FTIR AND DFT STUDIES OF GERMANIUM-CARBON CLUSTERS

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Fourier transform infrared studies have been intiated on germanium-carbon clusters formed by laser ablation and trapped in solid Ar. The determination of structures and vibrational fundamentals is facilitated by comparison of fudamental frequencies and isotopic shifts with the predictions of density functional theory calculations which are being carried out in concert with the experimental measurements. Of particular interest are comparisons with the previously reported structures and vibrations of a large number of related silicon-carbon clusters. [a]

[a] X.D. Ding, S.L. Wang, C.M.L. Rittby, and W.R.M. Graham J. Chem. Phys. 110, 11214 (1999) and references therein.