

UNCLASSIFIED

AD 401 107

*Reproduced
by the*

DEFENSE DOCUMENTATION CENTER

FOR

SCIENTIFIC AND TECHNICAL INFORMATION

CAMERON STATION, ALEXANDRIA, VIRGINIA



UNCLASSIFIED

NOTICE: When government or other drawings, specifications or other data are used for any purpose other than in connection with a definitely related government procurement operation, the U. S. Government thereby incurs no responsibility, nor any obligation whatsoever; and the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data is not to be regarded by implication or otherwise as in any manner licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use or sell any patented invention that may in any way be related thereto.

63-3-2

401 107

CATALOGED BY ASTIA
AS AD No. 401107

OFFICE OF NAVAL RESEARCH

Contract Nonr 3471(00)

Task No. 356-433

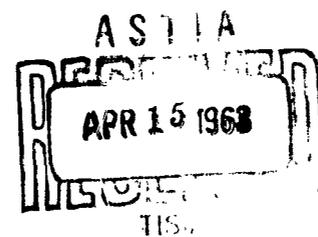
FINAL REPORT

Theoretical and Quantum Chemistry of Boron

Compounds and Related Molecules

by

Joyce J. Kaufman



RIAS
7212 Bellona Avenue
Baltimore 12, Maryland

March 15, 1963

Reproduction in whole or in part is permitted for any
purpose of the United States Government.

**Theoretical and Quantum Chemistry of Boron Compounds
and Related Molecules**

The theoretical boron research project under Contract Nonr 3471(00) for the Chemistry Branch of the Office of Naval Research has performed research in the development of methods to describe the valence structure, properties and behavior of boron compounds and related molecules.

This project has carried out investigations in:

- I. Theoretical Study of Charge Transfer Behavior of Boron-Containing Lewis Acid-Lewis Base Addition Compounds, especially those of the type $ZB_{10}H_{12}Z$.
- II. Rigorous Molecular Orbital Calculations of Boron Compounds.
 - a. Pentaborane
 - b. Calculation of Basic Parameters Necessary for Quantum Chemical Calculations on Boron-Containing Molecules: Modified (pp|pp) electron repulsion integrals and corresponding boron screening constants.
 - c. LCAO-MO-SCF (Self-Consistent Field) Calculations for Non-Saturated Boron-Containing Molecules.
- III. Ionization Potentials and Mass Spectral Fragmentation Patterns of Boron Compounds; also S_K values (the effects of substitution on ionization potentials) for cyclic radicals and for O and S compounds.

IV. Theoretical Study of Aluminum Coordination Numbers in
Various Compounds.

V. Theoretical Aspects of Bonding in Xenon-Fluorine Compounds.

Research on these and other topics is continuing under support from
the Air Force Office of Scientific Research, Directorate of Engineering
Sciences, Propulsion Division under Contract AF49(638)-1220.

I. Theoretical Study of Charge Transfer Behavior of Boron-Containing Lewis Acid-Lewis Base Addition Compounds, especially those of the type $ZB_{10}H_{12}Z$.

References: (A-TR-1) (S-2) (S-5)

A new class of Lewis acids and Lewis bases - delocalized electron-deficient molecules, such as the higher boron hydrides - with properties formally analogous to those of delocalized π -electron systems was defined. On this basis, the behavior of $ZB_{10}H_{12}Z$ and ZB_9H_{13} complexes (where Z is an electron pair donor) could be described in terms of charge transfer complex theory.

Treatment of the behavior of $ZB_{10}H_{12}Z$ compounds as a purely theoretical problem indicated the mechanism by which these complexes must be formed. Even more important, derivation of the correct quantum mechanical description of the valence structure and spectra of these $ZB_{10}H_{12}Z$ compounds and subsequent MO-LCAO calculations led unequivocally to the specific properties a Z molecule should have in order to be most effective in forming $ZB_{10}H_{12}Z$ compounds.

