

DETECTION OF TWO ISOMERS OF THE CYANOVINYL RADICAL: H₂CCCN AND CHCHCN BY FTMW SPECTROSCOPY

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The cyanoviny radical has been proposed to play important roles in the interstellar chemistry of neutral-neutral reactions and the combustion chemistry of heavy fuels. However, no spectroscopic study was available before. We have observed two isomers of this carbon chain form: H₂CCCN and CHCHCN in their X^2A' states with a Fourier transform microwave spectrometer, generating them in a pulsed-discharge nozzle with the CH₃CN/Ar or CH₂CHCN/Ar gas mixtures. The rotational constants from the observation are in good agreement with the values from *ab initio* calculations (RCCSD(T)/cc-PVTZ) by one percent. The observed spectra of both isomers showed very complicated patterns due to the comparable order of magnitude for the spin-rotation interaction and the nuclear hyperfine interactions from the three nuclei H and N, which made the traditional way of assignment incapable. An approach of maximizing a cross-correlation between experimental and simulated spectra has been applied to the assignment of the missing spectra. Result and progress will be presented.