HIGH ORDER CORRECTIONS TO ROTATIONAL CONSTANTS BY VIBRATION-ROTATION PERTURBATION THEORY

JUANA VÁZQUEZ and JOHN F. STANTON, Institute for Theoretical Chemistry, Department of Chemistry, University of Texas, Austin, Tx 78721.

Vibrational corrections to rotational constants due to second vibration-rotation interaction constants, i.e. γ_{ij}^{α} , are presented under the framework of fourth order Rayleigh-Schödinger perturbation theory. Applications to some asymmetric top molecules are analyzed and compared with corrections resulting from the first vibration-rotation constants, α_i^{α} .