OBSERVATION OF TWO La(C_3H_2) ISOMERS FORMED BY DEHYDROGENATION OF PROPYNE

DILRUKSHI HEWAGE, MOURAD ROUDJANE, and DONG-SHENG YANG, *Department of Chemistry, University of Kentucky, Lexington, KY 40506-0055*.

C-H bond activation of small hydrocarbons is of importance in chemistry and industrial applications. La(C_3H_2) was formed by the reaction of laser-ablated La atoms and propyne (C_3H_4) in supersonic molecular beams. Two isomers of La(C_3H_2) were detected for the first time by mass-analyzed threshold ionization (MATI) spectroscopy. From the MATI spectra, the two isomers exhibit origin bands at 42953(5) and 43609(5) cm^{-1} and vibrational intervals of 425 and 535 cm^{-1}, respectively. They were identified as La($CCCH_2$) formed from 1,3-dehydrogantion and La(HCCCH) formed by 3,3-dehydrogenation and were confirmed by measurements with deuterium substituted propyne (C_3D_4) as the precursor. The 1,3-dehydrogenated complex shows a higher ionization energy and larger metal-ligand stretching frequencies than the 3,3-dehydrogenated species. Based on DFT/B3LYP calculations, the electronic transitions responsible for the observed MATI spectrum of La(HCCCH)isomer is $^1A \leftarrow {}^2A$,and that of La($CCCH_2$)isomer is $^1A' \leftarrow {}^2A'$.