ASSIGNMENTS, PERTURBATIONS, PATHOLOGIES AND A ROTATIONAL ANALYSIS OF THE SPECTRUM OF CH_2DOH

JOHN C. PEARSON, SHANSHAN YU, BRIAN J. DROUIN, *Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Dr., Pasadena, CA 91109*.

Theory and analysis of three-fold internal rotors is a well established science allowing for a wide variety of molecules to be successfully analyzed to experimental accuracy. However, once the three-fold symmetry is broken with the substitution of a single deuterium, the problem becomes much less well described either theoretically or experimentally. CH_2DOH is rapidly formed on grains in the interstellar medium at low temperatures where it is energetically favorable for atomic deuterium to replace hydrogen in the methyl rotor of methanol. Additionally, the three equivalent ways to substitute in the methyl rotor suggest that CH_2DOH will be at least three times as abundant as CH_3OD. The observational evidence does not always support this assertion potentially because the intensities of CH_2DOH are poorly understood. An analysis of over 8000 transitions in the three torsional substates of the ground torsional state of CH_2DOH will be presented. Analysis of the data set shows a number of pathologies both in the energy level structure as well as with the labeling of transitions for this class of molecules. The analysis shows some surprising deviations from available theory. A number of assignments and pathologies in the excited torsional states will be presented as well.