

A NEW MULTI-STATE VIBRATION-TORSION-ROTATION FITTING PROGRAM FOR MOLECULES WITH A C_{3v} TOP AND C_s FRAME: APPLICATION TO THE ν_{10} BAND OF ACETALDEHYDE

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A new program is described for fitting several isolated small-amplitude fundamentals embedded in a pure torsional bath in molecules like acetaldehyde, in which the frame has C_s symmetry and the methyl top has C_{3v} symmetry. The program is based on the Longuet-Higgins group theoretical ideas and uses the Rho-axis method. In the talk the basic ideas, the structure of the program as well as the strategy for checking the program will be discussed. Also we present the first results^a of application of the new program to the spectrum of the ν_{10} vibrational state of acetaldehyde, CH_3CHO , near 509 cm^{-1} . The analysis of the 509 cm^{-1} band is accompanied by the analysis of microwave spectrum of the ν_{10} vibrational state and $\nu_t = 3,4$ torsional states of acetaldehyde.

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