MILLIMETER WAVE SPECTRUM OF N-PROPANOL IN THE GAUCHE-TRANS CONFORMER

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Recent millimeter-wave studies of ethanol with the FASSST apparatus have allowed further identification of strong interstellar lines. Propanol, C₃H₇OH, is the next largest alcohol after ethanol and is expected to be detected in high-mass star-forming regions. We have measured the millimeter wave spectrum of n-propanol in the region of 100 – 380 GHz with the FASSST spectrometer. N-propanol has five non-equivalent conformers, labeled Tt, Tg, Gt, Gg, and Gg’. The capital letter T (trans) or G (gauche) corresponds to the dihedral angle of CCCO, and the lower case designation to the dihedral angle of CCOH. As a result of the existence of five conformers, some of which are expected to be split due to hydroxyl and/or methyl top motions, more than 100,000 lines have been observed. Among the dense spectral features, series of a-, b- and c-type Q and R transitions have been successfully analyzed with a least-squares fitting method based on a Watson Hamiltonian, and assigned to the Gt conformer of n-propanol in the ground state. The rotational constants including sixth order centrifugal distortion parameters are determined to allow accurate transition frequency prediction for the Gt form through 400 GHz. The conformer assignment and isomerization in n-propanol will be discussed.