21:16:24 OCA PAD AMENDMENT - PROJECT HEADER INFORMATION 07/23/91

Active

Project #: G-33-525 Cost share #: Rev #: 3
Center # : P5065-0A0 Center shr #: OCA file #:
Work type : INST
Contract#: 813-2 Mod #: ADM REV Document : SUBCONT
Prime #: USE-8854202 Contract entity: GTRC

Subprojects ? : N CFDA: N/A
Main project #: PE #: N/A

Project unit: CHEMISTRY Unit code: 02.010.136
Project director(s):
BERTRAND J A JR CHEMISTRY (404)894-4050

Sponsor/division names: GEORGIA STATE UNIV / ATLANTA, GA
Sponsor/division codes: 400 / 034

Award period: 880501 to 911031 (performance) 911031 (reports)

Sponsor amount	New this change	Total to date
Contract value	0.00	51,628.00
Funded	0.00	51,628.00
Cost sharing amount		0.00

Does subcontracting plan apply ?: N

Title: GSU/UNDERGRADUATE FACULTY ENHANCEMENT IN CHEMISTRY

PROJECT ADMINISTRATION DATA

OCA contact: Kathleen R. Ehlinger 894-4820

Sponsor technical contact	Sponsor issuing office
DR CURTIS T SEARS, JR	MR CLYDE R APPLING, DIRECTOR
(404)651-3120	(404)651-0000
DEPT OF CHEMISTRY/UNIVERSITY PLAZA	GRANTS AND CONTRACTS/UNIV PLAZA
GEORGIA STATE UNIVERSITY	GEORGIA STATE UNIVERSITY
ATLANTA GA 30303	ATLANTA GA 30303-3080

Security class (U,C,S,TS) : U ONR resident rep. is ACO (Y/N): N
Defense priority rating : N/A N/A supplemental sheet
Equipment title vests with: Sponsor GIT
NONE PROPOSED.
Administrative comments -
NEW P.I., DR. J. AARON BERTRAND REPLACES DR. E. K. BAREFIELD.

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 05/19/92

Project No. G-33-525 | Center No. P5065-0A0

Project Director BERTRAND J A JR | School/Lab CHEMISTRY

Sponsor GEORGIA STATE UNIV/ATLANTA, GA

Contract/Grant No. 813-2 | Contract Entity GTRC

Prime Contract No. USE-8854202

Title GSU/UNDERGRADUATE FACULTY ENHANCEMENT IN CHEMISTRY

Effective Completion Date 911031 (Performance) 911031 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	920326
Final Report of Inventions and/or Subcontracts	N	
Government Property Inventory & Related Certificate	N	
Classified Material Certificate	N	
Release and Assignment	N	
Other	N	

CommentsPATENT REPORTING INCLUDED IN FINAL_(NSF GRANT-98A SUBMITTED)

Subproject Under Main Project No. ____

Continues Project No. ____

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

OMB Number 345-0058

NATIONAL SCIENCE FOUNDATION
1800 G STREET, NW
WASHINGTON, DC 20550

BULK RATE
POSTAGE & FEES PAID
National Science Foundation
Permit No. G-69

PI/PD Name and Address

Dabney White Dixon
Chemistry
Georgia State University
University Plaza, Atlanta, GA 30303-3083
Atlanta GA 30303

NATIONAL SCIENCE FOUNDATION FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION

1. Program Official/Org. William E. Haver - USE

2. Program Name FACULTY ENHANCEMENT PROGRAM

3. Award Dates (MM/YY) From: 05/88 To: 10/91

4. Institution and Address
Georgia State University
University Plaza
Atlanta GA 30303

5. Award Number 8854202

6. Project Title
Undergraduate Faculty Enhancement in Chemistry: A Series of National Workshops

This Packet Contains
NSF Form 98A
And 1 Return Envelope

NSF Grant Conditions (Article 17, GC-1, and Article 9, FDP-II) require submission of a Final Project Report (NSF Form 98A) to the NSF program officer no later than 90 days after the expiration of the award. Final Project Reports for expired awards must be received before new awards can be made (NSF Grant Policy Manual Section 677).

Below, or on a separate page attached to this form, provide a summary of the completed project and technical information. Be sure to include your name and award number on each separate page. See below for more instructions.

PART II - SUMMARY OF COMPLETED PROJECT (for public use)

The summary (about 200 words) must be self-contained and intelligible to a scientifically literate reader. Without restating the project title, it should begin with a topic sentence stating the project's major thesis. The summary should include, if pertinent to the project being described, the following items:

- The primary objectives and scope of the project
- The techniques or approaches used only to the degree necessary for comprehension
- The findings and implications stated as concisely and informatively as possible

PART III - TECHNICAL INFORMATION (for program management use)

List references to publications resulting from this award and briefly describe primary data, samples, physical collections, inventions, software, etc. created or gathered in the course of the research and, if appropriate, how they are being made available to the research community. Provide the NSF Invention Disclosure number for any invention.

	1/27/92
Principal Investigator/Project Director Signature	Date

IMPORTANT:
MAILING INSTRUCTIONS
Return this *entire* packet plus all attachments in the envelope attached to the back of this form. Please copy the information from Part I, Block I to the *Attention block* on the envelope.

PART IV — FINAL PROJECT REPORT — SUMMARY DATA ON PROJECT PERSONNEL

(To be submitted to cognizant Program Officer upon completion of project)

The data requested below are important for the development of a statistical profile on the personnel supported by Federal grants. The information on this part is solicited in response to Public Law 99-383 and 42 USC 1885C. All information provided will be treated as confidential and will be safeguarded in accordance with the provisions of the Privacy Act of 1974. You should submit a single copy of this part with each final project report. However, submission of the requested information is not mandatory and is not a precondition of future award(s). Check the "Decline to Provide Information" box below if you do not wish to provide the information.

Please enter the numbers of individuals supported under this grant.
Do not enter information for individuals working less than 40 hours in any calendar year.

	Senior Staff		Post-Doctorals		Graduate Students		Under-Graduates		Other Participants[1]	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
A. Total, U.S. Citizens	21	4							395	67
B. Total, Permanent Residents										
U.S. Citizens or Permanent Residents[2]:										
American Indian or Alaskan Native										
Asian										
Black, Not of Hispanic Origin										
Hispanic										
Pacific Islander										
White, Not of Hispanic Origin	21	4								
C. Total, Other Non-U.S. Citizens										
Specify Country 1.										
2.										
3.										
D. Total, All participants (A + B + C)	21	4							395	67
Disabled[3]										

☐ Decline to Provide Information: Check box if you do not wish to provide this information (you are still required to return this page along with Parts I-III).

[1]Category includes, for example, college and precollege teachers, conference and workshop participants.

[2]Use the category that best describes the ethnic/racial status for all U.S. Citizens and Non-citizens with Permanent Residency. *(If more than one category applies, use the one category that most closely reflects the person's recognition in the community.)*

[3]A person having a physical or mental impairment that substantially limits one or more major life activities; who has a record of such impairment; or who is regarded as having such impairment. *(Disabled individuals also should be counted under the appropriate ethnic/racial group unless they are classified as "Other Non-U.S. Citizens.")*

AMERICAN INDIAN OR ALASKAN NATIVE: A person having origins in any of the original peoples of North America, and who maintain cultural identification through tribal affiliation or community recognition.

