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) cm^{-1} for La(C_6H_4) and 36767 (5) 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.