DIVERGENT SERIES SUMMATION TECHNIQUE APPLIED TO MOLECULAR VIBRATIONAL ENERGY LEVELS CALCULATION

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The Rayleigh–Schrödinger perturbation theory is applied to energy levels calculation of the $HD^{16}O$ molecule excited vibrational states. The calculations are carried out for the vibrational states that correspond to three- to seven-fold vibrational excitations. Since the perturbation series diverge in the case of strong resonance interactions and their approximations by the Padé and Padé–Hermite methods do not yield sufficiently correct results as shown in our previous works [1], a calculation technique modifying the zero-order approximation is applied. The zero-order Hamiltonian is modified by shifting the vibrational frequencies, which decreases the mixing of states. The new Rayleigh–Schrödinger series can be summed using the quadratic Padé–Hermite approximation method.

REFERENCES

1. Bykov A.D., Kalinin K.V., Duchko A.N. Calculation of vibrational HDO energy levels: analysis of perturbation theory series, Optics and spectroscopy, 2013. Vol. 114. No 3. pp. 359-367.