

## Ce-PROMOTED BOND ACTIVATION OF PROPENE PROBED BY MASS-ANALYZED THRESHOLD IONIZATION SPECTROSCOPY

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The reaction of Ce + propene ( $\text{CH}_2=\text{CH}-\text{CH}_3$ ) was carried out in a laser-ablation supersonic molecular beam source.  $\text{CeC}_2\text{H}_2$ ,  $\text{CeC}_3\text{H}_4$ ,  $\text{CeC}_3\text{H}_6$ ,  $\text{CeC}_4\text{H}_6$ ,  $\text{CeC}_6\text{H}_{10}$ , and  $\text{CeC}_6\text{H}_{12}$  were identified by photoionization time-of-flight mass spectrometric measurements, and their structures and electronic states were investigated with mass-analyzed threshold ionization (MATI) spectroscopy and theoretical calculations. The metal complexes containing two or three carbon atoms were formed by the C-C bond breakage ( $\text{CeC}_2\text{H}_2$ ), dehydrogenation ( $\text{CeC}_3\text{H}_4$ ), or metal insertion into a C-H bond ( $\text{CeC}_3\text{H}_6$ ) of a propene molecule. The larger complexes with four to six carbons are formed through secondary reactions involving C-C bond coupling and dehydrogenation. The ground electronic states of the neutral  $\text{CeC}_2\text{H}_2$ ,  $\text{CeC}_3\text{H}_4$ ,  $\text{CeC}_3\text{H}_6$ , and  $\text{CeC}_4\text{H}_6$  complexes are triplets with a  $4f^1 6s^1$  electron configuration on the Ce center, and those of the corresponding ions are doublet with a  $4f^1$  configuration. Their MATI spectra are much more complex than those of the corresponding La species formed in the La + propene reaction previously observed by our group. The spectral complexity arises from possibly multiple electronic transitions due to the existence of a 4f electron of the Ce atom which could be located in any one of the seven f-atomic orbitals or involved in considerable spin-orbit interactions.