YTTRIUM-ASSISTED C-H AND C-C BOND ACTIVATION OF ETHYLENE PROBED BY MASS-ANALYZED THRESHOLD IONIZATION SPECTROSCOPY

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The reaction between Y atom and ethylene (CH_2=CH_2) was performed in a laser-ablation supersonic molecular beam source. Y(C_2H_2), Y(C_2H_4), and Y(C_4H_6) were observed by time-of-flight mass spectrometry and investigated with mass-analyzed threshold ionization (MATI) spectroscopy and theoretical calculations. Y(C_2H_2) is formed by hydrogen elimination, Y(C_2H_4) by simple association, and La(C_4H_6) by C-C bond coupling and dehydrogenation. Both Y(C_2H_2) and Y(C_2H_4) have a C_{2v} triangular structure with a C=C double bond in Y(C_2H_2) and a C-C single bond in Y(C_2H_4). Y(C_4H_6) has a five-membered metallacyclic structure (C_s) with Y binding to the two terminal carbon atoms of butene, which is the exactly same as that of Y(C_4H_6) formed in the Y + 1-butene reaction. For all three complexes, ionization has a small effect on the metal-carbon bond lengths because the rejected electron has basically a Y 5s character. The adiabatic ionization energies are measured to be 45679(5) $\mathrm{cm}^{-1}$for Y(C_2H_2), 45603(5) $\mathrm{cm}^{-1}$for Y(C_2H_4) and 43475(5) $\mathrm{cm}^{-1}$for Y(C_4H_6). The metal-ligand stretching frequencies of the three complexes are also measured from the MATI spectra.