STRUCTURES OF SMALL GOLD CLUSTER IONS

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The determination of gas phase structures is a central point in cluster physics. In particular the structures of small gold cluster ions have attracted much interest recently. For gold cluster anions experiment and theory have been at odds with respect to the specific size at which the transition from 2D to 3D structures occurs. By using the recently developed technique of trapped ion electron diffraction (TIED) we show that in combination with state of the art density functional structure calculations, experiment and theory can be reconciled. For Au_{11}^- best agreement between experimental data and theoretical model is found for a planar structure. The TIED result, in good agreement with former experimental investigations[a], indicate a 2D to 3D transition at a size of 12 gold atoms. Here a mixture of essentially iso-energetic 2D and 3D structures is found. Au_{13}^- to Au_{15}^- are flat 3D structures; a new structure hitherto unknown, was found for Au_{14}^-. Hollow cage structures were found for Au_{16}^-, Au_{17}^-, and Au_{18}^-. Au_{19}^- and Au_{20}^- are tetrahedral structures. In addition structures of selected gold cluster cations in this size range are presented. Distinct differences between the anion and cation structures are observed and discussed.

[a] F. Furche et al., J. Chem. Phys., **117**, 6982 (2002)