

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

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GeC_3Ge was first¹ 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 work² 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 $\nu_4(\sigma_u)=735.6\text{ cm}^{-1}$ and $\nu_6(\pi_u)=580.1\text{ cm}^{-1}$. In the present work using the same technique, GeC_3 trapped in solid Ar at $\sim 10\text{ K}$ 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.