NEW YORK UNIVERSITY
CHEMISTRY DEPARTMENT
UNIVERSITY HEIGHTS

6p

Contract No. NSG-76-60

Summary of work done in the period
November 1, 1962 to April 30, 1963

THEORETICAL STUDY OF ATOMIC AND MOLECULAR GASES AND THEIR REACTIONS IN THE UPPER ATMOSPHERE

Submitted to the National Aeronautics and Space Administration, Washington, 25, D.C. The report contains a brief summary of the work done during the period November 1, 1962 to April 30, 1963 and results are not necessarily in the final form.

Ralph C. Sahni

R. C. Sahni
Project Director

PERSONNEL

Dr. T. W. Davis	Director
Dr. R. C. Sahni	Senior Research Scientist and Chief Investigator
Dr. Donald LaBudde	Research Scientist
Dr. Franz-Josef Heinen	Assistant Research Scientist
Mr. E. J. DeLorenzo	Research Assistant
Mr. M. D. Sawhney	Research Assistant
Mr. Om Prakash Anand	Research Assistant
Mr. R. S. Bawa	Research Assistant

Work carried out during the period can be given under the following headings:

(1) Computation of Electronic Wave Functions of Different States of Diatomic Molecules. (Continued work of the previous report.)

(2) Thomas-Fermi Statistical Method for Atoms and Molecules.

(3) New Techniques for Diagonalization of Matrices.

(4) Electron Paramagnetic Resonance, Nuclear Magnetic Resonance, Quadrupole Resonance Studies of Well-defined Systems and Imperfect Crystals.

(1) COMPUTATION OF ELECTRONIC WAVE FUNCTIONS OF DIFFERENT STATES OF DIATOMIC MOLECULES

by E. J. DeLorenzo and R. C. Sahni

In the previous report we gave the procedure for computing different states of diatomic molecules. We stated in our earlier reports that although ground state functions of diatomic molecules have been computed, very little progress about the theoretical work of the ionized and excited states of diatomic molecules has been so far reported from any other center. We have, therefore, carried the work on the ionized and excited states very carefully comparing our data with the available experimental data. We have faced several difficulties in our work involving convergence and self-consistency of results. We are happy to report that we have overcome all these difficulties and we have now obtained reliable results. We intend to send shortly the following papers for publication:

1) Calculation of the Wave Functions, of Ionized States, Vertical Ionization Potentials and Adiabatic Ionization Potentials of CO, N_2, O_2 and NO Molecules.

2) Calculation of the Wave Functions, of Lower Excited States, Vertical Excitation Energies and Adiabatic Excitation Energies of CO, N_2, O_2 and NO Molecules.

(2) THOMAS-FERMI STATISTICAL METHOD FOR ATOMS AND MOLECULES

by R. C. Sahni and Franz-Josef Heinen

In the previous report we gave a brief summary of the statistical method of atoms. We also mentioned some of the difficulties that arise by including exchange forces in this method. Before tackling this problem and extending it to molecules, we have reviewed the whole literature and have critically examined different approaches to this problem. Most of the work on the statistical method exists in German and French literature. There is no book

available in the English literature dealing with the statistical method. Since this method will be very useful in a number of problems such as molecular structure and Plasma Physics, we are preparing a review article which will form the basis of our further work on this method.

(3) NEW IMPROVED TECHNIQUE FOR DIAGONALIZATION OF MATRICES
by C. D. LaBudde

Two new classes of algorithms for finding the eigenvalues and eigenvectors of real symmetric matrices are described. The algorithms described are essentially Jacobi-like iterative procedures employing Householder orthogonal similarity transformations and Jacobi orthogonal similarity transformations to reduce a real symmetric matrix to diagonal form. The convergence of the first class of algorithms depends upon the fact that the algebraic value of one diagonal element is increased at each step in the iteration and the convergence of the second class of algorithms depends upon the fact that the absolute value of one off-diagonal element is increased at each step in the iteration. Then it is shown how it is possible to combine one algorithm from each class together into a "mixed" strategy for diagonalizing a real symmetric matrix.

