

Spin-orbit effect into isomerization barrier of small gold Clusters. Oh ? D2h

Fluxionality of the Au₆²⁺ cluster Investigated by relativistic methods

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The Oh-[Au₆]²⁺ cluster exhibits an open-shell 1s²1p² which trend to a more stable D_{2h} isomer in 31.5 kcal/mol, as observed in the experimental [Au₆{P(C₆H₄Me-o)pH₂}₆] cluster. By taking into account the spin-orbit coupling (SOC) in Oh-[Au₆]²⁺, a resulting 1s_{1/2}²1p_{1/2}² closed-shell superatomic configuration is obtained stabilizing such structure by about 14.7 kcal/mol, decreasing the isomerization barrier. Thus, the spin-orbit term favors the Oh ? D_{2h} conformation rearrangement depicting a decrease in the calculated energy difference between both conformations, an interesting consequence which is not obtained in the hypothetical lighter counterparts. © 2017 Elsevier B.V.

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