ROTATIONAL SPECTROSCOPY AND CONFORMATIONAL STUDIES OF 4-PENTYNENITRILE, 4-PENTENENITRILE, AND GLUTARONITRILE

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The pure rotational spectra of 4-pentynenitrile, 4-pentenenitrile, and glutaronitrile were acquired using chirped pulse Fouirer transform microwave spectroscopy. 4-pentynenitrile and 4-pentenenitrile are the recombination products of two resonance stabilized radicals, propargyl + cyanomethyl or allyl + cyanomethyl, respectively, and are thus anticipated to be significant among the more complex nitriles in Titan's atmosphere. Indeed, these partially unsaturated alkyl cyanides have been found in laboratory analogs of tholins and are also expected to have interesting photochemistry. The optimized structures of all conformers below predicted energies of 500 cm^{-1}were calculated for each molecule. Both of the conformers, trans and gauche, for 4-pentynenitrile have been identified and assigned. Five conformers were assigned in 4-pentenenitrile. The eclipsed conformers, with respect to the vinyl group, dominate the spectrum but some population was found in the syn conformers including the syn-gauche conformer, calculated to be 324 cm^{-1}above the global minimum. The glutaronitrile spectrum contained only the two conformers below 500 cm^{-1}, with reduced amount of the gauche trans conformer. The assigned spectra and structural assignments will be presented.