RESOURCE - RELATED RESEARCH

COMPUTERS AND CHEMISTRY

(RR-00612 COMPETING RENEWAL APPLICATION)

Submitted to

BIOTECHNOLOGY RESOURCES BRANCH

OF THE

NATIONAL INSTITUTES OF HEALTH

May, 1976

site visit 1/7/77

DEPARTMENTS OF

CHEMISTRY, GENETICS, AND COMPUTER SCIENCE

STANFORD UNIVERSITY
GRANT APPLICATION

TO BE COMPLETED BY PRINCIPAL INVESTIGATOR (Items 1 through 7 and 15A)

1. TITLE OF PROPOSAL (Do not exceed 53 typewriter spaces)

RESOURCE-RELATED RESEARCH - COMPUTERS AND CHEMISTRY

2. PRINCIPAL INVESTIGATOR

Djerassi, Carl

Professor of Chemistry

2C. MAILING ADDRESS (Street, City, State, Zip Code)

Department of Chemistry
Stanford University
Stanford, California 94305

2D. DEGREE
Ph.D.

2E. SOCIAL SECURITY NO.

2F. TELEPHONE AREA CODE/TELEPHONE NUMBER/EXTENSION

415/555-1234

2G. DEPARTMENT, SERVICE, LABORATORY OR EQUIVALENT

Department of Chemistry

2H. MAJOR SUBDIVISION (See Instructions)

Department of Humanities and Sciences

7. Research Involving Human Subjects (See Instructions)

A. NO B. YES Approved:

C. YES - Pending Review

TO BE COMPLETED BY RESPONSIBLE ADMINISTRATIVE AUTHORITY (Items 8 through 13 and 15B)

9. APPLICANT ORGANIZATION(S) (See Instructions)

Stanford University
Stanford, California 94305
IRS No. 94-1156365
Congressional District No. 12

10. NAME, TITLE, AND TELEPHONE NUMBER OF OFFICIAL(S)
SIGNING FOR APPLICANT ORGANIZATION(S)

c/o Sponsored Projects Office
Telephone Number (415) 497-2883

11. TYPE OF ORGANIZATION (Check applicable item)

□ FEDERAL □ STATE □ LOCAL □ PRIVATE, NON-PROFIT UNIVERSITY

12. NAME, TITLE, ADDRESS, AND TELEPHONE NUMBER OF OFFICIAL IN BUSINESS OFFICE WHO SHOULD ALSO BE NOTIFIED IF AN AWARD IS MADE

K. D. Creighton
Deputy Vice Pres. for Business & Finance
Stanford University
Stanford, California 94305

Telephone Number (415) 497-2251

13. IDENTIFY ORGANIZATIONAL COMPONENT TO RECEIVE CREDIT FOR INSTITUTIONAL GRANT PURPOSES (See Instructions)

20 School of Humanities and Sciences

14. ENTITY NUMBER (Formerly PHS Account Number)

1941156365A1

15. CERTIFICATION AND ACCEPTANCE. We, the undersigned, certify that the statements herein are true and complete to the best of our knowledge and accept, as to any grant awarded, the obligation to comply with Public Health Service terms and conditions in effect at the time of the award.

SIGNATURES
(Signatures required on original copy only. Use ink. “Pen” signatures not acceptable)

A. SIGNATURE OF PERSON NAMED IN ITEM 2A

DATE

B. SIGNATURE(S) OF PERSON(S) NAMED IN ITEM 10

DATE

NIH 39B (FORMERLY PHS 39B)
## BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE</th>
<th>BIRTHDATE (Mo., Day, Yr.)</th>
<th>PLACE OF BIRTH (City, State, Country)</th>
<th>PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)</th>
<th>SEX</th>
</tr>
</thead>
<tbody>
<tr>
<td>CARL DJERASSI</td>
<td>Professor of Chemistry</td>
<td>10/29/23</td>
<td>Vienna, Austria</td>
<td>U.S. citizen</td>
<td></td>
</tr>
</tbody>
</table>

### EDUCATION

<table>
<thead>
<tr>
<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kenyon College</td>
<td>A.B. (summa cum laude)</td>
<td>1942</td>
<td>Chemistry, Biology</td>
</tr>
<tr>
<td>University of Wisconsin</td>
<td>Ph.D.</td>
<td>1945</td>
<td>Organic Chemistry (minor)</td>
</tr>
</tbody>
</table>