ASIAN: A person having origins in any of the original peoples of East Asia, Southeast Asia and the Indian subcontinent. This area includes, for example, China, India, Indonesia, Japan, Korea and Vietnam.

BLACK, NOT OF HISPANIC ORIGIN: A person having origins in any of the black racial groups of Africa.

HISPANIC: A person of Mexican, Puerto Rican, Cuban, Central or South American or other Spanish culture or origin, regardless of race.

PACIFIC ISLANDER: A person having origins in any of the original peoples of Hawaii; the U.S. Pacific Territories of Guam, American Samoa, or the Northern Marianas; the U.S. Trust Territory of Palau; the islands of Micronesia or Melanesia; or the Philippines.

WHITE, NOT OF HISPANIC ORIGIN: A person having origins in any of the original peoples of Europe, North Africa, or the Middle East.

Dixon, USE 8854202

Summary of Completed Project:

Georgia State University (GSU) and the Georgia Institute of Technology (GIT) have jointly coordinated an Undergraduate Faculty Enhancement Project in Chemistry for the southeastern United States. The project was designed to enhance the ability of faculty at two- and four-year institutions to teach a modern program in chemistry.

The major activities of the project were 15 one-week workshops and three 2-day mini-courses. Workshop topics were: (1) Molecular Modeling; (2) Mass Spectroscopy; (3) Instrument Interfacing; (4) FT-NMR Spectroscopy; (5) Chromatography; and (6) Molecular Orbital Theory. Mini-courses were held on: (1) Organometallic Chemistry/Catalysis; (2) Solid State Chemistry/Superconductivity; and (3) DNA Chemistry/Biotechnology. The workshops and mini-courses were taught by GSU and GIT faculty. Prominent specialists from other institutions served as keynote speakers. Annual reunions of all participants during the preceding 12 months were held to exchange experiences in implementing new methods in the curriculum.

Three Year Report

Undergraduate Faculty Enhancement in Chemistry

A Series of Regional Workshops

Georgia State University and
The Georgia Institute of Technology

July 1, 1988 - June 30, 1991

National Science Foundation
Grant Number USE 8854202

January 27, 1992

Submitted by:

Dabney White Dixon
Project Director

Table of Contents:

Project Description:

The goal of this project was to provide workshops and mini-courses designed to acquaint faculty who are engaged primarily in undergraduate teaching with recently developed experimental techniques, instrumentation and theoretical developments in chemistry. Table I lists the workshops and mini-courses held. Brief course descriptions and the names of the instructors are listed in the brochure (Appendix 1).

The sponsored workshops were held at Georgia State University and the Georgia Institute of Technology in Atlanta, Georgia. The Solid-State Chemistry/ Superconductivity mini-course was hosted by Savannah State College in Savannah, Georgia. The DNA Chemistry/Biotechnology mini-course was hosted by Mercer University in Macon, Georgia. The 1990 Reunion was held at Fort Valley State College in Fort Valley, Georgia and the 1991 Reunion was held in Atlanta, Georgia.

Statistics:

Participation by workshop is given in Tables I. We did not collect statistics on the race of the participants at the time of the workshops and it has not been possible to reconstruct this data.

The participants for the workshops and mini-courses covered by this report are from the following states: Georgia (41), North Carolina (33), Tennessee (21), Kentucky (17), South Carolina (16), Virginia (16), Alabama (10), Florida (10), Arkansas, (10) Missouri (9), Louisiana (9), Maryland (7), Mississippi (6), West Virginia (2), the Virgin Islands (1), Alaska (1), Puerto Rico (1), and New York (1).

Selection of Participants:

Participants for each workshop were selected by the Project Advisory Committee, a committee made up of the project director, the associate director, and five chemistry faculty members representing public and private two- and four-year colleges (see Appendix II), based on forms filled out by each applicant (see brochure in Appendix I). The selection criteria included: appropriateness of the workshop for the courses taught by the applicant; previous workshops or summer research programs attended; participation at regional and national meetings; elapsed time since receipt of last academic degree; and applicant's need for skill enhancement and updating. The lists of participants by workshop may be found in Appendix III.

Activity	Dates	Number of Attendees Proposed	Number of Attendees	Number of Applicants	Percentage Accepted Applicants
Chromotography Workshop	August 14-19, 1988	10	10	12	83%
Molecular Modeling Workshop	August 14-19, 1988	10	10	12	83%
Instrument Interfacing Workshop	December 11-16, 1988	10	10	43	23%
Mass Spectroscopy Workshop	December 11-16, 1988	10	10	19	53%
Organometallic/Catalysis Minicourse	March 17-18, 1989	40	24	24	100%
Annual Reunion	April 27-28, 1989	40	31	-	-
FT-NMR Workshop	June 11-16, 1989	20	20	26	77%
Molecular Modeling Workshop	August 20-25, 1989	10	10	23	43%
Instrument Interfacing Workshop	August 20-25, 1989	10	10	39	25%
FT-NMR Workshop	December 10-15, 1989	20	20	30	67%
Solid State Chemistry/ Superconductivity Minicourse	March 16-17, 1990	40	23	23	100%
Annual Reunion	April 27-28 , 1990	60	48	-	-
Molecular Modeling Workshop	June 10-15, 1990	10	10	35	29%
Chromatography Workshop	June 10-15, 1990	10	11	15	73%
Instrument Interfacing Workshop	August 19-24, 1990	10	11	28	39%
Mass Spectroscopy Workshop	August 19-24, 1990	10	10	17	59%
FT NMR Spectroscopy Workshop	December 9-14, 1990	20	20	24	83%
Chromatography Workshop	December 9-14, 1990	10	10	19	53%
DNA Chemistry/ Biotechnology Minicourse	March 15-16, 1991	40	38	40	95%
Annual Reunion	April 26-27, 1991	72	38	-	-
Instrument Interfacing Workshop	June 9-14, 1991	10	11	31	35%
Molecular Orbital Theory Workshop	June 9-14, 1991	30	30	39	77%
Molecular Modeling Workshop	August 18-23, 1991	12	13	16	81%
Polymer Chemistry Workshop	August 18-23, 1991	16	10	11	90%
Chemistry of Nucleic Acids Workshop	August 18-23, 1991	12	12	15	80%

Publicity:

The primary form of publicity for the regional workshops program was direct mailings of workshop brochures (Appendix I). The publicity was aimed at chemistry faculty of two- and four-year schools in the southeastern United States. There are approximately 1850 names on the mailing list which was obtained from the College of Chemistry Faculties, 7th Edition, published by the American Chemical Society. At the request of workshop participants, additional names were added to the mailing list. Additionally, for the Chemistry of Nucleic Acid Workshop, flyers publicizing the workshop were sent to approximately 100 Biology departments in the Southeast. Brochures were also made available at local, regional and national ACS meetings.

