ANHARMONIC VIBRATIONAL MØLLER-PLESSET PERTURBATION THEORIES USING THE DYSON EQUATION

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We have developed new second-order diagrammatic perturbation theories for the anharmonic vibrational structure of molecules and solids in the Møller-Plesset partitioning of the Hamiltonian which we refer to as XVMP2. XVMP2 uses the size-extensive vibrational self-consistent field (XVSCF) methods for the reference wave function. In lieu of calculating the total energies of excited vibrational states, XVMP2 calculates frequencies directly using the Dyson equation for the single-particle vibrational Green's function and a truncated diagrammatic sum for the Dyson self-energy. This method enables XVMP2 to predict accurate anharmonic frequencies even for methods affected by strong anharmonic resonance without any matrix diagonalization step.