VIBRATIONAL CONSTANTS FOR TRIATOMIC MOLECULES FROM FOURTH-ORDER PERTURBATION THEORY

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The second vibrational anharmonicity constants (y_{ijk}) for general non-linear triatomic molecules as derived from fourth-order Rayleigh-Schrödinger perturbation theory (VPT4) are presented. The derived constants include all force field and Coriolis terms from the Watson Hamiltonian except for the pseudopotential. The basic theory of VPT4 is discussed, particularly with application to molecular constants, as well as the computational methods used to derive the specific constants. Finally, the constants are analyzed in the context of model systems such as Morse and double-well potentials.