MILLIMETER-WAVE SPECTRUM OF ISO-PROPANOL

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With the aim of astronomical observation, the millimeter-wave spectrum of *iso*-propanol has been observed in the 100-370 GHz region with the FASSST spectrometer. Over 11000 transitions within three torsional substates and between two *gauche* substates have been successfully assigned up to J'' = 68 with the CAAARS program. The rotation of the hydroxyl portion gives *iso*-propanol three stable configurations labeled *trans*, *gauche* and *gauche*' corresponding to the dihedral angle of H-C-O-H. The two equivalent *gauche* forms interact through tunneling to split the degeneracy in energy. The resulting torsional substates can be characterized by the labels *gs* (symmetric *gauche*) and *ga* (anti-symmetric *gauche*). Previous microwave and infrared spectroscopic studies concluded that *gs* is the global minimum and *trans* is the highest in energy. In our new simultaneous fit of *gs* and *ga* data using a two-state Hamiltonian, it was necessary to include up to fifth-order torsion-rotation interaction terms as well as sextic centrifugal distortion terms to analyze the millimeter-wave spectrum of *iso*-propanol. The lease-square fit of *gauche* resulted in a RMS of 88 kHz. The *trans* substate was analyzed with a rotational Hamiltonian for a quasi-rigid molecule with up to sextic centrifugal distortion terms with a RMS of the fit 63 kHz. Despite a number of theoretical studies as well as experimental work, the torsional energy of the *trans* conformer has not yet been determined because of a lack of direct measurements of torsional transitions between the *trans* and *gauche* substates. We estimated the *trans-gauche* energy separation from relative intensity data.