Evaluation and Impact:

To assess the success of the program and to identify areas in need of strengthening, each participant filled out an evaluation form at the conclusion of the workshop (Appendix IV). On the whole, the evaluations were very good.

The best measure of the success of the workshop is its impact on chemistry instruction at the participants' colleges. All participants agreed at the time of acceptance to write a brief (2-3 page) report, due before the annual reunion, detailing what they had accomplished using the workshop material and their plans for future teaching endeavors in the area. The reports were photocopied and distributed to the reunion participants. Discussion at the reunion was based on the ideas and plans described in the reports. All workshops were asked to make a composite report and these are included in Appendix V.

An excellent benefit of this program has been the networking that has evolved among the participants. A number of them have met potential collaborators with similar interests and are now working on joint teaching or research projects. We have encouraged those who can to get on to BITNET. The Chemistry Educator's Discussion List is a good and lively BITNET forum with many postings of interest for this group. Also, the workshop instructors continue to serve as resource people for the participants and send out useful information (programs, references, etc.) to the participants.

Program Director Assessment of Successful/Unsuccessful Strategies in Running This Program

Number and Duration of Workshops:

We have run both two day mini-courses (Friday noon to Saturday 3 PM) and week-long (Sunday evening to Friday noon) workshops. Both are successful. Week-long workshops need a minimum of 10 people to work well. We have run them with as many as 30 people and have found no upper limit to the size of a successful workshop provided there are enough instructors and equipment. Beyond that number needed in one workshop, we find that a minimum total of 30 people are needed both for social interactions and for economies of scale. In particular, arrangements for room sharing, banquets, etc. are easier if there are more people. Therefore, we now run at least three 10-person workshops simultaneously.

We have run the DNA mini-courses and workshops with participants from both chemistry and biology departments. The mixture of people from the two departments was particularly exciting for both. This worked so well that the NSF might consider special sponsorship of chemistry/biology, chemistry/physics, chemistry/geology or chemistry/anthropology workshops.

Selection and Number of Instructors:

This is a critical aspect of the program. Participants come from a variety of institutions and have very different skill levels. We find that one faculty instructor is needed for each 6-10 participants. Graduate students and postdocs are useful in keeping the technical aspects of the workshops going, but cannot take the role of an instructor. When we try to run workshops with fewer faculty instructors, the participants feel frustrated and slighted and the instructors become too tired to do a first-rate job. Conversely, workshops run with two or three instructors have gone exceedingly well and received outstanding reviews from the participants.

Lecture/Laboratory Mixture:

A variety of strategies works well. Although most of the participants want to use the same equipment they will have when they return to their home institution, some want to work on advanced equipment not found at their college either in preparation for a grant proposal to acquire such equipment or because they have a scientific question that they want to answer rapidly. We have tried to accommodate both groups of people, and this strategy has worked well.

Post-Workshop Follow-up:

We run hold a reunion 6-9 months after the week-long workshops. Participants are required to agree to come when they are accepted into the workshop. Most participants feel that the reunion is a necessary part of the program for two reasons. First, it puts some pressure on them (and, if necessary, on their administration) to get experiments up and running at their home institutions. Second, the reunion serves as a problem solving time for the more subtle issues that become apparent after participants have worked on a project for a few months. However, it is quite expensive for many of them to return to Georgia and it is becoming increasingly difficult for participants to convince their Department Chairs and Deans to come up with the money. Some report that the trip back takes most of their discretionary funds for the year and that this is too high a price for the reunion. In the future, reunions at regional or national ACS meetings should be considered.

We have encouraged the participants of the reunions to choose one or two outstanding implementations of the course material and to work in groups to submit manuscripts to the Journal of Chemical Education or other forums. To date this has not resulted in the submission of a publication, although there are plenty of ideas and projects of publication quality generated by the participants. We have not yet determined how to encourage the participants more strongly along these lines.

In addition to reports and problem-solving sessions at the reunions, we have begun to have workshops/discussion sessions on obtaining grants and on getting connected to BITNET. Both measures have been exceedingly successful and are recommended to others running similar programs.

Many of our instructors stay in touch with the people in the workshops largely by mail or EMAIL. This provides the participants with useful information and with a continuing sense of being involved in the workshop community. Many of the participants also stay in touch with one another.

Workshop Participants as Instructors:

Many of the workshop participants are talented, resourceful teachers who can in turn help teach another group of participants. The little we have done along this line has been extremely successful. It is good to see this type of teaching being formalized in the new NSF proposal guides for the 1992 deadline.

Social Interactions:

The week-long workshops include three social events. On Sunday night we hold a reception and dinner followed by an informal time to talk. On Tuesday and Wednesday nights, we hold a dinner, followed by a lecture from an outside speaker and another informal time to get together. For some workshops, we have had different speakers on Tuesday and Wednesday; for others we have had the same speaker. Because we always have two or three workshops running simultaneously, the speakers are asked to give reasonably general lectures. One might think that two different speakers, one of special interest to one group and one of special interest to another, would work best, but in fact a single speaker for the two nights has been by far the most successful strategy. Well-known speakers are certainly appreciated but the speaker's enthusiasm and interest in the audience are far more important than a national reputation. We usually ask the Dean or another administrative official to welcome the people on the first night; this appears to have been quite important to some people.

Financial Considerations:

We provided \$50/day stipends for the people in these workshops and mini-courses. Administrations of colleges vary greatly in their support of additional training for their faculty. The \$50/day stipends are enough to cover most travel costs, and many faculties have used them for just that when their administrations would not or could not provide travel funds. In the Southeast during a recession, this stipend may be critical to a successful program.

Appendix I

National Science Foundation

Grant Number USE 8854202

Dabney W. Dixon, P.I.

Three Year Report

Appendix I USE 8854202

Workshop Opportunities in Chemistry for Undergraduate Faculty in Southeastern U.S.

Sponsored by

Georgia State University

and

Georgia Institute of Technology

Funded by

Office of Undergraduate Science,
Engineering and Mathematics Education,
National Science Foundation

Appendix II

National Science Foundation

Grant Number USE 8854202

Dabney W. Dixon, P.I.

Three Year Report

Appendix II
UFEC Advisory Committee
1990-91

Dr. Kent Barefield
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Department of Chemistry
225 North Avenue
Atlanta, GA 30332

Dr. Jeffrey James
Savannah State College
Department of Chemistry
Savannah, GA 31404

Dr. Alice Cunningham
Agnes Scott College
Department of Chemistry
Decatur, GA 30030

Dr. Janice Turner
Augusta College
Department of Chemistry
Augusta, GA 30904

Dr. David Dever
Macon Junior College
Department of Chemistry
Macon, GA 31206

Dr. Albert Thompson
Spelman College
Department of Chemistry
Box 287
Atlanta, GA 30314

Appendix III

National Science Foundation

Grant Number USE 8854202

Dabney W. Dixon, P.I.

