PHYSICAL INTERPRETATION OF TORSION-ROTATIONAL PARAMETERS IN METHANOL AND ITS ISOTOPOMERS: COMPARISON OF GLOBAL FIT AND CENTRIFUGAL CALCULATION RESULTS

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The molecular parameters for ^{12}C and ^{13}C methanol and its isotopomers CH_3OH, CH_3OD, and CD_3OD with O-16, 17 and 18 will be presented. Two methods have been used to determine the parameters. One uses the recent formulation of the centrifugal distortion effects in terms of the potential parameters for a molecule that contains a three-fold symmetric internal rotor[a b]. The other uses through a global fit to observed high resolution microwave, millimeter wave and Fourier transform far-infrared spectra based on a reduced torsion-rotational Hamiltonian model[c d e]. The calculated parameters, in particular the constants that represent interactions between torsion and rotation, are used to interpret the relationships among the terms in the reduced Hamiltonian. By calculating the molecular parameters from several potential energy functions for methanol isotopomers we can check the quality of these potentials. Finally, the calculated parameters are compared with the parameters that were obtained from global fits. The good agreement between the calculated centrifugal distortion terms and those derived from the fits to the spectra demonstrates that the derived formulae provide a useful tool for understanding the physical origins and mass dependence of fundamental molecular parameters[f g].

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