### HONORS

National Medal of Science ('73); Perkin Medal ('75); Am.Chem.Soc. Awards: Pure Chemistry ('58), Baekeland Medal ('59), Fritzche Award ('60), Award for Creative Invention ('73); Freedman Found. Patent Award ('71) and Chem. Pioneer Award ('73) of Am.Inst.Chem.; Intrasclence Res. Found. Award ('69); Hon. Member and Centenary Lecturer, Chem.Soc. (London); Intrascience Res. Found. Award ('69); Hon. Member and Centenary Lecturer, Chem.Soc. (London); Intrascience Res. Found. Award ('69); Hon. Member and Centenary Lecturer, Chem.Soc. (London);

### MAJOR RESEARCH INTEREST

Natural Products Chemistry and chemical applications of physical methods

### ROLE IN PROPOSED PROJECT

Principal Investigator

### RESEARCH SUPPORT

See attached.

HONORS (continued from above): Member of National Academy of Sciences, American Academy of Arts and Sciences, Royal Swedish Academy of Sciences, German Academy of Natural Scientists (Leopoldina), Honorary D. Sc. Kenyon, Mexico, Rio de Janeiro, Worcester Polytechnic, Wayne State.

### RESEARCH AND/OR PROFESSIONAL EXPERIENCE

**Academic Experience**

Professor of Chemistry, Stanford University, 1959-present

Assoc. Professor ('52-'54) and Professor ('54-'59), Wayne State University

**Industrial Experience**

Zoecon Corp., Palo Alto, Calif. Chairman of the Board and Chief Exec. Officer, '68-present

Syntex Corp.: Various positions in Mexico City ('49-'52, '57-'60) and Palo Alto, Calif. ('60-'72) ranging from Assoc. Director of Chemical Research to President of Syntex Research


**Miscellaneous**

Chairman of AAAS Gordon Res. Conf. on Steroids and Nat. Prod. ('52-'54). Member Amer. Pugwash Committee ('68-'75): Chairman, Latin American Science Board of National Academy of Sciences ('66-'68); Member ('68-'72) and Chairman ('73-'75) of Board on Science and Technology for International Development of National Academy of Sciences; Member, President's Advisory Group on Contributions of Technology to Economic Strength.

**Publications**

Author or co-author of six books (four dealing with organic mass spectrometry) and over 800 scientific publications. A selection of those dealing with mass spectrometry is given in the Bibliography.
RESEARCH SUPPORT: CARL DJERASSI

Agency: National Institutes of Health
Grant No.: GM-06840-18
Title of Grant: Marine Chemistry with Special Emphasis on Steroids
Period of Grant: 5/1/73-4/30/78
Current Budget: $101,490
Fraction of time committed: 15%

Agency: National Institutes of Health
Grant No.: AM-04257
Title of Grant: Mass Spectrometry in Organic and Biochemistry
Period of Grant: 10/1/75-9/30/79
Current Budget: $278,400
Fraction of time committed: 10%
# BIOPGRAPHICAL SKETCH

*(Give the following information for all professional personnel listed on page 2, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)*

<table>
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<tr>
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<tbody>
<tr>
<td>JOSHUA LEDERBERG</td>
<td>Professor and Chairman, Department of Genetics</td>
<td>5/23/25</td>
</tr>
</tbody>
</table>

**PLACE OF BIRTH** (City, State, Country):
Montclaire, New Jersey, U.S.A.

**PRESENT NATIONALITY** (If non-U.S. citizen, indicate kind of visa and expiration date):
U.S. citizen

**SEX**:
♂ Male  ♠ Female

## EDUCATION

*(Begin with baccalaureate training and include postdoctoral)*

<table>
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<tr>
<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tbody>
<tr>
<td>Columbia College, New York</td>
<td>B.A.</td>
<td>1944</td>
<td></td>
</tr>
<tr>
<td>Yale University</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**HONORS**

- 1957 - National Academy of Sciences
- 1958 - Nobel Prize in Medicine

**MAJOR RESEARCH INTEREST**
Molecular Genetics; Artificial Intelligence

**ROLE IN PROPOSED PROJECT**
Investigator

**RESEARCH SUPPORT** *(See instructions)*
Please see attached list.

**RESEARCH AND/OR PROFESSIONAL EXPERIENCE** *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

- **1959 - present** Professor and Chairman, Department of Genetics
  Stanford University School of Medicine