Three Year Report

Workshop Participants
Chromatography
August 14-19, 1988

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1001 Burkmont Avenue
Morganton, NC 28655
(704) 437-8688
SS# 239-40-1376

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Valdosta State University
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(404)
SS#

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SS# 406-52-2016

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(404) 864-3391 extension 296
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Dr. G. William Donaldson
East Georgia College
Metter, GA 30439
(912) 237-7831
SS#

Dr. Dwight Kinzer
Berry College
Department of Chemistry
Mount Berry, GA 30149
(404) 236-2237
SS# 418-50-2098

Dr. B. I. Naddy
Columbia State College
Columbia, TN 38402-1315
(615) 388-0120 extension 233
SS#

Dr. George N. Williams
Savannah State College
Savannah, GA 31404
(912) 356-2318
SS# 260-76-7448

Workshop Participants
Molecular Modeling
August 14-19, 1988

Dr. Julia P. Baker
Department of Chemistry
Armstrong State College
Savannah, GA 31419-1997
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Georgia Southwestern
Americus, GA 31709
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Transylvania University
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(606) 233-8156
SS# 032-34-2404

Dr. Tom Maier
Atlanta Metropolitan College
1630 Stewart Avenue SW
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Dr. Nancy C. McDonald
Athen State College
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Dr. Janice Turner
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Chemistry Department
Augusta, GA 30904
(404) 737-1541
SS# 253-52-3023

Dr. Alex N. Williamson
North Carolina A&T State University
300 Leland Drive
Greensboro, NC 27408
(919) 334-7565
SS# 587-38-4290

Workshop Participants
Mass Spectroscopy
December 11-16, 1988

Francis E. Chigbo
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Garry McGlaun
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Johnnie-Marie Whitfield
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Robert C. Wingfield, Jr.
Fisk University
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Nashville, TN 37208-3051
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Workshop Participants
Instrument Interfacing
December 11-16, 1988

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Greensboro, NC 27401-3239
(919) 370-8747

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Clare T. Furse
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Paul P. Hunt
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Michael D. Murphy
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Charlie M. Stinson, Jr.
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Jim C. Yu
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(816) 429-4948

Organometallic Chemistry Mini-course Workshop Participants:
March 17-18, 1989

Dr. Luz Marina Calle
Randolph-Macon Woman's College
Chemistry Department
Lynchburg, VA 24503

Dr. James C. Chang
University of Northern Iowa
Department of Chemistry
Cedar Falls, IA 50614

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Dr. W. H. Myers
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Appendix IV

National Science Foundation

Grant Number USE 8854202

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Three Year Report

Undergraduate Faculty Enhancement Program Evaluation

These activities are part of a three year program of workshops and mini-courses. Your comments concerning the organization and accommodations will be used in the planning of future activities. Comments specifically related to the workshop attended will be helpful for the next presentations of the workshop. If you prefer to remain anonymous, please provide the name of the workshop in which you participated.

Name ____

Organization

Was the organization of the week satisfactory; what changes would you suggest?

Workshops

Overall, did the workshop meet your expectations; in particular what, if anything, was missing?

Was the organization of the workshop satisfactory; what changes would you suggest?

Was the level of classroom instruction suitable; what changes might be made?

over

Were the laboratory sessions well organized and instructive? Suggest changes.

Was the mix of classroom and laboratory activities appropriate?

Do you consider the Keynote Lecture a significant feature of the program? Please comment specifically on the level and appropriateness of the topic.

Accommodations

Were your room and meal arrangements satisfactory?

Was the availability of the hospitality/evening discussion room a desirable feature?

The hotel was chosen because of its proximity to Lenox Square and the Buckhead area. Was the location suitable; did you find the area enjoyable and interesting?

Did travel by Marta present any problems?

Appendix V

National Science Foundation

Grant Number USE 8854202

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Three Year Report

Chromatography

We begin with short abstracts of each report submitted to the Director:

ACUFF: Report describes rebuilding inoperative GC and its incorporation and regular use in organic lab. Moreover, workshop attendance stimulated application to NSF for new equipment funding.

BAXTER: Report describes planned use of GC and HPLC for separation of essential oils and commmercial fragances in organic chemistry laboratory.

BREIVOGEL: Report describes successful introduction of TLC and HPLC to analysis of analgesics in organic lab.

DAVIS: Report describes use of chromatographic techniques in the majors organic chemistry course. The workshop emphasized the need to include chromatographic techniques whenever possible.

DEVER: Report described application of cellulose TLC to carboxylic acid/organic qualitative analysis in first quarter general chemistry lab. Further, anion exchange was applied to problem-oriented, open-ended, inorganic qualitative analysis scheme in second quarter, general chemistry lab.

DONALDSON: Report describes use of GC in sophomore organic lab to study reaction products of 1) dehydration of 2-methylcyclohexanol, and 2) nucleophilic substitution products of alkyl benzenes.

KINZER: Report describes HPLC analysis of benzene nitration products under various conditions; these data are then compared with IR analysis of some samples. Samples were also isolated by TLC and then analyzed by IR.

NADDY: Two laboratory periods were devoted to GC and TLC.

WILLIAMS: Report describes the separation of a mixture of blue dextran, cytochrome and DNP-glycine utilizing gel-filtration chromatography. Additionally, TLC was used in the identification of amino acids.

Future plans of group members run the full gamut of pedagogical activity. Some are going to introduce new courses to the curriculum or modify existing ones. Others plan to integrate chromatography with NMR and IR for identification. Also, there are plans to apply ion exchange techniques to inorganic analysis. One product of the workshop is the plan of several attendees to formally devote time to the design of experiments involving chromatography *per se*, as well as the incorporation of chromatographic techniques into existing programs. It is remarkable that many of these ideas come from the reunion and not just the workshop itself. Could we see more instruments?

Pedagogical Troubles Encountered

Pedagogical road-blocks were few. These seems to be too little time to introduce the new ideas into an already existing course. Poor results by students take time to discuss and rectify.

Equipment/Supply Problems

These were few and, in general, were those attendant to instruments in general. A great help would be catalogs, catalog numbers and a list of supplies for this specialty equipment.

Student Benefiting

Since the ultimate goal of this project is improvement in chemical education, the attendees were polled. It was revealed that 325 students, throughout the undergraduate range, had their theoretical and practical educations expanded as a result of this workshop. This number is expected to rise with time.

Benefits To Pre-College Students

Paper chromatography of ball-point inks and plant pigments has been used to interest pupils down to the 5th grade. SCOPE and other on-campus programs are benefiting from techniques learned at the workshop. We recommend paper and TLC demos during off-campus visits.

Changes For Future Workshops

There was not agreement on re-emphasizing different kinds of chromatography outside a slightly higher interest in HPLC. Some members would be willing to come back at night to get more time in lab.

Chromatography for Research

Since attendees are from colleges and junior colleges, only a few had research applications. Those applications mentioned include using HPLC for purity checks and following a kinetics study, analyzing reaction products and applying ion chromatography to water quality studies.

Colleague Acceptance

Resistance from colleages has not been a problem up to now and very little is anticipated. Attendees feel that student acceptance will swing any recalcitrant colleague, especially in allied health labs.

NOTE: As in no many other endeavors of this kind, meeting peers and experts must be put near the top of any "value" list. The friendship and comaraderie during the workshop will be built on in the future.

