**College of women for Arts,
Science and Education
Physics Department**

Quantum Dynamics as an Approach to Study Atomic and Molecular Structures of Some of The di-Atomic Molecules

A thesis presented
by

Rageh Attia Khalifa Hussien
B. Sc. in physics, 2001

for

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بِسْمِ اللهِ الرَّحْمنِ الرَّحِيمِ

﴿ إِنَّ فِى خَلْقِ ٱلسَّمَٰوَٰتِ وَٱلأَرضِ وَٱخْتِلَٰفِ ٱلَّيلِ وَٱلنَّهَارِ لَأَيَٰتٍ لِّأُوْلِى ٱلأَلْبَٰبِ (١٩٠) ٱلَّذِينَ يَذْكُرُونَ ٱللَّهَ قِيَٰمًا وَقُعُودًا وَعَلَىٰ جُنُوبِهِمْ وَيَتَفَكَّرُونَ فِى خَلْقِ ٱلسَّمَٰوَٰتِ وَٱلأَرضِ رَبَّنَا مَا خَلَقْتَ هَٰذَا بَٰطِلاً سُبْحَٰنَكَ فَقِنَا عَذَابَ ٱلنَّارِ (١٩١) ﴾

[ال عمران (190- 191)]

Dedicated

To

My parents (Father and Mother),

My sisters,

My brothers,

My cognates

and

My friends

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Abstract

Quantum Dynamics as an Approach to Study Atomic and Molecular Structures of Some of The di-Atomic Molecules

Rageh Attia Khalifa Hussien, B. Sc. in physics, 2001

The theoretical studies of molecular structure using the methods of quantum mechanics form a vast and very active research area. It would be very difficult to try to cover all recent advances in this area within a single work.

Most of the developments in the associated quantum-mechanics methodology are aimed at providing more and more accurate calculation of the structure of molecules, and this because the difficulties that were found to give the exact solution for Schrödinger equation.

All this theoretical investigation of the molecular structure has introduce Wide range of application to the branch of material science and chemists who interested in this field.

** In chapter one Literature Survey has been introduced to cover the molecular physics study from old to modern ideas , beginning with the first attempts to know the atomic and molecular structures of materials and the effort of all scientist that contribute to this subject.

** In chapter two all the theories that concerned with the work has been handled beginning with dividing the branch of physics that dealing with molecular structure into two sections:

- Molecular mechanics which use the laws of classical physics.

- Electronic Structure Methods which use the laws of quantum mechanics.

Electronic Structure Methods in turn divided into two sections:

a) The semi-empirical & b) The Ab-initio

a) The semi-empirical methods use parameters derived from experimental data to simplify the computation.

b) The Ab initio methods use no experimental parameters in their computations. Instead, their computations are based only on the laws of quantum mechanics-the first principles referred to in the name ab initio.

Theoretical model came as a tool to explore the investigation of the theories and give the result of work.

Theoretical model are characterized by the combination of:

a) Method (theoretical procedure) & b) Basis set

a) The theoretical models contain a hierarchy of procedures corresponding to different approximation methods in solving Schrödinger equation.

b) The basis set can be interpreted as any mathematical functions that can restrict each electron to a particular region of space.

Hartree use the variational principle and build Hartree fock self consistent field method that was finished by Roothaan and Hall and was found to be as a simple and a good approximated method.

Other methods like (CC), (CASSCF),….came later to fix some problems that Hartree fock self consistent field method cannot deal with.