ANALYTICAL COMPUTER CALCULATIONS FOR POLYATOMIC MOLECULES: ANHARMONIC, RESONANCE INTERACTION, RO–VIBRATIONAL, CENTRIFUGAL DISTORTIONAL PARAMETERS FOR ASYMMETRIC TOP MOLECULES

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Operator perturbation theory in the projector formulation was used as the basis for deriving general formulas which take into account possible as regular and accidental resonance interactions in asymmetric top molecules. MAPLE codes have been created which allowed us to derive in the analytical form
1) harmonic parameters $x_{\lambda\mu}$ and $y_{\lambda\mu\nu}$ in the expression

$$E_{v_1...v_n} = \sum_{\lambda} \omega_{\lambda} \left( v_{\lambda} + \frac{1}{2} \right) + \sum_{\lambda,\mu \geq \lambda} x_{\lambda\mu} \left( v_{\lambda} + \frac{1}{2} \right) \left( v_{\mu} + \frac{1}{2} \right) + \sum_{\lambda,\mu \geq \lambda,\nu \geq \mu} y_{\lambda\mu\nu} \left( v_{\lambda} + \frac{1}{2} \right) \left( v_{\mu} + \frac{1}{2} \right) \left( v_{\nu} + \frac{1}{2} \right);$$

2) parameters $F_0$ and $f_\lambda$ for different vibrational resonance interactions (Fermi, Darling-Dennison, etc.) $\sim [F_0 + \sum_{\lambda} f_\lambda b_\lambda]$, where $b_\lambda$ depend on the vibrational quantum numbers $v_\lambda$;

3) ro–vibrational coefficients $\alpha_{\lambda}^\beta$ and $\gamma_{\lambda\mu}^\beta$ in the expression

$$B_\beta = B_\beta^0 - \sum_{\lambda} \alpha_{\lambda}^\beta \left( v_{\lambda} + \frac{1}{2} \right) + \sum_{\lambda,\mu \geq \lambda} \gamma_{\lambda\mu}^\beta \left( v_{\lambda} + \frac{1}{2} \right) \left( v_{\mu} + \frac{1}{2} \right);$$

4) centrifugal distortion parameters $\Delta_i^e$ and $\delta_i^k$ in the expression

$$\Delta_i = \Delta_i^e + \sum_{\lambda} \delta_i^k \left( v_{\lambda} + \frac{1}{2} \right).$$

In the present version, results are obtained on the basis of the operator perturbation theory up to the fourth order and take into account sixth order parameters of the intramolecular potential function.

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