Molecular Modeling

Overview

Molecular modeling is a new field in chemistry. Historically, molecular modeling was almost exclusively done by quantum mechanicians and computational chemists. In addition, often only research groups at universities with extensive computer facilities were able to engage in serious molecular mechanical calculations. However, with the introduction of PC-based software, chemists at smaller colleges and universities have joined the molecular modeling community.

The results from these calculations have yielded excellent qualitative predictions of optimal three-dimensional structures. In addition, in many cases, quantitative results such as energy calculations have paralleled the qualitative results. The computer graphics output are both artistically exciting and intellectually intriguing to both faculty and students. And finally, we have begun to observe that high school students are able to utilize the results from the computer graphics to understand the shapes of molecules.

Unfortunately, there are areas in molecular mechanics that need addressing. Hardware requirements to do molecular modeling go beyond the equipment resources of most colleges. And software costs are still too high for most small liberal arts colleges to afford.

Usefulness of the Workshop

It is quite clear from the various reports that the molecular modeling workshop has started activity in this area at all the institutions represented. Although a variety of problems were encountered, there was very little discouragement expressed. The reunion conference has been very helpful because of the ease of idea exchange and it will probably generate renewed activity when we return to our individual institutions. While the members of our group may not interact with one another in any formal way in the future, we nevertheless know that helpful discussions are only a phone call away.

In a relative new area such as molecular modeling the workshop tone was more centered around expressing a variety of problems and possible solutions rather than simply a transfer of knowledge from the informed to the uninformed. For example, how we go about involving a class whether general, organic, physical chemistry students in molecular modeling has no simple answer. There are problems with either individual or group instruction when more than just a few students are involved. The workshop generated numerous questions but did not supply the answers. Because it did not supply answers, the workshop was more stimulating. The participants in this workshop may have a very significant impact upon the way molecular modeling will be introduced into an educational system at a college level and ultimately in high schools as well.

Uses of Molecular Modeling

The workshop felt that molecular modeling was of significant value particularly in expressing three aspects of chemistry to the students: the concepts of shape, symmetry and complexity. Beginning students generally have difficulty visualizing the three dimensional nature of molecules. Models have long been available but the students rarely spend enough time using models. The advent of computer molecular modeling provides another opportunity for the student to visualize the molecule in three dimensions.

Molecular symmetry is a fundamental aspect of chemistry from molecular spectroscopy to the allosteric interactions of multisubunit proteins. As with the idea of molecular shape, students rarely spend enough time working with models to develop an appreciation of symmetry. Molecular modeling offers a teaching tool in this area. The instructor can generate data sets illustrating various symmetry concepts and the students can use the molecular modeling software to visualize these. The color graphics currently available make this a visually, as well as intellectually, interesting experience.

Molecular complexity is a hallmark of biological chemistry. However, this complexity is not at all apparent to many students. For example, often students appear to view nicotinamide adenine dinucleotide as the letter (NAD^+) rather than as a pyridinium ring, phosphate linkage and adenosine moiety with the steric and electronic properties attendant to these groups. If biochemistry is to be more than simple memorization, students need to spend substantial time looking at biological structures. Professors have long used transparencies, and the new 4-color textbooks are often excellent in presenting the structures of biological molecules to the students. However, neither of these approaches is three dimensioanal. Molecular modeling has a number of other uses in the instructional setting. Dr. Williamson has used it successfully in the physical chemistry laboratory to generate data for molecular orbital calculations. It has also been used to determine the preferred sites of protonation in polyamines and to help explain the role of metal complex geometry in peroxide decomposition reactions.

The workshop participants felt that the visual aspects of molecular modeling are exciting for most students. The workshop participants hope that this visual aspect may reduce computer phobia in some students and allow them easy entry into the use of computers. At the other end of the computer use spectrum, workshop participants noticed that computer-literate students, particularly high school students, find molecular modeling very exciting. Molecular modeling may reveal the beauty of chemistry to students early in their studies.

National/Regional Symposia

Currently, a wide variety of types of software and the associated hardware are available to be used to show, at the CRT, the three dimensional nature of molecules. These representation range from the framework type to the space-filling variety. It is recommended that the use of these be encouraged by educators and vendors at future ACS meetings in the Division of Chemical Education and in the literature.

It is further suggested that at the 11th Biennel Conference on Chemical Education there be a symposium on the uses of Molecular Modeling in the Undergraduate Curriculum. This should go beyond the representation of the shapes of structures and include the various aspects related to the determination of structures, that have been minimized with respect to energy (stretching, bending, torsional, van der Waals, etc.).

Provisions should be made for presentation by authors of molecular mechanics software and by vendors of the software and required hardware. Presentation by undergraduate faculty currently using the technique of molecular mechanics in their courses might include, but not be limited to, the following applications: steneochemical difference in simple and complex systems, drug design, molecular dynamics and molecular beam collision, electrostatic interaction between molecules and ions, relationship to molecular and ion, relationship to molecular orbital calculations, etc.

Uses of Molecular Modeling in the Classroom

It is clear that molecular modeling can impact students from the very lowest grades though graduate studies. Some ways in which the methods could be used in teaching are as follows:

A. Lower Grades – Concept of two dimensional projection vs actual geometry – things as simple as triangles vs pyramids, squares vs cubes, etc.

B. Upper Grades – Again use to show geometry and also 3-D versions of molecules shown in chemistry texts. One idea that might be useful here would be for a good chemistry or science club to prepare video tapes that could be distributed in grammar schools and high schools in participant's area. Perhaps local ACS sections could underwrite such projects. Distribution could coincide with National Chemistry Day.

C. College Freshman – Same as for upper grades but more in depth including actual ideas of symmetry such as axes and planes. Here hopefully user friendly software could allow for direct student interaction to produce their own structures.

D. Upper Division – PC Model has parameters loaded to allow conformational analysis of organic structures. Stereochemistry can be displayed with clarity and avoid misconception between the speaker and the listener. It is very true that in this area, one picture, and especially one that can "move", is worth many frustrating moments of word use.

The ability to perform a calculation to produce the lowest energy structure is available in PC Model. This can be used to determine the direction for a project, to compare sites for possible reactivity, in reaction rate explanation and as yet to be determined areas in computational analysis.

The goal for the future of chemical modeling would be that in three to five years we would have the ability for a network and large screen projection equipment so students can (a) Construct their own models and have an instructor be able to access each computer from his unit and display the structure to the class. This utilizes all the interactive areas and the student actually "hands on" creates a structure. (b) The instructor can monitor progress and prevent total frustration. (c) Each student benefits from their colleagues' effort.

Hardware and Considerations

The one consensus of all participants was that excessive time was required to finally put together a hardware system which was compatible with the software acquired. A variety of different reasons were related by individual but the general problem is very real. Most campuses have not developed their computer labs for the needs of science students. Most campus PC's do not have math coprocessors which are necessary for any modeling program. By way of information, most art graphics programs are not usable on campus computer networks. These should be an immediate effort by everyone to encourage your own local situation to produce change in this area. NSF support for upgrading networks for this purpose would be most useful.

The modeling programs available are somewhat expensive and generally do not provide for licensing to the institution nor for networking. Both of those traits are desirable for academic usefulness.

