FORMATION OF LOW ATOMIC GOLD CLUSTERS AND DETERMINATION OF THEIR BINDING ENERGIES

Juraev Gulom Gofur ugli,
Kuldoshov Alikhon Bahtiyor ugli
Termiz State University
2nd year master's degree in physics

ABSTRACT

Complexes of atomic gold with a variety of ligands have been formed by passing helium nanodroplets (HNDs) through two pickup cells containing gold vapor and the vapor of another dopant, namely a rare gas, a diatomic molecule (H2, N2, O2, I2, P2), or various polyatomic molecules (H2O, CO2, SF6, C6H6, adamantane, imidazole, dicyclopentadiene, and fullerene).

Key words: *gold complexes, clusters, ligands, mass spectrometry*

АННОТАЦИЯ

Комплексы атомарного золота с различными лигандами были образованы путем пропускания нанокапель гелия (ГНД) через две пикап-ячейки, содержащие пары золота и пары другой легирующей примеси, а именно инертного газа, двухатомной молекулы (H2, N2, O2, I2, P2), или различные многоатомные молекулы (H2O, CO2, SF6, C6H6, адамантан, имидазол, дициклопентадиен и фуллерен).

Ключевые слова: *комплексы золота, кластеры, лиганды, масс-спектрометрия.*

INTRODUCTION

Gold has fascinated mankind for several thousand years . In its bulk form it exhibits a distinct yellow color which is considerably different from most other metals that reflect the complete visible range of light and have a shiny white appearance. This yellow color is the result of a relativistic contraction of the 6s orbital . This also leads to an exceptionally high atomic ionization energy for a metal of 9.225 eV , a large electron affinity of 2.3 eV] and it explains the shorter and stronger covalent bonds of gold which makes it often behave like a heavy hydrogen atom.

DISCUSSION AND RESULTS

A pronounced maximum at n = 12 was explained by the completion of an icosahedral shell and a local maximum at n = 14 by another stable structure where

two additional helium atoms can be squeezed into the first shell, similar to HenKr+, where also n = 14 turned out to be magic [38]. Pronounced magic numbers were also reported in a subsequent study where HNDs were doped with gold vapor and another rare gas Rg (Rg = Ne, Ar, Kr or Xe) [14]. For all four noble gases, the intensity of Rg2Au+ exhibits a local maximum which agrees in the case of Ar, Kr and Xe with a covalent character of the bonding [6]. In the case of He and Ne, intensity anomalies at n = 12 indicate an icosahedral shell closure and weak physical bonding. A clear intensity drop at Ar6Au+ suggests the closure of an octahedral solvation shell. Goulart et al. studied mixed cluster ions of gold and C60 [13]. For both polarities ions of the form (C60)2Au± are particularly abundant. Density functional theory calculations suggest a sandwich like structure similar to LAuL± ions previously reported for several smaller ligands L In the present study, we extend these ligand switching reactions to heavy rare gases and molecules including the diatomic species H2, N2, O2, P2, and I2, the molecules H2O, CO2, and SF6, and the carbonaceous species C6H6, C3H4N2, C5H6 (and its dimeric form), C10H16, and C60. In the case of adamantane, benzene and C60, anionic complexes with gold were also investigated.

CONCLUSION

The subsequent chemical reactivity of gold atoms or the cations might be unexpected for a metal that does not exhibit corrosion. In the low-pressure regime of a Fourier transform ion cyclotron resonance mass spectrometer, radiative association between Au+ and C6F6 leads to a weakly bound complex that was used by Schröder et al. as a precursor to generate other complexes by ligand-exchange reactions. In combined experimental and theoretical studies, they determined the binding energy of H2O to Au+ with 1.56 eV and benzene with 3.04 eV . Besides pristine gold cluster ions Aum+, binary cluster ions of the form HenAum+ were also observed .

REFERANCES

1. Hutchings G.J., Brust M., Schmidbaur H. Gold-an introductory perspective. Chem. Soc. Rev. 2008;37:1759–1765. doi: 10.1039/b810747p. [PubMed] [CrossRef] [Google Scholar]
2. Pyykkö P. Relativistic effects in chemistry: More common than you thought. In: Johnson M.A., Martinez T.J., editors. Annual Review of Physical Chemistry. Volume 63. Annual Reviews; Palo Alto, CA, USA: 2012. pp. 45–64. [PubMed] [Google Scholar]

3. Dyubko S.F., Efremov V.A., Gerasimov V.G., MacAdam K.B. Millimetre-wave spectroscopy of Au I Rydberg states: S, P and D terms. J. Phys. B-At. Mol. Opt. Phys. 2005;38:1107–1118. doi: 10.1088/0953-4075/38/8/003. [CrossRef] [Google Scholar]
4. Hotop H., Lineberger W.C. Dye-laser photodetachment studies of Au−, Pt−, PtN−, and Ag− J. Chem. Phys. 1973;58:2379–2387. doi: 10.1063/1.1679515. [CrossRef] [Google Scholar]
5. . Kapur S., Müller E.W. Metal-neon compound ions in slow field evaporation. Surf. Sci. 1977;62:610–620. doi: 10.1016/0039-6028(77)90104-2. [CrossRef] [Google Scholar]
6. Pyykkö P. Predicted Chemical Bonds between Rare Gases and Au+ J. Am. Chem. Soc. 1995;117:2067–2070. doi: 10.1021/ja00112a021. [CrossRef] [Google Scholar]