FTIR AND DFT STUDIES OF NOVEL GERMANIUM-CARBON AND MIXED GERMANIUM-SILICON-CARBON CLUSTERS

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The vibrational fundamentals and structures of novel germanium-carbon and mixed germanium-silicon-carbon clusters, formed by laser ablation and trapped in solid Ar, are currently under investigation. [a] Vibrational fundamentals and ground state geometries are characterized by comparison of Fourier transform infrared measurements of vibrational frequencies and ^{13}C isotopic shifts for the matrix isolated clusters with the predictions of density functional theory (DFT). Linear GeC_3Si has been detected, the first $Ge_jC_mSi_n$ species to be observed optically, and its ν_1 fundamental identified at 1939.0 cm^{-1}. The results are in excellent agreement with DFT predictions. Additional results and assignments for Ge_nC_m clusters will be reported.

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