VIBRATIONAL FUNDAMENTALS OF GeC_n CHAINS TRAPPED IN SOLID ARGON

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Experimental and theoretical studies on the structures and vibrational fundamentals of a novel family of germanium-carbon clusters (Ge_nC_m) that were initiated with our earlier identification of the GeC_3Ge cluster [a] have now been extended to include GeC_n chains. The new clusters, which are formed by the Nd-YAG laser ablation of germanium and graphite and are trapped in solid Ar at 10 K, have been identified using Fourier transform infrared (FTIR) measurements coupled with density functional theory calculations (DFT). The assignment of carbon stretching fundamentals for GeC_4, GeC_7, and Ge_9 will be discussed. FTIR measurements of ^{13}C isotopic shifts for the assignments are in good agreement with the DFT predictions.

[a] D. L. Robbins, C. M. L. Rittby, and W. R. M. Graham, J. Chem. Phys. 114, 3570 (2001).