DEHYDROGENATION AND C-H BOND INSERTION OF PROPENE: $La(\eta^2-C_3H_4)$ AND $HLa(\eta^3-C_3H_5)$

<u>SUDESH KUMARI</u> and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexing*ton, KY 40506-0055.

Dehydrogenation and C-H bond insertion are observed in the reaction of laser-ablated La atoms with propene (C_3H_6) in a pulsed molecular beam source. Several dehydrogenated and inserted products are identified by the time-of-flight mass spectrometry. La(C_3H_4) formed from H₂ elimination and HLa(C_3H_5) formed by C-H bond insertion are characterized by pulsed-field-ionization electron and ion spectroscopy, in combination with density functional theory. Two isomers of La(C_3H_4) are identified from 1,2- and 1,3-dehydrogenation. The adiabatic ionization energies of 1,2- and 1,3-dehydrogenated isomers are measured to be 40506(5) and 40941(5) cm⁻¹, respectively. For the inserted product HLa(C_3H_5), La atom is bound to the allyl radical in a three-fold binding mode (η^3). It is observed that the ionization energy of the HLa(η^3 -C₃H₅) insertion complex (41130(5) cm⁻¹) is close to that of the 1,3-dehydrogented La(η^2 -C₃H₄) species.