In $PyB_{10}H_{12}Py$, pyridines act as n-donors to $B_{10}H_{12}$ and then one gets reverse electron donation from $B_{10}H_{12}$ to the pyridine π -skeletons. The long wavelength transitions in $PyB_{10}H_{12}Py$ complexes were shown to be dependent on the energies of the lowest unfilled molecular orbitals (LUMO) of the substituted pyridines as calculated by MO-LCAO

methods (hence the transitions are confirmed as $B_{10}H_{12} \rightarrow Py$). From the differences in the wavelengths of analogous bands, the highest occupied molecular orbital (HOMO) of $B_{10}H_{12}$ would be estimated to be 0.83 eV above that of B_9H_{13} . For effective $ZB_{10}H_{12}Z$ formation it is confirmed that Z must not only be a good n-donor but should also be a good π -(or d-) acceptor.

Thus a purely theoretical study proved able to indicate to experimentalists the most judicious choice of which Z molecules should be used to form $ZB_{10}H_{12}Z$ compounds and why these particular Z molecules should be the most effective. An understanding of the theory of the bonding in these compounds also makes it possible to alter the Z molecule correctly in order to produce desired changes in behavior (A-1) (S-5).

A preliminary report of the application of charge transfer complex theory to delocalized electron-deficient boron hydrides was also made (S-2).

II. Rigorous Molecular Orbital Calculations of Boron Compounds.

a. Pentaborane.

Pentaborane, B_5H_9 , was chosen as the prototype boron hydride molecule on which to try several different rigorous and semi-rigorous molecular orbital calculational procedures. One of the main purposes of such a study is to determine what simplifying approximations can be made which will most closely match the results of a rigorous calculation and so

will make calculations on the higher boron hydrides more feasible.

Symmetry orbitals for pentaborane, B_5H_9 , were formulated for several different sets of basis orbitals, both hybridized and unhybridized. The elements of the 29x29 Hamiltonian matrices have been expanded in terms of individual atomic orbitals. Integrals are being evaluated two ways: First, have been estimated semi-empirically; Second, are being calculated rigorously by separating each matrix element into kinetic and potential energy and electron repulsion terms. This has necessitated our having to initiate setting up computer programs for the integrals involved (specifically the many-center integrals). A rigorous core approximation for integrals developed previously by Professor Daudel is being incorporated into the pentaborane calculations.

- b. Calculation of Basic Parameters Necessary for Quantum Chemical Calculations on Boron-Containing Molecules: Modified (pp|pp) electron repulsion integrals and corresponding boron screening constants.

References: (A-TR-7) (A-TR-8)

One major improvement in MO calculations of boron compounds would be the choice of a more correct boron screening constant, for use with Slater orbitals, which would embody electron correlation effects.

Modified one-center electron repulsion integrals (pp|pp) for B and B^- which take into account electron correlation effects have

been evaluated by expansion of the energies of the boron atom and its positive and negative ions as a function of spectroscopic term values.

The values for $(pp|pp)_B$ calculated from two different pairs of valence states 7.094 ev and 6.976 ev are very close. It is demonstrated that for boron in certain valence states the Pariser-Parr approximation $(pp|pp) = I-A$ and the more rigorous approximation of Julg $(pp|pp) = I-A - \epsilon(I+A)$ do not hold, because when the electron is put into a formerly empty orbital, an exchange term arises in addition to the Coulomb term.

For the calculation of $(pp|pp)_B^-$ it was necessary to evaluate the electron affinities of B^- to form $B^{=}$ in various valence states. This was done by adapting an existing rigorous extrapolation procedure to valence state calculations.

$(pp|pp)_B^-$ was calculated by expansion of the energies of B , B^- and $B^{=}$ as a function of spectroscopic term values. The value for $(pp|pp)_B^-$ calculated in this manner, 4.737 ev, and the value calculated using the Pariser-Parr approximation, $(pp|pp) = I-A = 4.015$ ev, are quite close. This is especially gratifying in view of the fact that the two calculations are independent and that each calculation depends on extrapolated values for the electron affinities of B^- in completely different valence states.

In addition a new general method for calculating (pp pp) [including correlation effects] for valence states of any arbitrary atom was derived and justified by a density matrix formalism for one and two electrons outside a "core". This general method of evaluating (pp pp) is expected to be of considerable use in all types of quantum chemistry calculations.

c. LCAO-MO-SCF (self-consistent field) Calculations for Non-saturated Boron-Containing Molecules.

