

Au₁₀₂⁺ and Au₆X₄₂⁺ clusters: Superatomic molecules bearing an SP³-hybrid Au₆ core

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The octahedral Au₆ core is explored for the formation of novel SP³-hybrid superatomic molecules by considering Au₁₀₂⁺ and Au₆X₄₄⁺ clusters (X= F, Cl, Br, I). The bonding between the four capping atoms and the Au₆ core requires a combination of 1S and 1P shells of the core leading to a set of four equivalent hybrid orbitals. Thus, combining the superatom concept with both the Lewis structure model and VSEPR theory contributes to the rationalization of structure and bonding in metal clusters. For example, our results consider the Au₆X₄₄⁺ clusters as analogues of the simplest perhalogenated hydrocarbon, CX₄. © 2016 Wiley Periodicals, Inc.

clusters

gold

halogens

hybridization

superatoms

Gold

Orbital calculations

clusters

halogens

Hybrid orbitals

hybridization

Lewis structure

Metal cluster

Superatoms

VSEPR theory

