THRESHOLD IONIZATION OF La(C₅H₈) FORMED BY La-MEDIATED DEHYDROGENATION OF 1-PENTENE

WENJIN CAO, YUCHEN ZHANG, DONG-SHENG YANG, Department of Chemistry, University of Kentucky, Lexington, KY, USA.

 $La(C_5H_8)$ was formed by La reaction with 1-pentene (CH_2 =CH- CH_2 - CH_3) in a laser-vaporization supersonic molecular beam source and characterized with mass-analyzed threshold ionization (MATI) spectroscopy. The MATI spectrum displays an origin band at 38988 (5) cm⁻¹ and three vibrational intervals of 130, 294, and 415 cm⁻¹. The $La(C_5H_8)$ complex is identified as a five-membered metallacycle in C_1 point group, with the doublet and singlet being the lowest energy states of the neutral and cation, respectively. The energy at 38998 cm⁻¹corresponds to the adiabatic ionization energy of the complex, and the three vibration intervals in the order of the frequency increase are assigned to the terminal CH_3 torsion, asymmetric La-ligand stretch, and symmetric La-ligand stretch excitation of the ion. The La+1-penetene reaction will also be compared with La reactions with other five-carbon hydrocarbon molecules, such as isoprene, 1-pentyne, and 1,4-pentadiene.