C-C BOND ACTIVATION AND COUPLING OF PROPENE INDUCED BY LA ATOM

DILRUKSHI HEWAGE, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*; HONG TAO, *Department of Chemistry, Southwest Forestry University, Kunming 650224, PR China*; RUCHIRA SILVA, SUDESH KUMARI, AND DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055.*

A series of La(C_nH_m) complexes with n $\leq$ 6 and m $\leq$ 12 were produced by the reactions between propene and La in a supersonic molecular beam source. Their formation and structures were investigated using mass-analyzed threshold ionization (MATI) spectroscopy in combination with theoretical calculations. Previously, we identified the formation of La(C_3H_4) and H-La(C_3H_5) through dehydrogenation and metal insertion mechanisms. In this work, we will discuss the formation of La(CH_2) and La(C_4H_6) by La induced C-C bond activation and coupling. La(CH_2) is formed by the C-C bond breakage and 1,2-hydride shift of propene and is a Schrock-type carbene complex. This complex is then coupled with the C=C bond of a second propene molecule to form La(C_4H_6) by removing two hydrogen atoms. The resultant La(C_4H_6) complex was idetified in two low-energy isomeric forms: one was a metallacycle (isomer A) and the other was lanthanum trimethylenemethane (isomer B). Both La(C_4H_6) isomers are in a doublet ground state, with isomer A in C_s point group and isomer B in C_{3v}. Adiabatic ionization energies and several vibrational frequencies of the two complexes were obtained from the sharp MATI spectra.