We need someone to provide the hardware to allow for direct recording of screen images in VGA/EGA graphics to a VCR tape. This would make it possible for high school teachers to come to their most convenient college campus and produce VCR tapes of shapes, etc., for use in their classes. This crosses over molecular modeling as a field into usefulness in other areas, i.e., kinetics. Since most of us have IBM compatibles that is the market of interest.

We would encourage *J. Chem. Ed.* to review new modeling software in a timely and thorough manner. We would encourage all members of these workshops to remain in contact and pass along information concerning new, usable software they encounter.

Instrument Interfacing

I. Instrument Access and Availability

A. Equipment Requirements

Research projects or any teaching applications of this workshop must involve computers, interfacing boards, appropriate software, other hardware, and a scientific instrument. These components are required to perform actual laboratory experiments.

B. Hardware and Software Acquisitions

All participants were able to access personal computers, usually, IBM's or compatibles. Some use Apple II. Between the December workshop and the April reunion all participants purchased or constructed interface boards. All have, as a result of the workshop, purchased, requisitioned, or plan (on next year's budget) to acquire software for data acquisition and/or control. The program of choice was one called UnkelsScope, which had been demonstrated and used at the workshop.

In using the hardware purchased, some problems were encountered because of lack of adequate documentation and technical support. Some individuals had access to expertise on their campuses, but those from small institutions were more dependent on information from suppliers, which was not always readily available.

C. Software Modifications

Some participants modified BASIC programs made available during the December workshop. At least one participant who had the ASYST scientific programs prior to the workshop, but who had not used it for acquiring data, learned more about its applications.

D. Instrument Modifications

Individual participants are working with a variety of laboratory apparatus, depending on their particular applications. One participant assembled and demonstrated a valve used for automatic titrations and brought enough valves to give one to each of the other participants. Others described their uses of a bomb calorimeter interface and polarograph.

II. Trouble Shooting and Maintenance

While maintenance once consisted of little more than soap & a test tube brush, the increasing complexity of chemical instrumentation, has left many instructors unable to properly maintain and troubleshoot the equipment they routinely use. To varying degrees, this posed a potential problem for each of the workshop participants, while some were perhaps a bit more skillful than other at things electronic, not one claimed any great expertise in the area, and not one had access to an on-campus electronics technician. Four had limited access to school personnel with other duties who had the expertise to help as time permitted. One had used the Ga. Tech traveling instrument repair service, but felt that many minor problems could be handled locally if phone advice were available.

III. Incorporation Into Teaching Activities

A. Rationale

The purpose of interfacing an instrument with a computer should be acquisition of better data without insulating the student from the experiment. The student is then freer to acquire data without feeling bogged down by the equipment.

B. Specific Applications

1. Integration of a computer interface with a polarograph was effected in Chem 201 at DeKalb College, Clarkston, GA. The software (Unkelscope) allows processing of the voltammogram data (integration and peak finding) to yield peak positions and areas.

2. Temperature and time measurement for a bomb calorimeter using a thermistor for temperature measurement was done in the physical chemistry course at Georgia Southern College, Statesboro, GA. The data acquisition board, signal conditioning electronics and data acquisition software permitted the students to concentrate on sample preparation and data analysis rather than tedious thermometer and stopwatch observations. The higher data quality and its availability in digital form allowed more shopisticated analysis of the data.

C. Projected goals

Most members of the group have or are purchasing the hardware and software required for instrument interfacing. Because each project is independent and because of time and/or economic considerations, some members have not yet been able to bring their projects to fruition.

IV. Incorporation Into Research Activities

Most participants in this workshop focused their activities on incorporating the workshop information into teaching. The research activities were very limited due in part to the short time between the workshop and the reporting reunion.

One area of research was addressed by a member of the group. A UV- visible spectrometer was interfaced with a lock-in amplifier to improve the signal-to-noise ratio. This is necessary to recover a signal from a very noisy background.

In addition, one member of the group is developing an inexpensive auto-tirating system to interface with a computer. The basic design was a low-amp relay, which opened and closed an externally-powered, solenoid-operated valve.

V. Instrument Interfacing – Colleague Acceptance

We experienced no difficulty with teaching colleague acceptance. Many colleagues were interested in what had been discussed at the Workshop, with some showing interest in attending subsequent workshops through the Faculty Enhancement Project.

In addition, colleagues were eager to ascertain if instrument interfacing could be applied in their area. As our group begins to complete their own individual projects, it is desirable that colleagues be included in future endeavors.

In general, acceptance by administrative colleagues was positive with a willingness to at least partially fund our projects.

Mass Spectroscopy

I. Overall Areas of Impact of the Workshop

The ten people who were selected to participate in the December 1988 mass spectroscopy workshop represented a wide range of institutions, both in size and scope. Their prior experience with mass spectroscopy ranged from active research to only brief introductions in courses. As a result of the workshop, all participants have reported more interest in this technique, greater emphases on instrumentation and stimulation toward professional growth.

Without exception, every participant gained something that he/she has already put to use in some professional activity. The areas represented by these activities include at least the following: 1. general information, 2. teaching, 3. research, 4. maintenance (tips), 5. resources, 6. professional contacts (colleagues), 7. trouble-shooting (vendors/local).

In the short time since the workshop, one instrument has been ordered, two are in the planning stage and two are being repaired to be put back into service. In addition, two colleges without instruments have taken field trips to existing Mass Spectroscopy research facilities and the subject has been more thoroughly covered in many classes.

In addition, one attendee from a relatively small two-year institution with a very limited budget became painfully aware of the minimum requirements for obtaining and maintaining any type of mass spectrometer. Having no research budget and teaching only lower division type courses makes it almost impossible to justify a MS lab on such a campus. The information gained at the workshop helped this individual make the logical and reasonable, though difficult, decision to decline the offer of a used mass spectroscopy instrument when it was offered to the institution approximately two months after attending the workshop. Not only the lack of financial resources, but also the realization that the lack of an adequately trained technician would make sustained and successful operation of the instrument unlikely.

However, since this institution is geographically located near Atlanta, this workshop participant and at least one other has, through contacts made at the MS Workshop included student visits to operating Mass Spectroscopy labs in their teaching activities. Field trips have included visits to the CDC in Atlanta, State Crime labs, and Georgia Tech.

The success of this workshop must be attributed to the quality of instruction and facilities provided. Dr. Moran and his staff provided an attitude and atmosphere very conducive to learning.

II. Impact on Teaching Activities

Participants in the workshop represented a wide variety of institutions and environments: large to small, 2- and 4-year, with and without access to MS instrumentation, with and without technical support where MS instrumentation is available. All, however, attested to the positive impact of workshop participation through the professional stimulation received from the workshop content, interaction with colleagues, and establishment of contacts at institutions with ongoing graduate-level programs.