- **1957 - 1959** Chairman, Department of Medical Genetics
  University of Wisconsin

- **1947 - 1957** Professor of Genetics
  University of Wisconsin

Selected publications appear in Bibliography Section.
Privileged Communication - Section II

Lederberg, Joshua

<table>
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<tr>
<th>GRANT NO.</th>
<th>TITLE OF PROJECT</th>
<th>CURRENT YEAR</th>
<th>PROJECT PERIOD</th>
<th>% OF EFFORT</th>
<th>GRANT AGENCY</th>
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<tr>
<td>Dr. Lederberg: personal research commitments</td>
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<tr>
<td>5ROI CA16896-18</td>
<td>Genetics of Bacteria</td>
<td>$70,000</td>
<td>5/76-4/77</td>
<td>15</td>
<td>NIH</td>
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<td></td>
<td></td>
<td>$195,000</td>
<td>5/74-4/77</td>
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<tr>
<td>NASI-9692</td>
<td>Viking Mission Participation</td>
<td>$42,500</td>
<td>1/76-6/76</td>
<td>5</td>
<td>NASA</td>
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<td></td>
<td></td>
<td>$62,572</td>
<td>1/75-3/77</td>
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<tr>
<td>Dr. Lederberg also functions as Principal Investigator ex officio on the following program-projects and training grants:</td>
<td></td>
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<tr>
<td>NGR-05-020-632</td>
<td>Analytical Methodology for Biochemical Monitoring</td>
<td>$60,000</td>
<td>5/75-4/76</td>
<td>2</td>
<td>NASA</td>
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<td></td>
<td></td>
<td>$180,000</td>
<td>5/73-4/76</td>
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<tr>
<td>NO1 CB 43902</td>
<td>Biomedical Markers that May Presage the Presence of Cancer</td>
<td>$95,000</td>
<td>6/75-6/76</td>
<td>5</td>
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<td>$183,108</td>
<td>6/74-6/76</td>
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<td>3TOI GM00295</td>
<td>Genetics Training Grant (graduate research training)</td>
<td>$121,000</td>
<td>7/75-6/76</td>
<td>10</td>
<td>NIH</td>
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<td>$916,637</td>
<td>7/74-6/79</td>
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<td>1T22 GM00198-02</td>
<td>Postdoctoral Training Medical Genetics</td>
<td>$48,133</td>
<td>7/75-6/76</td>
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<td>$144,133</td>
<td>7/74-6/79</td>
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<td>1PO/ KRU0/85-03</td>
<td>Stanford University Medical Experimental Computer: National Computer Resource for Research on AI in Medicine</td>
<td>$358,000</td>
<td>8/75-7/76</td>
<td>10</td>
<td>NIH</td>
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<td>$3,092,226</td>
<td>10/73-7/78</td>
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<td>NGR-05-020-004</td>
<td>Instrumentation for Planetary Exploration</td>
<td>$110,000</td>
<td>9/75-8/76</td>
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<td>NASA</td>
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<td>$110,000</td>
<td>9/75-8/76</td>
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<tr>
<td>GNZ0832-02</td>
<td>Genetics Research Project</td>
<td>$241,432</td>
<td>5/76-4/77</td>
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<td>NIH</td>
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<td>$1,292,113</td>
<td>5/74-4/79</td>
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## BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE</th>
<th>BIRTHDATE (Mo., Day, Yr.)</th>
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<tbody>
<tr>
<td>EDWARD A. FEIGENBAUM</td>
<td>PROFESSOR OF COMPUTER SCIENCE</td>
<td>1-20-36</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>PLACE OF BIRTH (City, State, Country)</th>
<th>PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)</th>
<th>SEX</th>
</tr>
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<tbody>
<tr>
<td>Weehawken, New Jersey, U.S.A.</td>
<td>U.S. citizen</td>
<td>☐ Male ☐ Female</td>
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### EDUCATION (Begin with baccalaureate training and include postdoctoral)

<table>
<thead>
<tr>
<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tbody>
<tr>
<td>Carnegie Institute of Technology</td>
<td>B.S.</td>
<td>1956</td>
<td>Electrical Engineering</td>
</tr>
<tr>
<td>Pittsburgh, Pennsylvania</td>
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<tr>
<td>Carnegie Institute of Technology</td>
<td>Ph.D.</td>
<td>1959</td>
<td>Industrial Administration</td>
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</table>

