FOURIER TRANSFORM INFRARED AND DENSITY FUNCTIONAL THEORY STUDIES OF THE VIBRATIONAL FUNDAMENTALS AND STRUCTURES OF Ge_n CLUSTERS TRAPPED IN SOLID Ar

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Fourier transform infrared measurements on germanium clusters formed by trapping in solid Ar at 12 K the products from the ablation of Ge rods using a Nd-YAG laser are being carried out in conjunction with density functional theory calculations on Ge_n structures, vibrational fundamentals, and isotopic shifts. Overlapping isotopic shifts from the large number of naturally occurring Ge isotopes complicate the FTIR spectra. Positive identification of the Ge_n species responsible, assignment of their vibrational fundamentals, and determination of their structures therefore depend on comparison of the observed FTIR spectra with simulated spectra based on DFT predictions. Structures of Ge_n clusters are compared with the structures previously determined for their Si_n counterparts.