MILLIMETER WAVE TUNNELING-ROTATIONAL SPECTRUM OF PHENOL

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The millimeter wave spectra of phenol in the vibrational ground state and the first excited states of the bending and torsion vibrational modes have been studied in the frequency regions of 140 – 170 GHz and 280 – 360 GHz. The internal rotation of the hydroxyl group is responsible for the observed tunneling splitting into two substates $(v_t, v_b)^+$ and $(v_t, v_b)^-$ and more than 3500 distinct tunneling-rotational ${}^bR$- and ${}^bQ$-type transitions between them were measured and analyzed. Furthermore, accidental near degeneracies of the $(+)$ and $(-)$ energy levels were observed in case of the ground state and the $v_b = 1$ excited state and the analysis using a two-state effective Hamiltonian including tunneling-rotational Coriolis terms was performed. The spectroscopic constants for the first excited states of the bending and the torsion vibrational modes have been determined for the first time. The analysis of the microwave data provided very precise values of the spectroscopic constants necessary for the astrophysical search of phenol. We report a tentative detection for this molecule in the IRAM 30m line survey of Orion KL.