HeI PHOTOELECTRON SPECTROSCOPY AND ELECTRONIC STRUCTURE OF ALKYL-LITHIUM CLUSTERS

G. TARCZAY, G. VASS, G. MAGYARFALVI, and L. SZEPES, *Department of General and Inorganic Chemistry, Eötvös University, P.O. Box 32, H-1518 Budapest 112, HUNGARY.*

HeI photoelectron spectra of some alkyl-lithium tetrameric and hexameric clusters have been recorded. In the low energy region (ca. 6.0-9.0 eV) bands have been assigned to ionization from the Li-C cluster orbitals. Ionization from the triply and doubly degenerate orbitals of the tetramers (T_d symmetry) and hexamers (D_{3d} symmetry), respectively, causes Jahn-Teller (JT) distortion of the clusters. *Ab initio* quantum chemical calculations have been performed to understand the nature and extent of the JT distortions.