

THE ROTATIONAL-TORSIONAL SPECTRUM OF METHYL FORMATE:PRECISE MEASUREMENTS ON AND INTERPRETATION OF MILLIMETRIC WAVE TRANSITIONS

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By using a cavity spectrometer with a helium-cooled detector and computerised methods of background removal, we have measured a total of 43 new lines of the ground torsional state of methyl formate with precision of 0.1 MHz. These include b-type transitions of high J and K quantum numbers. When combined with other literature reported data collected by conventional waveguide spectrometers [Plummer et al. 1984-1986], they are fitted to single-state Hamiltonians of internal axis method (IAM) in which the C-C bond is considered as one of the three mutually perpendicular axes of the molecular reference frame. In these Hamiltonians, we have allowed rotational parameters to differ between A and E torsional states because of coupling to other vibrations of corresponding symmetry [Oka et al. 1967]. As these interactions are symmetry dependent, it is not surprising that one obtains better fits by permitting different average parameters for the two species [Maes et al. 1987, Plummer et al. 1984]. The frequencies of the data were up to 355 GHz and 505 GHz for E and A species respectively. Rms deviations of 0.43 MHz for A and 0.27 MHz for E symmetry states were obtained. A total of 14 floating parameters and 3 fixed parameters were used in the fit. This very satisfactory results of the fit can be highly useful in precise prediction of line frequencies in other bands. The author would like to thank the council of research of Shiraz university for supporting this work. References Plummer,G.M., Herbst,E., Delucia,F.C., Blake,G.A., Ap.J.Suppl.,55,633,1984. Plummer,G.M., Herbst, E.,Delucia,F.C., Blake,G.a., Ap.J.Suppl.,60,949,1986. Blake,G.A., Sutton,E.C., Masson,C., Phillips,T.G., Ap.J.Suppl., 60, 357,1986. Oka,T., J. Chem. Phys., 47,12,1967. Maes,H., Wlodarczak,G., Banchert,D., Demaison,J.Z., Natureforsch., 429, 97, 1987.