References: (A-TR-5) (Db-3) (S-7)

An LCAO-MO-SCF (self-consistent field) computer program for non-saturated systems has been written and checked out for 7094 IBM computer. The problem of correct choice of input parameters for boron compounds was investigated (A-TR-5). Calculations are now being performed for boron-containing molecules to obtain resonance energies, amount of partial double-bond character, energy levels, charge distributions and hence reactivities.

A comparative evaluation was made of calculations employing only parameters α and β [corresponding to Coulomb integrals (valence state ionization potentials) and resonance integrals], with calculations including electron repulsion integrals - both with and without iteration to self-consistency. Boron ring compounds were used as a test case and

several quite different conceptual models for compounds such as borazoles were tried. These calculations were performed to ascertain how the various theoretically calculated properties such as energy levels, charge distributions, localization energies, spectra, etc. changed as a function of the calculational method employed. This problem was a continuation of the overall general problem which Dr. Kaufman carried out at the Centre de Mécanique Ondulatoire Appliquée, Paris, France, on comparison of calculations by the three techniques for all types of molecules. In order to be able to evaluate different calculational techniques for boron molecules, it was felt necessary to investigate this problem for molecules for which one had much more calculational experience. Consequently, during May - August 1962 these comparative calculations were carried out first for alternant hydrocarbons, second for non-alternant hydrocarbons, then for molecules containing heteroatoms. One wished to see if the geometry of the molecule or the fact it contained heteroatoms was the dominant factor governing its behavior. A most important finding was that for sites of chemical reactivities there is no consistent relation between charge distribution of the parent molecule and localization energies of the intermediate complex (using several different plausible models for the intermediate complexes). This is a point to be carefully considered for reactivities of boron hydrides, carboranes, etc. where charge distributions are often used as a criterion of reactivity (Db-3) (S-7).

III. Ionization Potentials and Mass Spectral Fragmentation Patterns of Boron Compounds; Also \mathcal{S}_K Values (the effects of substitution on ionization potentials) for cyclic radicals and for O and S compounds.

a. Calculations of Ionization Potentials and Mass Spectral Fragmentation Patterns of Boron Compounds.

References: (A-TR-2) (A-TR-4) (B-1) (B-5) (S-4)

1) Mass spectral fragmentation patterns of boron compounds.

The monoisotopic fragmentation pattern of a molecule is very important because it provides great insight into the mechanism of decomposition of the molecule under external influences and is directly related to its thermal and radiation stability. The problem of calculating monoisotopic fragmentation patterns for boron compounds containing the natural B^{10} - B^{11} abundances was very tedious due to the thousands of separate terms which had to be calculated.

A program for the calculation of monoisotopic fragmentation patterns for boron-containing molecules from mass spectral raw data was written and checked out with the generous cooperation of the Martin Company Computing Center. With this program, it is possible to calculate the monoisotopic fragmentation patterns of boron compounds labeled with both B^{10} and B^{11} as well as with two isotopes of another element such as H or D. The computer program is completely general and is applicable to any $X_m Y_n$ molecule with two different sets of isotopic labels. The availability of a computer program to calculate monoisotopic fragmentation

patterns should make possible a much wider use of mass spectrometry as a means of following the reactions and decomposition of boron compounds than has been previously possible.

Final calculations of fragmentation patterns of various isotopically labeled decaboranes prove that the commonly used method of estimating % B^{10} in a "normal" sample from the ratio of m/e 10 to m/e 11 is NOT valid and an alternate method must be chosen. This problem has far-reaching consequences in the boron field, especially when the B^{10} content of a "normal" sample is counted on as a neutron shielding or neutron absorbing agent. The error in estimating the % B^{10} from the ratio m/e 10 to m/e 11 can be as much as 40% of the total B^{10} content.

Final calculations of the monoisotopic fragmentation patterns of B_5H_9 and B_5D_9 provide an insight into the method of decomposition of pentaboranes which should bear a relationship to their behavior in electric discharge experiments such as are used to prepare $B_{10}H_{16}$ and carboranes.

2) Calculation of ionization potentials of boron compounds from mass spectral appearance potential data.

Calculations of the ionization potentials of B_5H_9 , B_5D_9 and the fragments formed from these molecules were completed during this past year. Comparison of the results indicated a very unusual reverse H-D isotopic effect on the ionization potentials which in turn seems

to have pertinent implications with respect to the valence structure of pentaborane and its fragments.

