Evaluation of Hollow Golden Icosahedrons: Bonding and Spherical Aromatic Properties of [Au11E]3? Superatoms (E=Se and Te) from Relativistic DFT calculations, Persistent Structures?

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Two novel clusters were proposed according to the superatom model involving a favorable inclusion of Se and Te into a Au12 cage leading to [Au11E]3? clusters. Such structures retain a hollow gold-based icosahedron with spherical aromatic character, according to the 18-valence electron rule. Interestingly, it is shown that despite the favorable electronic structure and aromatic behavior, the titled structure is further found to be a local minimum in the potential surface, which exhibits a planar isomer as a plausible candidate for the lowest-energy structure. The proposed strategy employed to vary the electron count of the cage is useful for the further design of novel spherical aromatic superatoms and ligand-protected clusters, for which the main variation is generated directly in the surface of the cluster, in addition to the extensive formation of endohedral clusters with different heteroatoms. © 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim

chalcogens

gold

hollow structures

p-block elements

superatoms