FTIR OBSERVATION AND DFT STUDY OF THE AlC_3 and AlC_3Al LINEAR CHAINS TRAPPED IN SOLID Ar

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The vibrational spectra of linear AlC_3 and AlC_3Al were observed after trapping the products of the dual laser evaporation of aluminum and carbon rods in solid Ar at $\sim$10 K. Fourier transform infrared (FTIR) measurements of ^{13}C isotopic shifts are in good agreement with the predictions of density functional theory (DFT) B3LYP/6-311G+(3*df*) calculations and have enabled the first identification of the $\nu_3(\sigma_u)$=1624.0 and $\nu_4(\sigma_u)$=528.3 cm^{-1} fundamentals of linear AlC_3Al and the tentative assignment of the $\nu_2(\sigma)$=1210.9 cm^{-1} fundamental of linear AlC_3.