Data from an earlier appearance potential study of decaborane was re-examined to gain more insight into the behavior of the $B_{10}H_{12}$ fragment. This $B_{10}H_{12}$ fragment seems to be quite closely related to the $B_{10}H_{12}$ portion of $ZB_{10}H_{12}Z$ addition compounds.

b. The Effect of Substitution on Ionization Potentials; δ_K Values.

References: (A-TR-3) (A-TR-9) (B-2) (B-3) (Da-2) (S-1)

It had been previously shown by Dr. Kaufman that the effect of substituent groups on ionization potentials of alkylamines (Y_3N), alkyl free radicals (Y_3C) and boryl radicals (Y_2B) were almost identical. From measured photoionization potentials of amines a new set of constants, δ_K values, which quantitatively reflect changes in ionization potentials were derived. That this δ_K method and the concepts on which it is based have a general validity and scope far beyond their use in predicting ionization potentials has recently been confirmed in an article by W. F. Libby, J. Chem. Phys., 35, 1714 (Nov. 1961) on radiation induced polymerization, in which our work on δ_K values is cited. δ_K values have also assumed importance recently because of the use of δ_K values as a measure of the magnitude of penetration integrals of neutral substituent groups in quantum chemical calculations. (Da-2) (S-1)

- 1) Estimation of the ionization potentials of cycloalkyl radicals and cyclic amines by δ_K values;
 δ_K values for alcohols, ethers and sulfides.

Research performed on this contract has shown that δ_K values obtained from linear and branched alkyl substituents proved to be extendable to cyclic substituents in which the carbon from whence the unpaired electron was being withdrawn was itself part of the ring. This fact would not have been apparent as simply a logical extension of our earlier work on S_K values.

Effects of substitution on ionization potentials were proved not to be the same for the series of alcohols and ethers as for the amines, a specific set of δ_K values for use with oxygen compounds was derived from photoionization measurements. The purpose of these values is twofold: first, to enable one to estimate ionization potentials of other oxygen-containing molecules and second, to permit one to differentiate effects of penetration integrals on different cores, $-\dot{C}$ and $-\dot{N}$: on one hand, and $-O-$ on the other hand. An analogous set of S_K values for S compounds proved to be different from that for O compounds and verifies the fact that the effect of substituent groups is different on first and second row cores. It is concluded that one should use different magnitudes for penetration integrals for substituents on first and second row elements. The observed differences in substituent group effects depending on whether an O (or S) radical or molecule is being ionized imply that one should

perhaps use different evaluations of penetration integrals depending upon whether one or two electrons from O (or S) are contributed to a delocalized system. (A-TR-3) (B-2) (B-3)

2) Extension of the density matrix treatment to a two-body model for electrons outside a "core".

Extension has been made to a two-body model for a pair of electrons outside a "core" of the treatment by density matrix formalism of a one-body model for an electron outside a "core". δ_K values [differences in ionization potentials between the parent compounds] for the π electron of alkyl radicals can be developed exactly as a one-body model problem in terms of density matrices. The derivation of the two-body model permits one quantum mechanically to describe the same δ_K effects on the ionization potentials of an electron from the lone pair of substituted amines by an analogous treatment using the same perturbation Hamiltonian as for substituted alkyl radicals with two electron functions for the lone pair of the nitrogen. (A-TR-9)

(C)

IV. Theoretical Study of Bonding in Aluminum Compounds.

A logical extension of our interest in boron compounds led us to examine analogous properties of aluminum compounds. The theory of charge transfer complexes was applied to the aluminum compounds and on this basis a great deal of regularity becomes apparent in the properties of

aluminum compounds with similar coordination numbers: tetra-, penta- or hexacoordinate. Infrared and NMR data on these compounds were examined and criteria for the determination of the aluminum coordination numbers in various compounds were formulated.

Definition used for electron donors in Mulliken charge-transfer theory are invoked in describing coordination to aluminum. Z, a neutral electron pair donor, and Y^- , an ion electron pair donor, are considered as equivalent.

