FTIR ISOTOPIC STUDY OF C-C STRETCHING MODES OF THE C_{12} CHAIN TRAPPED IN SOLID Ar

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The increasing length of carbon chains, which are being investigated, makes detailed isotopic studies to test vibrational assignments progressively more difficult. The large number of overlapping isotopomer bands resulting from ^{13}C enrichment can make unambiguous assignments problematical. We report here the results of an investigation of the linear C_{12} produced by laser ablation of graphite and trapped in solid Ar. The Fourier transform infrared spectrum is simplified by limiting the isotopomers produced to those with single ^{13}C substitutions. Comparison of measured frequencies and isotopic shifts with the results of density functional theory calculations at the B3LYP/cc-pVDZ level has resulted in the identification of the ν_8 = 1997.2 cm^{-1} and ν_9 = 1818.0 cm^{-1} stretching modes, with very good agreement between experiment and theory. Since bands close to these frequencies had previously been reported in Ne matrices and assigned to the anion, the Ar measurements have also been compared to DFT predictions and simulated spectra for C_{12}^-.