### HONORS


### MAJOR RESEARCH INTEREST

Artificial Intelligence

### ROLE IN PROPOSED PROJECT

Investigator

### RESEARCH SUPPORT (See instructions)

### RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

- Stanford University, Stanford, California
  - Chairman, Computer Science Department, 9/1976-
  - Professor of Computer Science, 1969-
  - Associate Professor of Computer Science, 1965-68
  - Director, Stanford Computation Center, 1965-68

- University of California, Berkeley
  - Associate Professor, School of Business Administration, 1964
  - Assistant Professor, School of Business Administration, 1960-63
  - Research Appointment, Center for Human Learning, 1961-64
  - Research Appointment, Center for Research in Management Science, 1960-64

- Editor, Computer Science Series, McGraw-Hill Book Company, New York, 1965-
  - Member, Computer and Biomathematical Sciences Study Section, National Institutes of Health, Bethesda, Maryland, 1968-72

- Ad-Hoc Mail Reviewer, National Science Foundation (various)
Selected Papers, 1965-76


Other papers in Information Processing Psychology (18)

Books and Monographs


RESEARCH SUPPORT AND PENDING APPLICATIONS: Edward A. Feigenbaum

Agency: Advanced Research Projects Agency
Contract Number: DAHC 15 73 C 0435
Title of Contract: Heuristic Programming Project
Period of Contract: July 1975-June 1977
Annual Budget Level: $203,000
Fraction of time committed: 40% Academic Yr.

Agency: National Science Foundation
Grant Number: MCS 76-11649
Title of Grant: MOLGEN: A Computer Science Application to Molecular Genetics
Period of Grant: 6/1/76-5/31/78
Annual Budget Level: $110,700 (2 yr. amount)
Fraction of time committed: 10% Academic Yr.; 100% Summer

PENDING:

Agency: National Library of Medicine
Title: Training Program in Biomedical Computing
Period: 6/77-5/82
Annual Budget Level: $334,193 (direct cost)
Fraction of time committed: 20%
**NAME**

BRUCE G. BUCHANAN

**TITLE**

Adjunct Professor

**BIRTHDATE (Mo., Day, Yr.)**

7-7-40

<table>
<thead>
<tr>
<th>PLACE OF BIRTH (City, State, Country)</th>
<th>PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)</th>
<th>SEX</th>
</tr>
</thead>
<tbody>
<tr>
<td>St. Louis, Missouri, U.S.A.</td>
<td>U.S. citizen</td>
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</tr>
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**EDUCATION (Begin with baccalaureate training and include postdoctoral)**

<table>
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<th>INSTITUTION AND LOCATION</th>
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<tbody>
<tr>
<td>Ohio Wesleyan University</td>
<td>B.A.</td>
<td>1961</td>
<td>Mathematics</td>
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<tr>
<td>Michigan State University</td>
<td>M.A.</td>
<td>1966</td>
<td>Philosophy</td>
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<tr>
<td>Michigan State University</td>
<td>Ph.D.</td>
<td>1966</td>
<td>Philosophy</td>
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</table>

**HONORS**


**MAJOR RESEARCH INTEREST**

Associate Investigator

**RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)**

1976 - Adjunct Professor, Computer Science Department
Stanford University, Stanford, California

1972-1976 Research Computer Scientist, Computer Science Department
Stanford University, Stanford, California

1966-1971 Research Associate, Artificial Intelligence Project
Stanford University, Stanford, California
Selected Publications:


RESEARCH SUPPORT AND PENDING APPLICATIONS: Bruce G. Buchanan

Agency: Advanced Research Projects Agency
Contract Number: DAHC 15 73 C 0435
Title of Contract: Heuristic Programming Project
Period of Contract: July 1975-June 1977
Annual Budget Level: $203,000
Fraction of time committed: 25%

Agency: National Science Foundation
Grant Number: MCS 76-11649
Title of Grant: MOLGEN: A Computer Science Application to Molecular Genetics
Period of Grant: 6/1/76-5/31/78
Annual Budget Level: $110,700 (2 yr. amount)
Fraction of time committed: 25%

PENDING:

Agency: National Library of Medicine
Title: Training Program in Biomedical Computing
Period: 6/77-5/82
Annual Budget Level: $334,193 (direct cost)
Fraction of time committed: 20%
BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME
Dennis H. Smith