Aluminum NMR absorptions should exhibit the same shift to higher field with increased Al coordination as do boron compounds. In addition, the magnitude of the coupling constant between hydrogen and aluminum should depend significantly on the percentage of s-character of the bonding hybrid of the directly bonded nucleus. NMR line widths of Al compounds have also been considered indicative of the cubic (octahedral or tetrahedral) or noncubic symmetry around the Al^{27} nucleus.

An Al-H stretch observed in the infrared has been reported to be indicative of whether an Al atom is tetra - (5.6μ) or pentacoordinate - ($5.8 - 5.9\mu$). This shift is easily understood, since the force constant of a bond to a tetraordinate Al must be stronger than that of a bond to a pentacoordinate Al, and $\nu \propto \sqrt{k}$.

All of these criteria should provide an indication of the coordination number of Al in a specific compound, and several examples are discussed.

V. Theoretical Aspects of Bonding in Xenon-Fluorine Compounds
(A-TR-10).

Theoretical concepts of bonding in xenon-fluorine compounds were developed to permit one to generalize and to predict the existence or non-existence of other closely related rare-gas compounds.

The combination of rehybridization of the xenon atom to utilize its d orbitals in valence-shell bonding and back-donation of π electrons from fluorine is the factor which contributes to the formation and stability of these Xe-F compounds.

The correct geometry for XeF_4 was predicted from these postulates, as well as the identification of the lower xenon-fluoride as XeF_2 and its correct geometry, and the existence of both Kr-F and Rn-F compounds.

PUBLICATIONS

A. ONR Technical Reports based on Research under this ONR Contract No. Nonr 3471(00).

1. Lewis Acid-Lewis Base Addition Compounds of Boron Containing Molecules and Their Charge Transfer Behavior, Joyce J. Kaufman, (Also RIAS TR-62-1), Jan. 25, 1962.
2. Appearance and Ionization Potentials of Selected Fragments from Decaborane, $B_{10}^{11}H_{14}$. Joyce J. Kaufman, W. S. Koski, L. J. Kuhns and R. W. Law. March 19, 1962 [published in J. Am. Chem. Soc., 84, 4198 (1962)]
3. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. Joyce J. Kaufman, March 1962. III. Estimation of the Ionization Potentials of Cycloalkyl Radicals and Cyclic Amines by σ_K Values. Published in J. Am. Chem. Soc., 84, 4393 (1962) IV. σ_K Values for Alcohols, Ethers, Thiols and Sulfides, [Published in J. Phys. Chem. 66, 2269 (1962)]
4. Appearance and Ionization Potentials of Selected Fragments from Isotopically Labeled Pentaboranes, Joyce J. Kaufman, W. S. Koski, L. J. Kuhns and Sally S. Wright. April 5, 1962 [Accepted for publication in J. Am. Chem. Soc.]
5. Automatic Computation of LCAO-SCF Molecular Orbitals for Non-Saturated Compounds, G. Berthier. January 1962 [also RIAS TR 62-5]
6. Comment Concerning the Effect on the Diborane-Pentaborane Exchange Reaction of the Reported Deuterium Isotope Effect in the Decomposition of Diborane, Joyce J. Kaufman, May, 1962. [Published in Inorg. Chem. 1, 973 (1962)]
7. Calculation of Basic Parameters Necessary for Quantum Chemical Calculations on Boron-Containing Molecules I. One-Center Electron Repulsion Integral $(pp|pp)_B$, Joyce J. Kaufman, Gaston Berthier, December, 1962. [Also RIAS TR-62-2]
8. Calculation of Basic Parameters Necessary for Quantum Chemical Calculations of Boron-Containing Molecules. II. $(pp|pp)_B$ - and Valence State Electron Affinities of B^- , Odilon Chalvet, Joyce J. Kaufman, December, 1962. [Also RIAS TR-62-2]

9. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. V. Extension of the Density Matrix Treatment to a Two-Body Model for Electrons Outside A "Core". Joyce J. Kaufman, December, 1962. [Also RIAS TR - 62-22]
 10. Some Theoretical Aspects of Bonding in Xe-F Compounds, Joyce J. Kaufman, December, 1962.
- B. Papers published based on Research under this ONR Contract No. Nonr 3471(00).
1. Appearance and Ionization Potentials of Selected Fragments from Decaborane, $B_{10}^{11}H_{14}$. Joyce J. Kaufman, W. S. Koski, L. J. Kuhns, and R. W. Law. J. Am. Chem. Soc., 84, 4198 (1962)
 2. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. III. Estimation of Ionization Potentials of Cycloalkyl Radicals and Cyclic Amines by δ_K Values. Joyce J. Kaufman. J. Am. Chem. Soc. 84, 4393 (1962)
 3. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. IV. S_K Values for Alcohols, Ethers, Thiols and Sulfides. Joyce J. Kaufman. J. Phys. Chem. 66 2269 (1962)
 4. Comment concerning the Effect on the Diborane - Pentaborane Exchange Reaction of the Reported Deuterium Isotope Effect in the Decomposition of Diborane. Joyce J. Kaufman. Inorg. Chem. 1, 973 (1962)
- Accepted for Publication:
5. Appearance and Ionization Potentials of Selected Fragments from Isotopically Labeled Pentaboranes. Joyce J. Kaufman, W. S. Koski, L. J. Kuhns, and Sally S. Wright. J. Am. Chem. Soc.
- C. New Paper Based on Research Under this ONR Contract No. Nonr 3471(00) Presented at National Meeting
1. Criteria for the Determination of the Aluminum Coordination Numbers in Various Compounds. Joyce J. Kaufman. 142nd National American Chemical Society Meeting, Washington, D. C. before the Division of Inorganic Chemistry, March, 1962.

D. Additional Publications since May 15, 1961

a. Research Predated Start of this ONR Contract

1. Some Theoretical Aspects of Bonding in N-F Compounds. Joyce J. Kaufman, J. Chem. Phys. 37, 759 (1962) (also RIAS TR-62-6, April 1962)

2. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. II. Theoretical Interpretation of σ_K Values for Alkyl Radicals and Amines. Joyce J. Kaufman. RIAS TR-62-8, April, 1962

b. Research performed May-Aug. 1962 at Centre de Mecanique Ondulatoire Appliquee, Paris, France

1. Comparison of Various Techniques for Calculation of Localization Energies. I. Alternant and Non-alternant Hydrocarbons. Odilon Chalvet, Raymond Daudel and Joyce J. Kaufman. (accepted for presentation before the Physical Chemistry at the National American Chemical Society National Meeting, Los Angeles, Calif. April 1963)

LECTURES

A. Speeches on Results of New Research presented by Dr. Joyce J. Kaufman
May 15, 1961 - January 30, 1963.

1. The Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. I. A New Set of Constants, the S_K Values. Conference of International Union of Pure and Applied Chemistry, Montreal, Canada.
2. Charge Transfer Complexes of Boron-Containing Molecules. Office of Naval Research, Boron Research Planning Meeting, New Haven, Conn.
3. Some Theoretical Aspects of Bonding in N-F Compounds. American Chemical Society, National Meeting, Chicago, Division of Inorganic Chemistry.
4. Appearance and Ionization Potentials of Selected Fragments from Isotopically Labeled Pentaboranes. American Chemical Society, National Meeting, Chicago, Division of Physical Chemistry.
5. Lewis Acid-Lewis Base Addition Compounds of Boron Containing Molecules and Their Charge Transfer Behavior. American Chemical Society National Meeting, Washington, D.C., Division of Physical Chemistry.
6. Criteria for the Determination of the Aluminum Coordination Numbers in Various Compounds. American Chemical Society National Meeting, Washington, D. C. Division of Inorganic Chemistry.
7. Comparison of Localization Energies Calculated by Various Techniques. Centre de Mecanique Ondulatoire Appliquee, Paris, France. O. Chalvet, R. Daudel and Joyce J. Kaufman.

