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Guide to the Robert S. Mulliken Papers 1908-1985



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Descriptive Summary

Identifier	ICU.SPCL.MULLIKEN
Title	Mulliken, Robert S. Papers
Date	1908-1985
Size	63 linear ft. (130 boxes)
Repository	Special Collections Research Center University of Chicago Library 1100 East 57th Street Chicago, Illinois 60637 U.S.A.

Abstract The papers of Robert S. Mulliken, comprising 63 linear feet, document most aspects of his long and successful career in the field of chemical physics from the 1920s through 1985. They include correspondence, lectures and writings, research and teaching materials, and files from his affiliations at the University of Chicago and with other scientific organizations.

Information on Use

Access

No restrictions

Citation

When quoting material from this collection, the preferred citation is: Mulliken, Robert S. Papers, [Box #, Folder #], Special Collections Research Center, University of Chicago Library

Biographical Note

Robert Sanderson Mulliken was born in Newburyport, Massachusetts on June 7, 1896. His father, Samuel Mulliken, was a chemistry professor at the Massachusetts Institute of Technology, where Robert Mulliken received his B.S. degree in chemistry in 1917. During World War I, Mulliken worked under James B. Conant of the Chemical Warfare Service doing research on poison gases. He began graduate work in the Chemistry Department at the University of Chicago in 1919 under the supervision of William D. Harkins. He received a National Research Fellowship upon completing his Ph.D. degree in 1921 with a thesis on the partial separation of mercury isotopes by evaporation. Mulliken continued this research at the University of Chicago until 1923, when he went to Harvard University to learn spectroscopy and to study theoretical physics. Visiting Europe in the summers of 1925 and 1927, he met many of the most important physicists of the day including Niels Bohr and Erwin Schrödinger, along with a number of younger scientists. He returned to Europe as a Guggenheim Fellow in 1930 and again in 1932-1933, accompanied by his wife, Mary Helen Von No, Mulliken, whom he married on

December 24, 1929. The Mullikens had two daughters, Lucia Maria born in 1934, and Valerie No, born in 1948.

Mulliken joined the faculty of New York University as an assistant professor of physics in 1926 and remained there until 1928, when he returned to the University of Chicago as Associate Professor of Physics. He was made Professor of Physics in 1931, and Ernest DeWitt Burton Distinguished Service Professor of Physics in 1956. He remained an active member of the faculty after official retirement as Distinguished Service Professor of Physics and Chemistry from 1961 through 1985. He also held an appointment as Distinguished Research Professor of Chemical Physics during winter quarters at Florida State University in Tallahassee from 1964-1971. Mulliken died in Alexandria, Virginia on October 31, 1986.

Mulliken's postdoctoral work at Harvard led him to explore the relations between molecules and atomic electronic states through analysis and classification of band spectra. Following the establishment of the new quantum theory in the 1920s, Mulliken (contemporaneously with Friedrich Hund) applied group theoretical methods to these phenomena and developed the molecular orbital, or MO, method for explaining molecular structure. At the same time, he continued the work in experimental spectroscopy he began at Harvard and was instrumental in the design and construction of a spectroscopic laboratory at the University of Chicago. This extensive theoretical and experimental work in the study of molecules was highlighted in the 1930s with the publication of a series of papers on electronic structures of Polyatomic Molecules and valence. It was this foundational work that is largely credited for his receipt of the Nobel Prize in chemistry in 1966. Mulliken followed this work in the late 1930s by extending the MO theory to the study of the absolute strengths of electronic transitions in molecules.

The MO theory was one of two descriptive theories developed in this period to apply the ideas and formalisms of quantum mechanics to the problems of molecular structure. While the valence bond theory (articulated primarily by Heitler, London, and Pauling) treated molecules as made of interacting but individual atoms, each maintaining its own electrons, the MO theory as developed by Mulliken and others treats the electrons of a molecule as being spread out in wave functions, or orbitals, over all the atoms in a chemical bond of molecule. This model gave predictive equations describing properties of spatial structure, chemical binding energies, ionization potentials, and molecular spectra.

While Mulliken's early work provided the MO theory with a rigorous mathematical form, the complexity of the equations makes their exact solution impossible. Attempts were made during the 1940s and 1950s to improve available approximations through the use of semi empirical methods, and beginning in the late 1940s, Mulliken and his collaborators were engaged in research using new wholly theoretical techniques and increasingly sophisticated computers to improve the accuracy of calculations based on the MO theory. During the 1950s and 1960s, he pursued research on the study of donor-acceptor relations and charge-transfer complexes,

conjugation and hyper conjugation in ions, and population analysis on LCAO-MO wave functions.

