

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Probing the existence of energetically degenerate cluster isomers by chemical tagging QIAN WANG, Virginia Commonwealth University, QIANG SUN, PURU JENA — Current methods for identifying the ground state geometry of a cluster require synergy between theory and experiment. However, this becomes a difficult problem when the accuracy of the theoretical methods is not sufficient to distinguish between nearly degenerate isomers. Using density functional theory based calculations we show that the near degeneracy between the planar and cage structures can be lifted by tagging these with halogens and superhalogens moieties such as Cl and BO₂. The energy of the planar Au₁₆⁻ isomer is lowered from 0.15 eV before tagging to 0.51 ~ 0.55 eV after tagging, thus providing a way to probe its coexistence.

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Date submitted: 19 Nov 2010

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