MICROWAVE AND MILLIMETER WAVE SPECTRUM OF STYRENE OXIDE C₆H₅C₂H₃O

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Ever-increasingly complex molecules are being searched for in the interstellar medium, and following the detections of propylene oxide a and benzonitrile b, chiral and aromatic molecules are becoming appealing targets for laboratory studies and interstellar searches. The chiral molecule styrene oxide (C₆H₅C₂H₃O), also known as phenyloxirane, is an epoxide (R – C₂H₅O) with a phenyl ring as the (-R) substituent. With a single conformer and a permanent dipole moment of about 1.8 Debye, styrene oxide emerges as an interesting chiral molecule for astrochemical investigations. We investigated the microwave and millimeter wave spectrum of styrene oxide and analysed the ground-state rotational spectrum as well as rotational transitions from low-energy vibrationally excited states. Chirped-pulse Fourier-transform microwave and millimeter-wave spectroscopy and frequency modulation absorption spectroscopy were used to record spectra in the regions of 2-12 GHz, 75-110 GHz, 170-220 GHz, and 260-330 GHz. From the spectral analysis, a set of precise rotational and centrifugal distortion parameters up to the sextic order was obtained. Our accurate predictions of styrene oxide into the (sub-)millimeter range are mandatory for radio astronomy searches with state-of-the-art observational facilities, such as ALMA. In addition, we assigned the spectra of all singly-substituted ¹³C and ¹⁸O isotopologues, which allowed us to determine the gas phase structure of the molecule experimentally.