Eigenfunction, uncertainties and thermal properties of the Schrodinger equation with Screened modified Kratzer potential for diatomic molecules.

Collins Edet[1], Akpan Ikot[1], Uduakobong Okorie[2], Hewa Abdullah[3], and Idris Salah[3]

[1]University of Port Harcourt
[2]Akwa Ibom State University
[3]Tishk International University

June 1, 2020

Abstract

In this work, we proposed a screened modified Krazer potential and use the newly proposed Nikiforov-Uvarov-Functional Analysis (NUFA) method to obtain the energy spectrum and the corresponding wave function. With the obtained energy spectrum, we studied the numerical results for some selected diatomic molecules and our results are in good agreement with other analytical method. We also evaluated the vibrational partition function for , and diatomic molecules via the Euler–Maclaurin approach and other thermodynamic functions such as free energy, entropy, mean energy and specific heat Capacity. The expectations values of and are also calculated numerically for different diatomic molecules using the normalized wave function for the two low lying states corresponding to the ground and first excited states. Our numerical results for the selected diatomic molecules validate the Heisenberg uncertainty relation, .

Hosted file

`Screened Modified Kratzer potential IJQC.docx` available at https://authorea.com/users/328236/articles/455637-eigenfunction-uncertainties-and-thermal-properties-of-the-schrodinger-equation-with-screened-modified-kratzer-potential-for-diatomic-molecules