FTIR AND DFT STUDIES OF NOVEL,SMALL GERMANIUM-CARBON CLUSTERS

D.L.ROBBINS,C.M.L.RITTBY, and W.R.M.GRAHAM, *Department of Physics and Astronomy, TCU, Fort Worth, TX 76129.*.

The vibrational fundamentals and structures of germanium-carbon clusters formed by laser ablation and trapped in solid Ar, are currently under investigation. The determination of the ground state geometries and vibrational fundamentals are facilitated by the comparison of frequencies and ^{13}C isotopic shifts measured by Fourier transform infrared spectroscopy with the predictions of density functional theory. The identification of the ν_3 fundamental of linear GeC_3Ge at 1920.7 cm^{-1} has been made,[a] and the results of further calculations and assignments will be reported.

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