Predicting the Photoelectron Spectra of Quasi Octahedral Al_6Mo^- Cluster

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Abstract

We have recently developed a computational methodology to separate the effects of size, composition, symmetry and fluxionality in explaining the experimental photoelectron spectra of mixed-metal clusters. This methodology was successfully applied first in explaining the observed differences between the spectra of Al_{13}^- and $Al_{12}Ni^-$ and more recently to explain the measured spectra of Al_nMo^-, n=3-5,7 clusters. The combination of our approach and new synthesis techniques can be used to prepare cluster based materials with tunable properties. In this work we use the methodology to predict the spectrum of Al_6Mo^-. This system was chosen because its neutral counterpart is a perfect octahedron and it is distorted to a D_{3d} symmetry and was not observed in the recent experiments. This high symmetry cluster bridges the less symmetric Al_5Mo^- and Al_7Mo^-structures. The measured spectra of Al_5Mo^- has well defined peaks, while that of Al_7Mo^-does not. This can be explained by the fluxionality of Al_7Mo^-, as at least 6 different structures lie within the range that can be reached by thermal effects. We predict that Al_6Mo^- has well defined peaks, but some broadening is expected as there are two low-lying isomers, one of D_{3d} and the second of D_{3h} symmetry that are only 0.052 eV apart.

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