PREDICTION OF VIBRATIONAL ENERGY LEVELS USING A MIXED APPROACH OF NUMERICAL AND ANALYTICAL INTEGRATION

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A method for the computation of vibrational energy levels based on Watson's simplified form of the complete rotation-vibration nuclear Hamiltonian[a] is presented. The Hamiltonian matrix is constructed within a harmonic oscillator product basis using a discrete variable representation of the potential energy and a quasi-analytic treatment of the remaining terms. The latter are obtained by an expansion of the modified reciprocal moment of inertia with respect to the normal coordinates and the integration is carried out using a string-based formalism. Results for linear and nonlinear molecules demonstrate the excellent performance of the present implementation.

[a] J. K. G. Watson, *Mol. Phys.*, 15, 479 (1968):19, 465 (1970).