

COMBINATION BANDS OF SMALL CARBON CLUSTERS: AN ISOTOPIC INFRARED STUDY

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The $^{12,13}\text{C}$ isotopic substitution method applied to IR absorption spectra has been successful in identifying the size and the geometry of many molecular systems, including carbon clusters.^a Using this method we obtained ^{13}C -labeled IR spectra in the $\nu > 2200\text{ cm}^{-1}$ region for linear carbon clusters isolated in an Ar matrix. By comparison to the calculated isotopomer frequencies at the B3LYP/6-31G* level, the observed bands have been assigned to combination modes of $^{12,13}\text{C}_n$ clusters. In addition, from these combination band frequencies the few symmetrical mode vibrations in the linear C_n ($n < 10$) clusters have been deduced.

^aA. Van Orden and R. J. Saykally, Chem. Rev. 98, 2313 (1998), and references therein.