

Symmetry collapse due to the presence of multiple local aromaticity in Ge₂₄⁴⁻

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Abstract

Understanding the structural changes taking place during the assembly of single atoms leading to the formation of atomic clusters and bulk materials remains challenging. The isolation and theoretical characterization of medium-sized clusters can shed light on the processes that occur during the transition to a solid-state structure. In this work, we synthesize and isolate a continuous 24-atom cluster Ge₂₄⁴⁻, which is characterized by X-ray diffraction analysis and Energy-dispersive X-ray spectroscopy, showing an elongated structural characteristic. Theoretical analysis reveals that electron delocalization plays a vital role in the formation and stabilization of the prolate cluster. In contrast with carbon atoms, 4 s orbitals of Ge-atoms do not easily hybridize with 4p orbitals and s-type lone-pairs can be localized with high occupancy. Thus, there are not enough electrons to form a stable symmetrical fullerene-like structure such as C₂₄ fullerene. Three aromatic units with two [Ge₉] and one [Ge₆] species, connected by classical 2c-2e Ge-Ge σ -bonds, are aligned together forming three independent shielding cones and eventually causing a collapse of the global symmetry of the Ge₂₄⁴⁻ cluster. © 2022, The Author(s).