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Title: Possible Precursors of Endohedral-Metallofullerene

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Abstract:

Metal-carbon binary clusters generated by the laser-vaporization cluster beam-source were directly injected and tested with the FT-ICR mass-spectrometer. In order to probe the structure of clusters appearing in mass spectra, reactivity of negative carbon clusters and metal-carbon binary clusters to nitric oxide were examined. Systematic experiments showed that odd-numbered empty carbon clusters were much more reactive than even-numbered clusters. Furthermore, carbon clusters with La atom such as LaC_{44}^- were very much unreactive to NO. The reactivity of clusters contaminated with a hydrogen atom was very curious. One hydrogen atom made odd-numbered clusters less reactive and even-numbered clusters more reactive. These experimental results were perfectly explained by a consideration of number of dangling bonds based on the random-raged geometric structure predicted by the molecular dynamics simulations. Even-numbered carbon cage can be well annealed to non-dangling-bond caged structure that is not necessarily made of only pentagons and hexagons.