More directly, however, has been the appearance of new or expanded MS content in their undergraduate teaching, appearing in instrumental analysis courses, but also in organic (lecture and/or laboratory), organic qualitative analysis or physical chemistry. While exposure to MS hardware varied, simulation softwares and "paper" unknowns have been utilized as alternatives. Most reported a rather direct adaptation of workshop content and materials to their purpose, ranging from an overview of the instrument and its capabilities to more detailed coverage of equipment, sample presentation and analysis of spectra. Many have used field trips to MS facilities to span the gap where operational MS instrumentation was available.

All participants are involved in a student "pipeline" operation from 2- to 4-year programs, to graduate/professional postbaccalaureate study, or to industry. Instrumentation utilized in any of these environments is constantly evolving, inevitably toward greater sophistication. We as classroom teachers must find ways to remain current and ensure that this currency is appropriately reflected in our instruction.

One participant from Millsaps' plans to use information from the workshop in part of another workshop this summer. She is co-director of the Howard Hughes Medical Institute (HHMI) Workshop for high school teachers. The five Chemistry participants will be exposed to current research tools and techniques such as GC-MS, FT-IR, HPLC, AA, and NMR for an intense two weeks (Phase I). During this time, the teachers will plan Phase II which is for two additional weeks after a two week break. In Phase II, the five teachers will each return with one or two of their students. At the close of Phase II, they will submit research proposals for consideration for modest funding by the Hughes Grant committee.

III. Impact on Research Programs Involving Use of Mass Spectrometry

Among the participants in the Mass Spectroscopy workshop, three are associated with active programs involving the application of MS to research projects.

1. At Western Kentucky University, the benchtop MSD unit is being used extensively to support an undergraduate research program. The project includes the preparation of a series of unsaturated substituted amines for which MS is the primary means of structural confirmation. These compounds will be used to study ion-radical transformations.

2. At Savannah State College, one on-going project directed by Kamalakar Rant involves the synthesis of compounds with potential pharmaceutical activity. One known active compound is perhexilene, 2,2- dicyclohexyl-1-(2-piperdyl)ethane, which is effective in the treatment of angina pectoris. Its use is limited by toxic side effects such as neuropathy and hepatoxicity. The project at SSC has led to the preparation of a number of analogues of 2,2-diphenyl-(N-phenyl)ethylamine. It is proposed that the substitution of phenyl groups in place of the cyclohexyl groups and the removal of the N from the piperidyl ring will diminish or eliminate the toxicity while maintaining physiological activity.

Although no MS instrumentation is available on the campus at SSC, FAB analyses obtained at Georgia Tech (as a direct consequence of this workshop) and elsewhere have confirmed the identity of several of the newly synthesized compounds. These will now be subjected to tests regarding their physiological activity.

3. Mass Spectroscopy has been used by Jing-Fong Wei of Southern University as an effective tool for her DOE funded research project. She applied gas chromatography/mass spectrometry to identify the products from derivatization of aromatic amino and phenolic compounds.

When trifluoroacetyl chloride was used as the derivatizing agent and pyridine was used as the base catalyst, all amino compounds, like anilines and tetrahydroquinolines, were quantitatively converted to trifluroacetyl amides. The formation of these trifluoroacetyl amides was confirmed by comparing the m/e values of the molecular ions of the derivatized products with those of the original compound. A m/e increase of 96 resulted from the exchange of a hydrogen atom (mass unit 1) with a trifluoroacetyl group (mass unit of 97). However, little derivatization was observed for phenolic compounds, which has been previously reported in the literature. It is attributed to the highly labile characteristic of the trifluoroacetyl group in esters. To increase the derivatization yield for phenols, the following method was applied. The trifluoroacetyl chloride was again used but was accompanied with an alkanoic acid (e.g. butyric acid). Phenolic and amino compounds exhibited very different behavior toward derivatization as described in the following chemical reactions

$$\text{phenols} + CF_3C(O)Cl + C_3H_7C(O)OH \longrightarrow \text{phenyl butyrate}$$

$$\text{amino compounds} + CF_3C(O)Cl + C_3H_7C(O)OH \longrightarrow \text{trifluoroacetyl amides}$$

For phenol derivatization, trifluoroacetyl chloride served as catalyst rather than as derivatizing agent. The products of reaction with phenols were confirmed to be butyrates by the observation of a m/e value of molecular ion increase of 70 (resulted from addition of the $C(O)C_3H_7$ group, mass 71, and loss of the hydroxyl hydrogen, mass 1)

Gas chromatography was used to determine the percent derivatization of a model compound in a model compound mixture. However, gas chromatography was not used for derivatized products' indentification because the following reasons. (1) standard compounds are often not available from chemical companies, therefore, a retention-time confirmation is not feasible; (2) for some amino compounds (e.g. 2 aminobiphenyl), the retention time of the original compound may be the same as that of its derivatized product; (3) coeluted peaks are often present. Therefore, gas chromatography/mass spectrometry must be used for compound identification.

IV. Equipment Maintenance and Problem Areas

The MS Workshop presented participants with information and catalogs for parts and specialized services which were most appreciated. Basic guidelines for trouble shooting were given, and were used by several participants since December 1988. (by Rita Hessley at Western Kentucky for example.) Other schools were able to get yearly service contracts (Millsaps) whereas others utilized "per incident" service visits and and the CHEMS service from Georgia Tech. Other schools such as Southern University and Jacksonville State University have their own service technicians in house, the ideal situation. Southern University, however, had their technician resign this year as the mass spec went down. Hewlett-Packard came to fix it, but funds ran out before they completed the job. As soon as Southern obtains the necessary funds, HP will return.

Two participant's schools – West Georgia College in Carrolton, Georgia and Millsaps College in Jackson, Mississippi – have recently purchased Ion Trap Detectors coupled with GC's that have had extensive problems and are currently not operational. West Georgia's is a Finnegan and Millsaps' is a Finnegan inside of a Perkin-Elmer labeled box. Neither instrument has worked properly since installation. West Georgia's problems ballooned when the warranty expired and the administration canceled service contracts. When service visits quickly exhausted the funds for manufacturer instrument repair that were available, West Georgia switched to CHEMS at Georgia Tech where their instrument is currently being repaired. Millsaps' problems were compounded by being one of the first in the mid-south to purchase a Perkin-Elmer GC-ITD. Millsaps' was also the first one installed and serviced by their P-E service rep. When one problem was fixed, one or two more suddenly appeared. The last trip in March to correct a problem caused in November before warranty expired resulted in the service rep "frying" both columns available. He had "sandwiched" Millsaps in an installation visit to another lab in Jackson. Because of the many problems, Millsaps Chemistry Department was able to convince their administration to purchase a service contract for the ITD as well as several other new P-E instruments.

V. Colleague Acceptance

There is general agreement among the participants of the mass spectroscopy that very positive colleague acceptance and interest exists, not only among the members of the workshop, but even more importantly from their colleagues on their home campus. This is evidenced by the questions many of us have been asked by fellow faculty members.

The two major categories that the questions generally relate to are either about the specific subject matter covered in the workshop or involve requesting information about how they can make application to attend one of the future workshops.

At this point, the members of the Mass Spectroscopy Workshop wish to express their sincere thanks and appreciation to all those individuals and institutions responsible for any part of the planning, development and conductance of this workshop and the follow-up reunion conference. All of us have benefited in a number of ways from our attendance at this workshop. Thank you all – faculty and staff – Georgia State University, Georgia Tech, Berry College – for sharing your time, efforts and expertise.

