INFRARED OBSERVATION OF THE $\nu_2(\sigma)$ STRETCHING MODE OF LINEAR GeC_3

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GeC_3Ge was first[1] produced by dual laser ablation of germanium and carbon rods, and the $\nu_3(\sigma_u)$ stretching fundamental was assigned at 1920.7 cm^{-1}. Later work[2] enhanced the production of the molecule via laser ablation of a single, sintered germanium-carbon rod, thus enabling the identification of two additional infrared active vibrational fundamentals $\nu_4(\sigma_u)$=735.6 cm^{-1} and $\nu_6(\pi_u)$=580.1 cm^{-1}. In the present work using the same technique, GeC_3 trapped in solid Ar at $\sim$10 K has been observed by FTIR spectroscopy . Comparison of ^{13}C isotopic shift measurements with the predictions of density functional theory (DFT) calculations at the B3LYP/cc-pV(D,T)Z level confirm the identification of the $\nu_2(\sigma)$ stretching fundamental at 1279.6 cm^{-1}.

[1] D.L. Robbins, C.M.L. Rittby, and W.R.M. Graham, J. Chem. Phys. **114**, 3570 (2001).
[2] E. Gonzalez, C.M.L. Rittby, and W.R.M. Graham, J. Chem. Phys. in press.