During World War II, Mulliken served as Director of the Information Division of the Plutonium Project at the Metallurgical Laboratory of the University of Chicago. In 1944, he helped to draft the Plutonium Project's first "Prospectus on Nucleonics" on peaceful uses of atomic energy. Following the war, Mulliken's active research group in spectroscopy resumed its activities, and from 1952 were officially designated the Laboratory of Molecular Structure and Spectra. Dozens of researchers from all over the world, both theoreticians and experimentalists, spent time at LMSS as students, postdoctoral fellows, or research associates. Mulliken spent a year in Oxford as a Fulbright Fellow in 1953, and served as scientific attach, at the United States Embassy in London during 1955. He maintained extensive contacts with scientists throughout Europe, India, and Japan and attended many international scientific meetings.

In the course of his career, Mulliken published over 200 papers. In addition, he collaborated on the publication of three review volumes in the 1960s and 1970s. His autobiography, *Life of a Scientist*, was edited by Bernard Ransil and published posthumously by Springer-Verlag in 1989.

Mulliken received many honorary degrees and most of his profession's highest honors, including the G. N. Lewis Medal, the Peter Debye Award, the J. Willard Gibbs Medal, and the Priestley Medal of the American Chemical Society. He was awarded the Nobel Prize in Chemistry in 1966. He was a member of many scientific societies both in the U.S. and abroad, including the National Academy of Sciences to which he was elected in 1936. A member of the American Physical Society from the 1920s, he was in 1944-1945 chairman of a committee to organize a Division of Spectroscopy. Their work led to the establishment of the Division of Chemical Physics, with Mulliken as its inaugural chairman, in 1951.

Scope Note

Mulliken maintained extensive files of his correspondence, and other materials concerning research and professional activities through most of his long career. The papers have been arranged in four series:

Series I: BIOGRAPHICAL MATERIALS

Series I begins with items associated with Mulliken's youth, his hometown of Newburyport, Massachusetts, and his college days at the Massachusetts Institute of Technology. Items in BOX 1, Folders 10-12 possibly came to Mulliken from his father Samuel Mulliken. The collection of memorabilia that follows consists of materials from Mulliken's travels abroad and from the period surrounding his receipt of the Nobel Prize. Filed with his personal memorabilia

are biographical items about Mulliken and his collection of biographical reprints about other scientists. Some other memorabilia (honorary certificates and degrees) can be found in BOX 131. The final section of this series includes material from Mulliken's various political and extrascientific activities, including records from his year as science attach, in London.

Series II: CORRESPONDENCE

Series II includes Mulliken's correspondence from the 1920s through 1985 and is arranged in four subseries. The first and largest part of the series consists of his correspondence with individuals, mostly though not exclusively fellow scientists. It is arranged alphabetically by the last name of correspondent, with the exception of some files of correspondence with Indian colleagues collected together as "India correspondence" in BOX 25.

The second section contains his correspondence with various institutions, including professional societies, corporations for whom he did consulting work, and funding agencies. This correspondence is arranged alphabetically by name of institution.

The next subseries includes most of Mulliken's correspondence with editors and publishers about his work, arranged alphabetically by name of publisher or publication. The final subseries contains correspondence about particular books. Filed with this correspondence are typescripts and related material.

Series III: SCIENTIFIC AND PROFESSIONAL ACTIVITIES

Series III consists of four subseries, corresponding to different aspects of Mulliken's scientific work. The first part of this series includes material from Mulliken's extensive attendance at conferences and symposia. This material is arranged in two sections. The first of these contains material, arranged alphabetically by conference name, from a select group of special annual conferences which Mulliken attended in several years. The second contains material from all other conferences, symposia, and certain visits, arranged chronologically.

The next subseries contains materials associated with many of Mulliken's talks to scientific and popular audiences from the 1920s through 1981. Arranged chronologically, the material includes drafts, typescripts, and photocopies of slides from talks on a wide range of Mulliken's research interests. A small collection of tape recordings is also included (BOX 79).

The third subseries contains Mulliken's research materials from the 1920s through the 1970s. It includes notes, drafts and typescripts for published and unpublished research, and annotated reprints arranged roughly chronologically in Boxes 80-100. Boxes 101-104 contain glass photographic plates of spectra from Mulliken's work in the 1920s.

The final section of this series contains copies of many of Mulliken's published papers, arranged chronologically.