(4) ELECTRON PARAMAGNETIC RESONANCE, NUCLEAR MAGNETIC RESONANCE AND QUADRUPOLE RESONANCE STUDIES OF WELL-DEFINED SYSTEMS AND IMPERFECT CRYSTALS
by R. C. Sahni

During my discussions at the National Aeronautics and Space Administration University Conference in Chicago and my visits to other National Aeronautics and Space Administration Centers, I find there was much interest in the above mentioned fields because of their application to materials. Since these fields are outgrowths of Quantum Chemistry, therefore, I have included them in our research program. These studies will be helpful to our general study of the molecular structure and will also indicate the importance of our basic work on atoms and diatomic molecules to other fields.

PROGRAMS FOR ELECTRONIC DIGITAL COMPUTERS

The group has utilized the following electronic computers for studying various problems:

1) 7090 IBM Electronic Digital Computer, Institute for Space Studies, 475 Riverside Drive, New York, N.Y.

2) 1620 IBM Electronic Digital Computer, New York University, University Heights, New York 53, N.Y.

3) 1604 CDC Electronic Digital Computer, New York University, University Heights, New York 53, N.Y.

The following programs were prepared for different computers:

1) Programs using Linear Combination of Atomic Orbitals, Self-Consistent Field Method of Computing Wave Functions of Different States of Diatomic Molecules for 1620 Electronic Computer
by Eugene DeLorenzo

2) A program of Diagonalization of Matrices Using Dr. LaBudde's Method for 7090 Electronic Computer
by M. D. Sawhney

3) A program of Diagonalization of Matrices Using Jacobi's Method for 7090 Electronic Computer
by Franz-Josef Heinen and R. S. Bawa

GROUP ACTIVITIES

1) Dr. R. C. Sahni and Dr. Franz-Josef Heinen attended the National Aeronautics and Space Administration University Conference on the Science and Technology of Space Exploration in Chicago, Illinois, November 1 - 3, 1962.

2) Dr. R. C. Sahni visited the Universities of Chicago and Columbus, Ohio, for discussions on Molecular Structure, June 8 - 14, 1963.

3) Dr. R. C. Sahni was invited to give a paper at the American Society for Testing and Materials Conference in Atlantic City, New Jersey on June 25, 1963 on the following topic:

"Comparison of Electron Paramagnetic Resonance Studies of Well Defined Systems and Irradiated Substances."

4) Dr. C. D. LaBudde and other members of the group attended the Mathematical Society Meeting in New York on May 27, 1963 and had fruitful discussions with a number of scientists including Dr. A. S. Householder.

5) Dr. C. D. LaBudde was invited to give a talk on his Method of Diagonalization of Matrices at the International Business Machines Center, Time and Life Building, New York, New York on June 19, 1963.

PUBLICATIONS

The following papers have been accepted for publication:

1) Comparison of Electron Paramagnetic Resonance Studies of Well Defined Systems and Irradiated Substances
by R. C. Sahni
Journal American Society for Testing and Materials (in press)

2) The Reduction of an Arbitrary Real Square Matrix to Tri-diagonal Form Using Similarity Transformation
by Dr. C. D. LaBudde
Mathematics of Computation (in press)

3) A New Algorithm for Diagonalizing A Real Symmetric Matrix
by Dr. C. D. LaBudde
Mathematics of Computation (in press)

The following papers are being prepared for publication:

1) Comparison of Different Methods of Diagonalizing A Matrix
by M. D. Sawhney

2) Quantum Mechanical Study of Ionized States of Some Diatomic Molecules
by Eugene DeLorenzo and R. C. Sahni

3) Quantum Mechanical Study of Lower Excited States of Some Diatomic Molecules
by R. C. Sahni and Eugene DeLorenzo

4) Thomas-Fermi Statistical Method of Atoms and Molecules; (a review article)
by R. C. Sahni and Franz-Josef Heinen

5) Two New Classes of Algorithms for Finding the Eigenvalues and Eigenvectors of Real Symmetric Matrices
by C. D. LaBudde