

HIGH RESOLUTION INFRARED SPECTROSCOPY OF CYANO-OXIRANE (c-C₂H₃OCN)

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Oxiranecarbonitrile (cyano-oxirane, c-C₂H₃OCN) is of interest as a possible chiral precursor molecule of evolution^a. We have calculated parity violation in this molecule^b in view of possible experiments and biomolecular homochirality^c. The spectrum of the molecule has been investigated in the millimeter, submillimeter^d and terahertz^e regions. Here we report high resolution (0.0011 cm⁻¹) measurements of the infrared spectrum of this molecule at room temperature using the Zurich Prototype ZP 2001 FTIR Spectrometer, and a rovibrational analysis of about two thousand transitions associated with the ν_{12} (915.3 cm⁻¹) and ν_{13} (848.2 cm⁻¹) fundamentals using a Watson Hamiltonian and the WANG program^f, including also molecular parameters and ground state energies from our work in the THz region^e. Accurate spectroscopic parameters were obtained. The results are discussed in relation to astrophysical spectroscopic searches and the evolution of biomolecular homochirality^g.

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