TITLE
Research Associate

BIRTHDATE (Mo., Day, Yr.)
11/12/42

PLACE OF BIRTH (City, State, Country)
New York

PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)
USA

SEX
\( \square \text{ Male } \quad \square \text{ Female } \)

EDUCATION (Begin with baccalaureate training and include postdoctoral)

<table>
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<th>INSTITUTION AND LOCATION</th>
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<tbody>
<tr>
<td>Massachusetts Inst. of Technology</td>
<td>S.B.</td>
<td>1964</td>
<td>Chemistry</td>
</tr>
<tr>
<td>Cambridge, Mass.</td>
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</tr>
<tr>
<td>University of California, Berkeley</td>
<td>Ph.D.</td>
<td>1967</td>
<td>Chemistry</td>
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<tr>
<td>Berkeley, California</td>
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</tbody>
</table>

HONORS
Alfred P. Sloan Foundation Scholarship
NASA Predoctoral Traineeship
Phi Lambda Upsilon, Sigma Xi

MAJOR RESEARCH INTEREST
Mass Spectrometry and A.I. in Chemistry

ROLE IN PROPOSED PROJECT
Research Associate

RESEARCH SUPPORT (See instructions)
N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

1971-Present Research Associate, Stanford University, Stanford, Ca.
1970-1971 Visiting Scientist, University of Bristol, Bristol, England

Publications: See attached list.


N. Mancuso, R. Murphy, D.A. Flory, and M.A. Reynolds, "Preliminary Organic 
Analysis of the Apollo 12 Cores," Proceedings of the Apollo 12 Lunar Science 


of Low Resolution Mass Spectra-Application to Geochemical and Environmental 

"Complex Mixture Analysis – Geochemical and Environmental Applications of a 
Compound Classifier Based on Computer Analysis of Low Resolution Mass Spectra," 

18. P. Longevialle, D.H. Smith, H.M. Fales, R.J. Highet, and A.L. Burlingame, 
"High Resolution Mass Spectrometry in Molecular Structure Studies. V. The 
7, 401 (1973).

of Real-time Mass Spectrometric Techniques to Environmental Organic Geochemistry. 

20. G. Loew, M. Chadwick, and D.H. Smith, "Applications of Molecular Orbital 
Theory to the Interpretation of Mass Spectra. Prediction of Primary Fragmentation 

and Stereochemical Problems, CCXXXVIII. The Effect of Heteroatoms upon the 

Structural and Stereochemical Problems. CCXLII. Analysis of Mixtures Based on 
the Distribution of Fragment Ions Arising from Unimolecular Decomposition of 


Spectrometric Techniques to Environmental Organic Geochemistry. I. Computerized 
High Resolution Mass Spectrometry and Gas Chromatography-Low Resolution Mass 

Elucidation. Modelling Chemical Reaction Sequences Used in Molecular Structure 
Chemical Society, Washington, D.C., in press.


See also Bibliography.
BIographiesKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME: RAYMOND EDGAR CARHART
TITLE: RESEARCH ASSOCIATE
BIRTHDATE (Mo., Day, Yr.): 10/4/46

PLACE OF BIRTH (City, State, Country): Evanston, Illinois, U.S.A.
PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date):
U.S. citizen
SEX: M

EDUCATION (Begin with baccalaureate training and include postdoctoral)

<table>
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<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tbody>
<tr>
<td>Northwestern University</td>
<td>B.A.</td>
<td>1968</td>
<td>Chemistry</td>
</tr>
<tr>
<td>California Institute of Technology</td>
<td>Ph.D.</td>
<td>1973</td>
<td>Physical Organic Chemistry</td>
</tr>
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HONORS: Phi Beta Kappa; Sigma Xi; Phi Lambda Upsilon; NSF pre-doctoral fellowship 1968-72; NIH post-doctoral fellowship 1972-74.

MAJOR RESEARCH INTEREST: Applications of Computer Science to Organic Chemistry

ROLE IN PROPOSED PROJECT: Research Associate

RESEARCH SUPPORT: N/A

RESEARCH AND PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

1974-
Research Associate, Department of Computer Science, Stanford University

1972-1974 NIH Post-doctoral Fellow, Department of Computer Science, Stanford University

1969(summer) Visiting Scientist, IBM Research Laboratory, San Jose, California

Recent Publications:


**SECTION II - PRIVILEGED COMMUNICATION**

**BIOGRAPHICAL SKETCH**

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE</th>
<th>BIRTHDATE (Mo, Day, Yr.)</th>
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<tbody>
<tr>
<td>Gretchen Maria SCHWENZER</td>
<td>Research Associate</td>
<td>2/6/49</td>
</tr>
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</table>

**PLACE OF BIRTH (City, State, Country)**

Buffalo, New York, U.S.A.

**PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)**

U.S.

**SEX**

☐ Male ☑ Female

**EDUCATION (Begin with baccalaureate training and include postdoctoral)**

<table>
<thead>
<tr>
<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tbody>
<tr>
<td>State University of New York at Buffalo</td>
<td>B.A.</td>
<td>1971</td>
<td>Mathematics &amp; Chemistry</td>
</tr>
<tr>
<td>University of California, Berkeley</td>
<td>Ph.D.</td>
<td>1975</td>
<td>Chemistry</td>
</tr>
<tr>
<td>Institute in Quantum Chemistry, Solid State Physics &amp; Quantum Biology, Uppsala, Sweden</td>
<td>Summer 1973</td>
<td></td>
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</tbody>
</table>

**HONORS**

- Phi Beta Kappa, Pi Mu Epsilon, Alpha Lambda Delta
- Graduated Magna Cum Laude with Highest Distinction; Allied Chemical Scholar, 1971; Award of American Institute of Chemists for Scholastic Achievement.

**MAJOR RESEARCH INTEREST**

Application of Computers in Chemistry

**ROLE IN PROPOSED PROJECT**

Direct C13 NMR with attention to the structural nature of the problem

**RESEARCH SUPPORT (See instructions)**

N/A

**RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)**

- Stanford University
  - Computer Science Department, Stanford, Calif. 1976 -

- IBM, San Jose Research Division, San Jose, Calif. 1975

- University of California, Berkeley, Calif. 1971-1975
  - Thesis: The Excited Electronic States of HCN and HNC; a New Method to Obtain Wave Functions of SCF Quality Configuration Interaction Wave Functions to Obtain Optimized Minimum Basis Set Potential Surfaces

State University of New York at Buffalo, Buffalo, N.Y.


"Documentation of ALCHEMY", Gretchen M. Schwenzer, IBM Report.
**SECTION II - PRIVILEGED COMMUNICATION**

**BIOGRAPHICAL SKETCH**

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

<table>
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<th>NAME</th>
<th>TITLE</th>
<th>BIRTHDATE (Mo., Day, Yr.)</th>
</tr>
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<tbody>
<tr>
<td>HAROLD D. BROWN</td>
<td>Research Associate</td>
<td>7-12-34</td>
</tr>
</tbody>
</table>

<table>
<thead>
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<th>PLACE OF BIRTH (City, State, Country)</th>
<th>PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)</th>
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<td>South Bend, Indiana, U.S.A.</td>
<td>U.S. citizen</td>
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<tr>
<th>SEX</th>
</tr>
</thead>
<tbody>
<tr>
<td>☑ Male</td>
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</table>

**EDUCATION** (Begin with baccalaureate training and include postdoctoral)

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<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tr>
<td>University of Notre Dame</td>
<td>M.Sc.</td>
<td>1963</td>
<td>Mathematics</td>
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<tr>
<td>Ohio State University</td>
<td>Ph.D.</td>
<td>1966</td>
<td>Mathematics</td>
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**HONORS**

**MAJOR RESEARCH INTEREST**

**ROLE IN PROPOSED PROJECT**

Research Associate

**RESEARCH SUPPORT** (See instructions)

Proposed Amount: $42,733
Period: 11/1/75-10/31/77
Source: National Science Foundation

**RESEARCH AND/OR PROFESSIONAL EXPERIENCE** (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

- 1971-72: Associate Professor, Computer Science Department, Stanford University
  1973-
- 1973-: Research Associate, Medical School, Stanford University
- 1963-75: Instructor/Assistant Professor, Assistant Chairman/Associate Professor, Mathematics, The Ohio State University
- 1964-70: Director/Associate Director, National Science Foundation SSTP
- 1967-68: Visiting Member, Courant Institute of Mathematical Sciences, New York University
- 1960-63: Assistant to the Chairman, Mathematics, University of Notre Dame
Publications:


Basic Computations for Orders, Stanford CS Report STAN-CS-72-208.


Applications of Artificial Intelligence for Chemical Inference XVIII. An Approach to Computer-Assisted Elucidation of Molecular Structure (with R. Carhart and D. Smith), JACS (in press).
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