## METHANOL AS A FLEXIBLE MODEL

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A method based on the semi rigid bender and the flexible model approaches has been developed for the internal rotation motion in methanol. For construction of the torsion Hamiltonian matrix a $K$-dependent trigonometric variational basis set adapted to $C_{3v}$ symmetry was employed. Functions of molecular geometry parameters were chosen as a Fourier series in the torsional angle $\rho$ allowing geometry relaxation of both the top and the frame during the revolution of the top. It was found that when considering certain idealized cases of structure variation with torsional angle, an unusual splitting of the $A_1$ and $A_2$ energy levels occurs in the extreme case of a free rotor.

It was shown how the results of the *ab initio* calculations for $C_{3v}$(M)-molecules could be linked to the developed flexible model by using the approximation of equality of the torsional angle $\rho$ and the average of the three top-frame dihedral angles $\tau_{\text{eff}}$.

An analysis of the process of determining the methanol molecular geometry employing the developed model was performed. Two of the zero-order parameters were fixed at the values obtained from electron diffraction measurement and the remaining zero-order parameters and some of the parameters describing variation of the geometry during the torsion as well as the potential energy function were determined for various $J_{\max}$. The fitted values for the bending semirigidity parameters were found to be broadly consistent with those from the MO calculations, whilst the fitted bond stretching parameters were generally in poor agreement.

Line strength calculations have also been performed using the wave functions of various Hamiltonians. It was confirmed that the main contribution to the line strengths comes from the permanent components of the dipole moment whilst the dipole variation with torsion produces little contribution to the methanol line strengths.

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