Dear Dr Weaver: Here is my little report. I have enjoyed meeting you.

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Biology + Chemistry

October 24, 1933. Brief Account of Research in Chemistry Supported by Grant from the Rockefeller Foundation.

The general plan of the research involves an experimental and theoretical attack on important problems of ~~this~~ structural chemistry through the use of recent developments in physics. The experimental methods principally used are x-ray diffraction by crystals and electron diffraction by gas molecules. The latter procedure was originated by Mark and Wierl in 1930; our own work in this field was the first done in America. The theoretical work involves the application of quantum mechanics to complex molecules.

In developing structural chemistry we have not drawn a line between inorganic and organic substances, and at first most of our work, covering compounds of all elements, dealt with organic compounds to only a small extent. However, our methods have been found to be particularly valuable in the treatment of the complicated problems of organic chemistry, and we are now devoting the major part of our effort to these problems. The first applications of our method of solving the Schrödinger wave equation for complex molecules were to aromatic molecules, leading to the complete determination of the nature of benzene, naphthalene, and other aromatic hydrocarbons, and of the hydrocarbon free radicals, whose structure had been the focus of attention ever since their discovery by Gomberg thirty years ago. The treatment has been applied to conjugated systems of double bonds and aromatic nuclei (such as exist in carotene, for example), and is now being extended to heterocyclic rings, such as pyrrole, with the hope that ultimately an attack can be made in this way on the purpurins, chlorophyll, hemoglobin, and other substances of biological importance.

The electron-diffraction method has shown itself to be particularly useful in treating organic molecules. We have discovered a relation between interatomic separation and bond type or electronic structure which permits the

deduction of the electronic structure from the experimental determination of the configuration of the molecule, and which in particular permits the experimental determination of the existence and extent of resonance of a molecule among several electronic structures. Thus we have shown the azide group in methyl azide to be linear rather than cyclic, settling a question of structure left unsettled by the organic chemists despite investigations extending over many years. The experimental study of resonance in conjugated systems (which is closely correlated with our quantum-mechanical work) has been begun, cyanogen, diacetylene, and carbon suboxide having been already investigated, with benzene, pyrrole, cyclopentadiene, furane, and many similar molecules now being studied.

The study of crystals with x-rays has led to very valuable results regarding inorganic substances, the general principles determining the structure of ionic crystals such as the silicates having been formulated three or four years ago. We are now studying the sulfide minerals and other similar crystals to obtain information regarding the covalent bond, and in addition investigating organic and inorganic crystals which promise to throw light on one of our general problems. (For example, the study of NH_4HF_2, containing hydrogen bonds, may help in the determination of the structure of proteins, in which these bonds without doubt play a part.) With the completion of the new ionization spectrometer, designed by Dr. Sturdivant especially for structure investigations, we hope to pay more attention to organic crystals, ultimately investigating crystalline substances of biological importance, such as hemoglobin.

The men working with me are the following:

Research Fellows on Rockefeller Fund:

Dr. J.H.Sturdivant, constructing ionization spectrometer.
Dr. L.O.Brockway, electron diffraction.
Dr. G.W.Wheland, organic preparations, quantum mechanics of organic molecules. (Harvard)
Dr. E.B.Wilson, Jr. quantum mechanics.
Dr. J. Sherman) Calculators in quantum mechanics and crystal
Dr. S. Weinbaum) structure.

Additional Research Fellows:

Dr. L.E.Sutton, International Fellow in Organic Chemistry, (Oxford), Electron diffraction of organic molecules.
Dr. L. LaCoste, Texas, quantum mechanics.
Dr. L. Helmholtz, Johns Hopkins, crystal structure.
Dr. H.P.Klug, Ohio State, crystal structure.

Graduate Students:

J.Y.Beach, electron diffraction.
F.T.Wall, electron diffraction.
W.V.Medlin, crystal structure.
D.Harker, Crystal structure.
J.B.Howard, crystal structure.

The complex and difficult nature of most of our problems, especially the quantum-mechanical ones, makes them unsatisfactory for graduate students.

Linus Pauling

Summary of investigations completed or well under way.
(July 1, 1932 - October, 1933)
(* indicates research published or in hands of publisher.)

Crystal Structure:

Ionic crystals:
* Zunyite, $Al_{13}Si_5O_{20}(OH)_{18}Cl$
* $RbNO_3$
* $Na_7(PO_4)_2F.19H_2O$

Sulfide minerals:
* Chalcopyrite, $CuFeS_2$
* Sulvanite, Cu_3VS_4
* Binnite, $Cu_{12}As_4S_{13}$
* Enargite, Cu_3AsS_4
  Tetradymite, Bi_2Te_2S
  Pentlandite, (Fe,Ni)S

Organic crystals:
  $C_2H_4I_2$
  $C_2H_2I_2$
* Ortho-C_6H_4ICOOH
  1,3,5-$C_6H_3(C_6H_5)_3$

Other substances:
* CaB_6
* $KAg(CN)_2$
* KSCN
* K_2SeBr_6
* $Pd(NH_3)_4Cl_2.H_2O$
  $(NH_4)_6Mo_7O_{24}.4H_2O$

Electron diffraction:

* SF_6, SeF_6, TeF_6
* ClO_2
* CH_3N_3, C_3O_2
* C_2N_2, C_4H_2
  PF_5, C_6H_6, C_4H_4NH, and many other molecules.

