

CYCLOPOLYMERIZATION OF ACETYLENE TO BENZYNE AND NAPHTHALENE

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Reactions of acetylene (C_2H_2) with laser-vaporized La atoms produced $La(C_6H_4)$ and $La(C_{10}H_8)$ in supersonic molecular beams. The organic fragments in these complexes were benzyne and naphthalene. The benzyne species was produced by the La-mediated cyclotrimerization of three acetylene molecules, whereas naphthalene was formed likely by the cyclization of the transient benzyne with two additional acetylene molecules. These cyclized products were identified by mass-analyzed threshold ionization mass spectroscopy, which measured adiabatic ionization energies and several vibrational frequencies. The measured ionization energies were $40875(5) \text{ cm}^{-1}$ for $La(C_6H_4)$ and $36767(5) \text{ cm}^{-1}$ for $La(C_{10}H_8)$. The most active vibrational transitions of both complexes were metal-ligand stretching with 326 cm^{-1} for $La(C_6H_4)$ and 286 cm^{-1} for $La(C_{10}H_8)$. By combining the spectra with theoretical calculations, the ground electronic states of the neutral complexes were determined to be $^2A_1(C_{2v})$ and $^2A'(C_s)$ and those of the corresponding ions were $^1A_1(C_{2v})$ and $^1A'(C_s)$ for $La(C_6H_4)$ and $La(C_{10}H_8)$, respectively.