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Entitled

THEORETICAL AND COMPUTATIONAL ASTROCHEMISTRY: A VARIATIONAL QUANTUM MONTE CARLO (VQMC) STUDY OF THE TRIHYDROGEN MOLECULE CATION (H_3^+)

By

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Abstract

H_3^+ is the simplest three-center two-electron molecule and it is of much interest in astrochemistry due to its high occurrence in the outer space, high reactivity, and strong acidic properties. In addition, H_3^+ is involved in many chemical reactions in the interstellar medium (ISM) and its significant ability to absorb energy contributed to the cooling of the universe during its early stages.

The main objective of this thesis is to approximate the ground state electronic energy of H_3^+ by using a simple trial wavefunction consisting of a doubly occupied molecular orbital multiplied by a Jastrow factor. The latter factor allows us to introduce some degree of electron correlation and obey the electron-ion cusp condition. With this trial wavefunction, we derived an expression for the local energy which was then implemented in a Variational Quantum Monte Carlo (VQMC) code in line with a Metropolis algorithm sampling technique. Moreover, the computer code was written in Python 3.6 language and was first tested on an analytically solvable system which is the quantum harmonic oscillator (QHO). Finally, the equilibrium H-H bond length at the fixed equilateral geometry and the normal breathing frequency were estimated. The calculated equilibrium H-H bond length of the equilateral triangular geometry is 1.800 Bohr (0.95 Å) which is only 1.8 % as a deviation from the experimental value of 1.833 Bohr (0.97 Å). Furthermore, the symmetric normal breathing frequency was also calculated to be 3240 cm^{-1} with a small error percentage of 1.7 % from the obtained experimental value of 3185 cm^{-1}. Thus, both values of bond length and frequency are in good agreement with the experiment and prior theoretical studies on the molecule. Last but not least, the calculated ground state energy value was -1.256458 Hartree. As a conclusion, the theory developed in this thesis goes beyond the independent-particle approximation and leads to promising, reliable, and reproducible results despite the simplicity of the used trial wave function.

Keywords: Astrochemistry, H_3^+, Theoretical/Computational Chemistry, Quantum Chemistry, Variational Theorem, Quantum Monte Carlo Methods, Metropolis algorithm.