

A THEORETICAL SEARCH FOR AN ELECTRONIC SPECTRUM OF THE He-BeO COMPLEX

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The surprisingly high dissociation energy of the He-Be bond in the He-BeO complex was first reported 25 years ago.^a Following which, a number of theoretical studies have investigated similar closed shell helium containing complexes. However, despite these investigations, a complex containing a strong He-X bond has thus far eluded experimental detection. In this work, potential energy surfaces of electronically excited states of the He-BeO complex have been calculated employing high level CASSCF+MRCI+Q methodologies and utilizing extended basis sets. Several excited states show strong interactions between helium and BeO lying in Franck-Condon accessible windows of electronic transitions arising from the vibrationless electronic ground state. It is hoped that the conclusions of this study will result in the observation an electronic spectrum of this long hypothesized strongly bound complex in the near future.

^aW. Koch, J. R. Collins and G. Frenking, *Chem. Phys. Lett.* 1986, **132** 330-333.