B. Additional Invited Seminars Presented by Dr. Joyce J. Kaufman.

8. Effect of Substitution on Ionization Potentials of Free Radicals and Molecules. University of Delaware

9. Electron-Deficient Boron Compounds. University of Minnesota Chemistry Department.
10. The Effect of Substitution on Ionization Potentials of Free Radicals and Molecules. Theoretical Interpretation of δ_K Values. University of Wisconsin, Chemistry Department.
11. The Future of Chemistry in Space Travel. Franklin School, Reisterstown, Maryland - Science Club.
12. Lewis Acid - Lewis Base Addition Compounds of Boron Containing Molecules and Their Charge Transfer Behavior. Cambridge University, England - Dept. of Theoretical Chemistry.
13. Lewis Acid - Lewis Base Addition Compounds of Boron Containing Molecules and their Charge Transfer Behavior. King's College, Newcastle-upon-Tyne, England, Chemistry Department.
14. Lewis Acid - Lewis Base Addition Compounds of Boron Containing Molecules and Their Charge Transfer Behavior. University of Sheffield, England - Chemistry Department.
15. Theoretical Interpretation of the Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. University of Manchester, England - Chemistry Department.
16. Theoretical Interpretation of the Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. University of Nottingham, England - Department of Applied Mathematics.
17. Theoretical Interpretation of the Effect of Substitution on the Ionization Potentials of Free Radicals and Molecules. Oxford University, England - Dept. of Applied Mathematics.

Project Personnel

Dr. Joyce J. Kaufman

Principal Investigator

Mrs. Sally Wright

Research Assistant

Dr. Gaston Berthier

Research Associate - 3 months

Dr. Klaus Ruedenberg

Consultant - 5 days

TECHNICAL REPORT DISTRIBUTION LIST

Contract - Nonr 3471(00)

NR # 356-433

No. of Copies

Commanding Officer Office of Naval Research Branch Office The John Crerar Library Building 86 East Randolph Street Chicago 1, Illinois	1
Commanding Officer Office of Naval Research Branch Office 346 Broadway New York 13, New York	1
Commanding Officer Office of Naval Research Branch Office 1030 East Green Street Pasadena 1, California	1
Commanding Officer Office of Naval Research Branch Office Box 39 Navy # 100 Fleet Post Office New York, New York	7
Director, Naval Research Laboratory Washington 25, D. C.	
Attn: Technical Information Officer	6
Chemistry Division	2
Chief of Naval Research Department of the Navy Washington 25, D. C.	
Attn: Code 425	2
DDR&E Technical Library Room 3C-128, The Pentagon Washington 25, D. C.	1
Technical Director Research & Engineering Division Office of the Quartermaster General Department of the Army Washington 25, D. C.	1

Technical Report Distribution List ... cont. Contract Nonr 3471(00)

	<u>No. of Copies</u>
Research Director Clothing & Organic Materials Division Quartermaster Research & Engineering Command U. S. Army Natick, Massachusetts	1
Air Force Office of Scientific Research (SRC-E) Washington 25, D. C.	1
Commanding Officer Diamond Ordnance Fuze Laboratories Washington 25, D. C. Attn: Technical Information Office Branch 012	1
Office, Chief of Research & Development Department of the Army Washington 25, D. C. Attn: Physical Sciences Division	1
Chief, Bureau of Ships Department of the Navy Washington 25, D. C. Attn: Code 342C	2
Chief, Bureau of Naval Weapons Department of the Navy Washington 25, D. C. Attn: Technical Library Code RRMA-3	3 1
ASTIA Document Service Center Arlington Hall Station Arlington 12, Virginia	10
Director of Research U.S. Army Signal Research & Development Laboratory Fort Monmouth, New Jersey	1
Naval Radiological Defense Laboratory San Francisco 24, California Attn: Technical Library	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)

	<u>No. of Copies</u>
Naval Ordnance Test Station China Lake, California Attn: Head, Chemistry Division	1
Code 40	1
Code 50	1
Commanding Officer Army Research Office Box CM, Duke Station Durham, North Carolina Attn: Scientific Synthesis Office	1
Brookhaven National Laboratory Chemistry Department Upton, New York	1
Atomic Energy Commission Division of Research Chemistry Programs Washington 25, D. C.	1
Atomic Energy Commission Division of Technical Information Extension Post Office Box 62 Oak Ridge, Tennessee	1
U. S. Army Chemical Research and Development Labs. Technical Library Army Chemical Center, Maryland	1
Office of Technical Services Department of Commerce Washington 25, D. C.	1
Bureau of Naval Weapons Representative Westinghouse Electric Corporation P. O. Box 746 Baltimore 3, Maryland	1
Commanding Officer Office of Naval Research Branch Office 1000 Geary Street San Francisco 9, California Attn: Dr. P. A. Miller	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)No. of Copies

