A coupled cluster study of the stability of lithium clusters. Foerner, Wolfgang; Seel, Max

Abstract

Coupled-cluster studies on Li2, on the Li6 ring, and on other Li6 clusters are reported. In its linear approxn., the coupled-cluster method gives a larger fraction of the correlation energy for Li2 than the nonlinear version, although other phys. properties like force consts. and bond lengths are described unsatisfactory. The planar Li6 ring was predicted to be stable in the equidistant form. Larger rings tend to have a Peierls-distorted alternant geometry on the Hartee-Fock level. Thus, Li behaves somewhat similar to (CH)n; while for Hn, also the n = 6 ring is distorted. The stability of equidistant six-membered rings was therefore attributed to the existence of rather delocalized 2s-electrons. Comparison of the results for Li6 clusters having different symmetries (D6h, Oh, C5v) with similar calcns. reported in the literature indicated that the inclusion of p-functions is essential; whereas, the size of the s-function subspace is not very important.