STEP-SCAN FOURIER TRANSFORM INFRARED ABSORPTION SPECTROSCOPY OF CUBIC SOLID ACETYLENE CLUSTERS

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The infrared spectra of large acetylene clusters formed in pulsed supersonic jets have been measured in the 800-5000 cm^{-1}region using step-scan Fourier transform infrared (FTIR) absorption spectroscopy.[a] The ν_3 band of $\mathrm{C_2H_2}$ cluster was reproduced well by two Lorentzian profiles peaked at 3234 and 3241 cm^{-1}. From comparison with the spectral positions of small clusters and two solid phases in the C-H stretching region, the 3234 cm^{-1}band was assigned to the solid in the high temperature cubic phase. Another feature is invariant at 3241 cm^{-1}under various supersonic jet conditions and is therefore likely attributed to the large clusters with stable structure. The relative intensity for monomer vibration-rotation lines gives the rotational temperature of 12 K at 10% $\mathrm{C_2H_2}$ in Ar. The infrared absorption band of $\mathrm{C_2D_2}$ clusters has also been measured at 2399 cm^{-1}. The deuterium isotopic shift is in good agreement with the predictions based on the harmonic oscillator model and confirms the assignment of cubic $\mathrm{C_2H_2}$ and $\mathrm{C_2D_2}$. This is the first infrared observation of cubic solid $\mathrm{C_2D_2}$. Although the experimental data do not allow us to estimate the precise size of cubic acetylene clusters, the cluster size is likely to be $\sim$10 nm.

[a] S. Hirabayashi and Y. Hirahara, *Chem. Phys. Lett.* **361**, 265 (2002).