Commanding Officer Office of Naval Research Branch Office 495 Summer Street Boston 10, Massachusetts Attn: Dr. A. L. Powell	1
Dr. H. S. Gutowsky Department of Chemistry University of Illinois Urbana, Illinois	1
Dr. D. A. Brown Department of Chemistry University College Upper Merrion Street Dublin, Ireland	1
Dr. J. T. Vanderslice Institute of Molecular Physics University of Maryland College Park, Maryland	1
Dr. Anton B. Burg Department of Chemistry University of Southern California University Park Los Angeles 7, California	1
Dr. E. G. Rochow Department of Chemistry Harvard University Cambridge 38, Massachusetts	1
Dr. T. D. Parsons Department of Chemistry Oregon State College Corvallis, Oregon	1
Dr. T. P. Onak Department of Chemistry Los Angeles State College Los Angeles, California	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)No. of Copies

Dr. Robert W. Taft, Jr. Department of Chemistry Pennsylvania State University University Park, Pennsylvania	1
Dr. J. D. Roberts Department of Chemistry California Institute of Technology Pasadena, California	1
Dr. J. E. Leffler Department of Chemistry Florida State University Tallahassee, Florida	1
Dr. M. J. S. Dewar Department of Chemistry University of Chicago Chicago, Illinois	1
Dr. T. L. Heying Olin Mathieson Chemical Corporation 275 Winchester Avenue New Haven, Connecticut	1
Dr. G. Barth-Wehrenalp, Director Inorganic Research Department Pennsalt Chemicals Corporation Box 4388 Philadelphia 18, Pennsylvania	2
Mr. K. Warren Easley Monsanto Research Corporation Everett Station Boston 49, Massachusetts	1
Dr. Hans H. Jaffe Department of Chemistry University of Cincinnati Cincinnati, Ohio	1
Dr. Murray S. Cohen Chief, Propellant Synthesis Section Reaction Motors Division Thiokol Chemical Corporation Denville, New Jersey	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)No. of Copies

Professor W. S. Koski Chemistry Department The Johns Hopkins University Baltimore, Maryland	1
Dr. Vernon H. Dibeler, Chief Mass Spectrometry Section National Bureau of Standards Washington 25, D. C.	1
Dr. E. J. Prosen, Chief Thermochemistry Section National Bureau of Standards Washington 25, D. C.	1
Dr. L. J. Edwards Manager of Programs Callery Chemical Company Callery, Pennsylvania	1
Dr. Edgar W. Fajans Assoc. Director of Chemical Research U.S. Borax Research Corporation 412 Crescent Way Anaheim, California	1
Dr. R. W. Parry Department of Chemistry University of Michigan Ann Arbor, Michigan	1
Commanding Officer Frankford Arsenal Philadelphia 37, Pennsylvania Attn: ORDBA-LCO	1
Dr. Riley Schaeffer Department of Chemistry Indiana University Bloomington, Indiana	1
Dr. S. Golden Department of Chemistry Brandeis University Waltham 54, Massachusetts	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)No. of Copies

Dr. M. F. Hawthorne Rohm and Haas Company Philadelphia 5, Pennsylvania	1
Dr. W. N. Lipscomb Department of Chemistry Harvard University Cambridge 38, Massachusetts	1
Dr. H. C. Clark Department of Chemistry University of British Columbia Vancouver, British Columbia Canada	1
Dr. H. B. Jonassen Department of Chemistry Tulane University New Orleans, Indiana	1
Dr. M. M. Chamberlain Department of Chemistry Western Reserve University Cleveland, Ohio	1
Dr. D. C. Bradley Department of Chemistry University of Western Ontario London, Canada	1
Dr. Henry Taube Department of Chemistry Stanford University Stanford, California	1
Dr. C. E. Nordmann Department of Chemistry University of Michigan Ann Arbor, Michigan	1
Dr. Ross I. Wagner American Potash & Chem. Corporation Research Department Whittier, California	1

Technical Report Distribution List ... cont.Contract Nonr 3471(00)No. of Copies

Dr. E. C. Ashby
Ethyl Corporation
Baton Rouge, Louisiana

1

Dr. George F. Huff, Vice President
Research and Development
Callery Chemical Company
Callery, Pennsylvania

1

Dr. David Chamberlain, Jr.
Stanford Research Institute
Menlo Park, California

1