

Thermodynamic properties and the approximate solutions of the Schrodinger equation with the shifted Deng–Fan potential model

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With the introduction of a new improved approximation scheme (Pekeris-type approximation) to deal with the centrifugal term, the energy eigenvalues and the wave functions of the Schrodinger equation of the shifted Deng–Fan molecular potential are obtained, via the asymptotic iteration method. Rotational–vibrational energy eigenvalues of some diatomic molecules are presented, these results are in good agreement with other results in the literature. For these selected diatomic molecules, energy eigenvalues obtained are in much better agreement with the results obtained from the rotating Morse potential model for moderate values of rotational and vibrational quantum numbers. Furthermore, thermodynamic properties such as the vibrational mean U , specific heat C , free energy F and entropy S for the pure vibrational state in the classical limit for these energy eigenvalues are studied.

Keywords: shifted Deng–Fan molecular potential; Pekeris-type approximation; asymptotic iteration; eigenvalues;

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