Series IV: THE UNIVERSITY OF CHICAGO

This series is divided into five subseries. The first three contain general material about the University of Chicago, the Physical Sciences Division and the Physics Department. These are followed by material from the Laboratory of Molecular Structure and Spectra. The LMSS material is broken into general material, research reports, personnel, grants and contracts, and miscellaneous. The next subseries contains records of Mulliken's activities with the Department of Chemistry and the final subseries contains notes from various courses taught by Mulliken from 1928 through the 1970s, arranged chronologically.

Series V: OVERSIZE

Related Resources

The following related resources are located in the Department of Special Collections:

<http://www.lib.uchicago.edu/e/spcl/select.html>

A large collection of Mulliken's scientific offprints and related material is held separately in the archives. Other material related to Mulliken can be found in the University Presidents' Papers, the John A. Simpson Papers, and records of the Department of Physics and the Physical Sciences Division. The papers of his father-in-law, Adolf Carl Noe, are also located in the archives.

Subject Headings

- Clementi, Enrico
- Coulson, C. A. (Charles Alfred), 1910-1974
- De Maine, Paul A. D
- Duchesne, J. (Jules)
- Fernández Morán Villalobos, Humberto, 1924-
- Herzberg, Gerhard, 1904-
- Libby, Leona Marshall, 1919-
- Löwdin, Per Olov, 1916-
- Mulliken, Robert Sanderson
- Parr, Robert G., 1921-

- Person, Willis B., 1928-
- Platt, John Rader, 1918-
- Price, William Charles, 1909-
- Slater, John Clarke, 1900-1976
-
- University of Chicago. Dept. of Chemistry
- University of Chicago. Dept. of Physics
- University of Chicago. Division of the Physical Sciences
- University of Chicago. Laboratory of Molecular Structure and Spectra
- Chemistry
- Physics
- Molecular orbitals
- Molecular spectroscopy

INVENTORY

Series I: Biographical Materials

Subseries 1: Personal

Box 1

Folder 1

Letters to Katherine Mulliken, ca. 1910

Box 1

Folder 2

Newburyport, Massachusetts, miscellaneous

Box 1

Folder 3-5

Newburyport, Massachusetts, high school, commencement programs

Box 1

Folder 6

"Electrons; What they are and what they do," correspondence, ca. 1960s

Box 1

Folder 7

Student essays, 1908, 1913-1914

Box 1

Folder 8

Massachusetts Institute of Technology, Themes, English class, 1913-1914

Box 1

Folder 9

Massachusetts Institute of Technology, Class of 1917, 50th reunion

Box 1

Folder 10

National Research Council, Division of Chemistry, minutes, April 27, 1921

Box 1

Folder 11

Massachusetts Institute of Technology, "Proposal to establish a graduate school," 1932

Box 1

Folder 12

Massachusetts Institute of Technology, chemistry department, miscellaneous material, ca. 1930s

Box 1

Folder 13-15

Autobiographical notes

Box 1

Folder 16

Autobiography, notes and correspondence, ca. 1980s

Box 1

Folder 17-20

Autobiography, drafts

Box 2

Folder 1-4

Autobiography, drafts

Box 2

Folder 5-10

Christmas cards, ca. 1970s-1980s

Subseries 2: Memorabilia

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Europe, 1948, memorabilia

Box 3

Folder 2

Europe, 1948, personal correspondence

Box 3

Folder 3

Europe, 1948, Paris, posters

Box 3

Folder 4-6

Europe, 1953, memorabilia

Box 3

Folder 7

Russia, 1958

Box 3

Folder 8

University of Chicago, Citizens' Board Dinner, December 1966

Box 3

Folder 9

Chicagooan of the Year, Award Dinner, January 1967

Box 3

Folder 10-20

Nobel prize, autograph requests

Box 4

Folder 1-10

Nobel prize, congratulatory letters and telegrams

Box 4

Folder 11

Nobel prize, invitations

Box 4

Folder 12-14

Nobel prize, lecture

Box 4

Folder 15

Nobel prize, miscellaneous

Box 4

Folder 16

Student inquiries

Box 5

Folder 1-2

Miscellaneous invitations

Box 5

Folder 3

Invitations declined, 1966-1981

Box 5

Folder 4

Guest of honor, recruit graduation review, Great Lakes Naval Training Center, March 19, 1976

Box 5

Folder 5

Biography entries

Box 5

Folder 6-7

Articles about Mulliken

Box 5

Folder 8-12

Scientists' biographical reprints

Box 6

Folder 1-3

Scientists' biographical reprints

Box 6

Folder 4

Miscellaneous correspondence and memorabilia

Box 7

Folder 1

Plaque, guest of honor Great Lakes Recruit Training Command, 1976

Box 7

Folder 2

National Academy of Sciences Centennial Medal

Box 7

Folder 3

Chicago Press Club, Chicagoan of the Year, 1966, inscribed plaque from commemorative statue

