

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 ¹³C isotopic shifts for the matrix isolated clusters with the predictions of density functional theory (DFT). Linear GeC₃Si 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.

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