HIGH RESOLUTION INFRARED SPECTROSCOPY OF AZIRIDINE-2-CARBONITRILE ($C_3H_4N_2$)

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Molecular parity violation has been critically discussed in relation to biomolecular homochirality in the early evolution of life [a]. In this context molecules of potential importance for prebiotic chemistry like the small, chiral three-membered heterocyclic molecule aziridine-2-carbonitrile (2-cyanoaziridine) are of interest [b]. Indeed, this molecule has been previously examined [c] and the parity violating energy difference between the enantiomers in their ground state has also been calculated [d]. Molecular parameters for the ground state of this molecule are available from earlier microwave studies [e], and its conformations have been examined by $ab\ initio$ theory [f]. Here we report initial results of a high resolution spectroscopic study of cyanoaziridine, carried out at room temperature with an instrumental resolution of 0.0011 cm^{-1} in the 800-1000 cm^{-1} region using the Bruker IFS125 Zurich Prototype (ZP2001) Fourier transform spectrometer [g]. Transitions in the ν_{15} and ν_{16} bands have been assigned, and molecular parameters have been determined using the Watson Hamiltonian. Simulations performed using these parameters reproduce the observed spectra well. The results are discussed in relation to astrophysical spectroscopy and recent efforts on parity violation in chiral molecules [h].

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