ROTATIONAL AND ROVIBRATIONAL CONSTANTS FOR TRIATOMIC MOLECULES FROM FOURTH-ORDER PERTURBATION THEORY

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Rotational and rovibrational constants including the quadratic vibration-rotation interaction constants (the "γ"s), vibrationally-dependent quartic centrifugal distortion constants, and equilibrium hexic centrifugal distortion constants for general non-linear triatomic molecules as derived from fourth-order Rayleigh-Schrödinger perturbation theory (VPT4) are presented. The derived constants include all terms from the Watson Hamiltonian except for the pseudopotential. The resulting expressions are applied to a model molecular system, and issues such as vibrational resonance are discussed.