Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Geometry and Electronic Structure of Nickel Benzene Complexes

A. K. KANDALAM, S. N. KHANNA, PURU JENA, Virginia Commonwealth University — A synergistic approach combining the negative ion photo- detachment spectroscopy and the first principles density functional calculations is used to probe the geometrical structure, nature of electronic bonding and the magnetic moment of anionic and neutral nickel- benzene (Bez) complexes. It is shown that, contrary to the previously published results, the ground state of a Ni-Bez anion is a structure where the Ni atom is inserted in one of the C-H bonds of the benzene molecule. However, a detailed investigation of the reaction barrier shows that this ground state may be inaccessible in ordinary experiments and the observed structures in negative ion photo- detachment spectra may be the higher energy structure where a Ni atom occupies a hollow site above the benzene molecule. The stability of inserted structures in multiple Ni-Bez complexes and how they may be attained in carefully planned experiments will be highlighted.

Anil Kandalam
Virginia Commonwealth University

Date submitted: 29 Nov 2004 Electronic form version 1.4