suited for studying gas-phase fragmentation of complex ions such as ligated gold clusters. The energetics, dynamics, and mechanisms of cluster ion fragmentation in the absence of solvent are determined through RRKM modeling of time and kinetic energy dependent SID spectra. This approach provides quantitative information on the ligand binding energies in phosphine-ligated gold clusters important for understanding their formation in solution. Furthermore, ligand binding energies derived from SID data provide the first benchmark values for comparison with electronic structure calculations.

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