

Structure determination of coinage metal cluster ions by Trapped Ion Electron Diffraction

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The structures of transition metal cluster ions have been studied by the recently developed technique of trapped ion electron diffraction (TIED)¹. In brief, cluster ions are generated by a magnetron sputter source and injected into a cooled (100 K) quadrupole ion trap. After mass selection and thermalization, the trapped ions are irradiated with a 40 keV electron beam. The resulting diffraction pattern is integrated with a CCD detector. The assignment of the structural motif is done via a comparison of the experimental and simulated scattering function, calculated from density functional theory structure calculations.

The structures of mass selected silver cluster cations Ag_{19}^+ , Ag_{38}^+ , Ag_{55}^+ , Ag_{59}^+ , Ag_{75}^+ and Ag_{79}^+ have been investigated². The resulting experimental data are best described by structures based on the icosahedral motif, while closed packed structures could be ruled out. Additionally, we present a comparison of the structures of $\text{Cu}_{20}^{+/-}$, $\text{Ag}_{20}^{+/-}$ and $\text{Au}_{20}^{+/-}$. Our findings show unambiguously that the structure of Au_{20}^- is predominantly given by a tetrahedron in agreement with previous results³. In contrast, structures of Ag_{20}^- and Cu_{20}^- based on the icosahedral motif agree best with the experimental data. The possibilities and limitations of the TIED method are discussed.

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- (3) J. Li, X. Li, H. J. Zhai, and L. S. Wang, *Science* **299**, 864 (2003).