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

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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 H_2 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-C_3H_5) insertion complex (41130(5) cm^{-1}) is close to that of the 1,3-dehydrogented La(η^2-C_3H_4) species.