Quantum mechanics:

Simple atoms and molecules:
* He_2^+, He_2^{++}
* H_2^+, H_2
* Li, Be^+, ---
  Be, B, C, N, O, F
  Li_2^+

Complex molecules:
* Calculation of matrix elements for molecules.
* Benzene, naphthalene, and free radicals.
* Values of resonance energy of molecules.
* Conjugation in organic molecules.
* Keto-enol isomerism.
  Heterocyclic compounds.
  Acid strengths of aromatic substances.
  Quinones.
  Chromophore groups.

Miscellaneous investigations:
* Tables of sin x/x (for electron diffraction).
* The structure of the antimonates.
* Magnetic properties of KO_2.
* Madelung constant of cuprite.

Published Papers, 1932-3.

1. The Formulas of Antimonic Acid and the Antimonates. Linus Pauling, J.Am.Chem.Soc., 55, 1895-1900 (1933).

2. Note on Dr. Wheeler's Discussion of the Madelung Constants for Some Cubic Crystal Lattices. J.Sherman, Phil.Mag., 14 (7), 745 (1932).

3. The Determination of the Structures of the Hexafluorides of Sulfur Selenium and Tellurium by the Electron Diffraction Method. L.O.Brockway and Linus Pauling, Proc.Nat.Acad., 19, 68-73 (1933).

4. The Crystal Structure of Zunyite, $Al_{13}Si_5O_{20}(OH,F)_{18}Cl$. Linus Pauling. Zeit.f.Krist., 84, 442-452 (1933).

5. Note on the Structure of Rubidium Nitrate. Linus Pauling and J. Sherman, Zeit.f.Krist., 84, 213-216 (1933).

6. The Crystal Structure of Ammonium Hydrogen Fluoride, NH_4HF_2. Linus Pauling. Zeit.f.Krist., ~~(in press)~~ 85, 380-391 (1933)

7. Röntgenographische Untersuchung an Natriumfluorophosphat. Edward Neuman Zeit.f.Krist. ~~(submitted for publication)~~ 86, 298-300 (1933)

8. The Crystal Structure of Chalcopyrite, Linus Pauling and L.O.Brockway Zeit.f.Phys.Chem., 82, 188-194 (1932).

9. The Crystal Structure of Sulvanite. Linus Pauling and Ralph Hultgren. Zeit.f.Krist., 84, 204-212 (1933).

10. The Crystal Structure of Potassium Bromoselenite. J.L.Hoard and B.N.Dickinson. Zeit.f.Krist., 84, 436-441 (1933).

11. The Crystal Structure of Potassium Thiocyanate. Harold P. Klug. Zeit.f.Krist., 85, 214-221 (1933).

12. Wave Functions for the Ground State of Lithium and Three-Electron Ions. E.Bright Wilson, Jr. J.Chem.Phys., 1, 210-218 (1933).

13. The Normal State of the Hydrogen Molecule-Ion. B.N.Dickinson. J.Chem.Phys., 1, 317-318 (1933).

14. The Normal State of the Hydrogen Molecule. Sidney Weinbaum. J.Chem.Phys., ~~(Submitted for publication)~~ 1, 593-596 (1933)

15. The Calculation of Matrix Elements for Lewis Electronic Structures of Molecules. Linus Pauling. J.Chem.Phys., 1, 280-283 (1933).

16. The Nature of the Chemical Bond. V. Quantum Mechanical Treatment of Aromatic Substances and Hydrocarbon Free Radicals. Linus Pauling and G.W.Wheland. J.Chem.Phys. 1, ~~(in press)~~ 362-374 (1933)

17. Nature of the Chemical Bond. VI. The Energy of Resonance of Molecules among Several Electronic Structures from Thermochemical Data. Linus Pauling and J. Sherman. J. Chem. Phys. ~~(submitted for publication)~~ 1, 606-617 (1933)

18. The Crystal Structure of ortho-benzoic Acid. H.P. Klug. Iodo J. Am. Chem. Soc., 55, 1430-1437 (1933)

19. The Normal State of the Helium Molecule-Ions He_2^+ and He_2^{++}. Linus Pauling, J. Chem. Phys., 1, 56-59 (1933).

20. The Three-Electron Bond in Chlorine Dioxide. L.O. Brockway Proc. Nat. Acad., 19, 303-307 (1933).

Papers published or in process of publication, October 24, 1933.

21. Electron-diffraction Investigation of Methyl Oxide and Carbon Suboxide, L.O. Brockway and Linus Pauling, P.N.A. Sept. 1933.

22. Determination of the Structure of Cyanogen and Diacetylene by Electron Diffraction. L.O. Brockway, P.N.A. Sept. 1933.

23. The Nature of the Chemical Bond. VII. The Calculation of Resonance Energy in Conjugated Systems. L. Pauling and J. Sherman. J.C.P. 1, 679-86 (1933)

24. A Calculation of the Equilibria in Keto-enol Isomerism. G.W. Wheland, J. Chem. Phys. 1, 731-736 (1933)

25. The Crystal Structure of Binnite. L. Pauling and E.W. Neuman, Z. Krist., in press.

26. The Crystal Structure of Enargite, L. Pauling and S. Weinbaum, submitted to Z. Krist.

27. Atomic Radii in Crystals Containing Covalent Bonds, L. Pauling and M.L. Huggins, Z. Krist., in press.

28. A Four-place Table of $\sin x / x$, J. Sherman, Z. Krist. 85, 404-19 (33)

29. Note on the Madelung Constant of Cuprite, J. Sherman, submitted to Phil. Mag.

30. The Crystal Structure of Tetramminopalladous Chloride, B.N. Dickinson, submitted to Z. Krist.