Box 8

Folder 1-3

Indian decorative memorabilia

Subseries 3: Political and special interest activities

Box 9

Folder 1

Gamma Alpha fraternity, Chicago chapter

Box 9

Folder 2-7

American Association of Scientific Workers

Box 10

Folder 1-2

Scientists' Committee on Loyalty Problems, 1948-1950

Box 10

Folder 3

"Loyalty tests," talk, 1949

Box 10

Folder 4

Atomic Scientists of Chicago, ca. 1950s

Box 10

Folder 5

Geneva Atomic Energy Conference, 1955

Box 10

Folder 6-7

American Embassy, London, personal correspondence, 1955-1961

Box 10

Folder 8

Science attache, activities, ca. 1955

Box 10

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Science attache, diary

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Folder 10

Science attache, personal papers

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Folder 11

Science attaché, personal correspondence

Box 10

Folder 12-13

Science attache, engagement calendar

Box 10

Folder 14-18

Science attache, personal contacts

Box 11
Folder 1
Embassy activities, miscellaneous

Box 11
Folder 2
Embassy period material

Box 11
Folder 3-4
Science and the state, correspondence, 1956-1958

Box 11
Folder 5
Japan Council Against Atomic and Hydrogen Bombs

Box 11
Folder 6
Science and Foreign Relations

Box 11
Folder 7
Center for the Study of Democratic Institutions

Box 11
Folder 8-9
Committee on the Present Danger

Box 11
Folder 10
Congressional correspondence file

Box 11
Folder 11
Cosmos Club, Washington, D.C.

Box 11
Folder 12
Federation of American Scientists, ca. 1960s-1970s

Box 11
Folder 13-14
International Cultural Foundation

Box 11
Folder 15
International Conference on the Unity of the Sciences, London, 1974

Box 12
Folder 1-4
International Conference on the Unity of the Sciences, New York, 1975

Box 12
Folder 5
International Conference on the Unity of the Sciences, Washington, D. C., 1976

Box 12
Folder 6
International Conference on the Unity of the Sciences, 1977-1978

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Folder 7

International Conference on the Unity of the Sciences, Los Angeles, 1979

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International Conference on the Unity of the Sciences, Miami Beach, Florida, 1980

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Folder 9

International Conference on the Unity of the Sciences, Seoul, Korea, 1981

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Negative Population Growth, Inc.

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Sakharov, Andrei, tribute, May 19, 1981

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Sakharov, Andrei, efforts to assist

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Folder 13

Savile Club

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Folder 1-4

Scientists and Engineers for Secure Energy

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Folder 5-6

Weizmann Institute of Science

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Folder 7-8

World Cultural Council

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Folder 9-10

Miscellaneous political groups, correspondence

Box 13

Folder 11

Astrology

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Futurology

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Ball lightning

Box 13

Folder 14

"Through ZPG to NPG," typescript and correspondence

Series II: Correspondence

Subseries 1: Individuals

Box 14

Folder 1

Abelson, Phillip

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Adler, B.

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Allen, L. C.

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Allison, Michael D.

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Altman, S. L.

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Anderson, Herbert L.

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- Araki, Gentaro
- Aronson, Harmon
- Atkinson, Edward R.
- Auterhoff, H.

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A, general

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Bader, R. F. W.

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Bak, Borge

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Barrow, R. F.

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Barton, Henry A.

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Basu, S., with Bhattacharya, R.

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Bates, D. R.

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Bidelman, William P.

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- Brown, H. C.
- Brown, M. G.
- Brown, R. D.
- Brown, W. G.
- Browne, J. C.

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Buenker, Robert J., 1969-1982

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Bunnett, J. F.

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- Buraway, Ida
- Burke, Mrs. Edmund
- Burnelle, Louis
- Burton, Milton

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B, general

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Cade, Paul E.

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- Calais, Jean-Louis
- Callomon, J. H.
- Carrington, Alan

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Carroll, Peter K., 1960-1963

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- Castex, M. C.
- Certain, Phillip R.
- Chandrasekharan, V.
- Chisolm, S. L.

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Chiu, Lue-yung chow

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- Closs, G. L.
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Coleman, G. H.

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Condon, Edward U.

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Coon, Jesse B.

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Cotton, F. Albert

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Coulson, Charles A., 1948-1975

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