ON THE POSSIBILITY OF ESTIMATION HARMONIC FREQUENCIES OF MOLECULES (INTRAMOLECULAR FORCE FIELD PARAMETERS) ON THE BASE OF INFORMATION ABOUT ITS PURE ROTATIONAL SPECTRUM

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In the process of study near local mode XY_2 and XY_3 molecules we found[a] that all properties of spectroscopic parameters of such type molecules are determined, considerably, by the simplest solutions of equations, which connect ambiguous parameters $\sin\gamma_i$ with the parameters of intramolecular potential function and masses of molecular nucleus. As the analysis of other solutions of above mentioned equations shown, simple (nondepended on intramolecular force constants) results for $\sin\gamma_i$ parameters can be obtained in general enough case (with only one limitation $m/M \ll 1$) for XY_2 and XY_3 molecules. On this base it is shown that for molecules of such types experimental information on rotational and quartic centrifugal distortion parameters (e.g., determined from microwave spectra) allows one to predict with high enough accuracy harmonic frequencies and quadratic force constants of intramolecular potential function even without any additional information about fundamental or overtone bands. Calculations for different real molecules are presented, as an illustration. Attempt of expansion of results to more complicated molecular systems is discussed.
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[a] O.N.Ulenikov and R.N.Tolchenov, Abstr.XIV Colloq.High Resolution Molecular Spectroscopy, F23, Dijon (France), 1995.