VI. Summary

The value of this workshop can be summarized by two quotes from written reports of participants:

> "In closing, I want to say that both my students and myself are much better informed and aware of what mass spectroscopy is, what it can do and how it is currently being used. We are all better educated as a result, and I'm very appreciative of having had the opportunity to attend the workshop."

Gary McGlaun
Gainesville College

> "Over the years, I have participated in a number of instrument training-type programs, most with the same general goals as this one. Some were of marginal value, and others almost a waste of time. None was even comparable to this workshop which was excellently planned, smoothly executed and outstandingly staffed. The opportunity to participate is sincerely appreciated."

Richard Legendre
University of South Alabama

FINAL REPORT OF THE FT-NMR SPECTROSCOPY WORKSHOP REUNION

I. INTRODUCTION

Forty people participated in two workshops (June and December, 1989) on FT-NMR held at GSU. Thirty of the participants attended a reunion symposium held in Savannah, Georgia to formulate this report. We would like to thank Dr. Curtis Sears, Dr. Ronald Jones, and Dr. Thomas Farrar for their hard work and NSF for funding this program.

The workshops involved hands-on use of FT-NMR spectrometers with their associated superconducting magnets for acquisition of time-domain spectra (FID's), network transfer of the FID's to VAX computers, and both on-line and off-line Fourier transformation and plotting of the frequency-domain spectra. Different computer programs were used on the VAX terminals and IBM 80386 powered PC's. The program *PC-NMR+* for processing of FID's previously collected on Brucker or Varian spectrometers and which runs on IBM PC-AT computers equipped with a math-coprocessor and a three-button mouse seems to be very powerful to many participants in that it can be used at home institutions with minimal cost.

Without any reservations, all who attended the workshop recommend continuation of this program. Even though instruments may be limited, IBM PC programs and access to remote FT-NMR facilities allow the participants the ability to incorporate this technique in research and teaching. The report includes a statistical survey of participants as well as a number of conclusions.

II. STATISTICAL SURVEY OF FT-NMR GROUP

TOTAL RESPONDENTS = 30

INSTITUTIONS:

INSTITUTIONS OFFERING TWO YEAR DIPLOMAS.............. 5
iNSTITUTIONS OFFERING FOUR YEAR DEGREES................25

COURSEWORK:

HAVE INSTRUMENTAL ANALYSIS COURSE.............. 18
INCORPORATE FT-NMR INTO ADV. ORGANIC.......... 10
INCORPORATE FT METHODS INTO ORGANIC.......... 2

INSTRUMENTATION:

PLAN/HOPE TO ACQUIRE FT-NMR.........14
HAVE ACCESS TO FT-NMR..................... 13
HAVE OPERATIONAL FT-NMR................. 4
HAVE CW-NMR.. 19
HAVE NO CW-NMR.................................. 9

COMPUTER HARDWARE AND SOFTWARE:

HAVE IBM PC OR COMPATIBLE (80286+MOUSE)............... 16
HAVE/PLAN TO ACQUIRE PC-NMR+.................................... 18
USE OTHER SOFTWARE (SERAPHIM, TRINITY, ETC)...... 13

III. INCORPORATION OF FT-NMR INTO TEACHING

A. The majority of participants in this conference have limited access to spectrometers. Even for those who have such instruments, hands-on use of these instruments by undergraduates is limited because of operational complexities and for protection of the instrumentation. For these reasons it seems necessary to focus on instructional strategies that make knowledge of FT-NMR spectroscopy accessible to a larger population of students. We believe that FT-NMR can be incorporated into the chemistry curriculum at several levels of complexity, depending on the sophistication of the students.

1. Introduction at the Freshman Level is possible when application is stressed (i.e. MRI Magnetic Resonance Imaging). This has been employed successfully in chemistry courses for students in allied health programs. This approach could be extended to courses designed for students majoring in science programs.

2. At the sophomore organic chemistry level, interpretation of proton ^{1}H-n.m.r. and ^{13}C-n.m.r. spectra should be the main focus. In the laboratory, student operation of FT-NMR instruments should not be expected, but examples of spectra can demonstrate the power of the FT and CW techniques. Comparison of these techniques in structure elucidation problems has been used as a successfully pedagogical tool by some participants.

3. Juniors and Seniors can be exposed to principles and theory of more advanced techniques, and interpretation of two-dimensional spectra (COSY and HETCOR), etc. This type of presentation has been done successfully by several workshop participants.

4. Advanced undergraduate students are generally ready for hands-on operation of FT-NMR spectrometers. In FT-NMR usage at all levels of instruction, students must develop an appreciation for the importance of meticulous sample preparation.

B. Computer software currently available can extend the teaching of FT-NMR techniques to those institutions which are unlikely to own or have immediate access to an FT-NMR spectrometer. The *Felix* and *PC-NMR+* software packages will allow students to produce, examine, and plot their own spectra from previously accumulated FID's without the physical presence of a complete FT-NMR spectrometer. With cooperation from institutions having appropriate spectrometers, a large library of FID's for standard compounds could be made available in appropriate file format for use with these software packages. It should be emphasized that these programs are not simulators. Rather, they allow relatively inexpensive computers and plotters to do real-time Fourier transformation, along with the use of apodization functions, and other processing of FID's that have been previously accumulated. From the student point of view, this is about half of the total process of production of FT-NMR spectra.

   In addition to these computer programs and FID files, we would like to see the development of software packages that would simulate the hands-on operation of an FT-NMR spectrometer for the acquisition of FID's. This should be designed to give students experience in dealing with the various parameters that must be considered in the process.

IV. HARDWARE SPECTROMETER AVAILABILITY

Several topics were discussed by a group of participants who have secured FT-NMR spectrometers or funding to buy one in the near future. The issues discussed are delineated below.

A. FUNDING SOURCES: NSF(ILIP), Camille-Dreyfus Foundation and corporate funding for matching money.

B. SPECTROMETER: High-field multi nuclei FT-NMR spectrometers are preferred.

C. MAINTENANCE: Service contracts. Cost of helium and an electronics person.

D. SITE PREPARATION: Very important to have a dust free magnetically shielded, air-conditioned room. Power supply of 220 V with appropriate stabilization is necessary. A participant quoted a cost of $10,000 for site preparation.

E. OPERATORS: Faculty and trained (advanced) students. One faculty member is designated as the principal operator.

F. WHERE IN CURRICULUM: Organic I & II (lab and theory), Spectroscopy course, Physical Chemistry, Advanced Organic Lab, Instrumental Analysis, Biochemistry, and (most definitely) Undergraduate Research.

V. CONCLUSIONS

A. The cost of acquisition and maintenance of a modern Pulsed Fourier Transform-NMR spectrometer with a superconducting magnet is prohibitive at typical smaller colleges. Lower field continuous wave instruments with permanent magnets are more feasible and relatively commonly encountered. Unfortunately, they severely limit applications relative to those available with pulsed FT systems.

B. There is a need for a commercially available teaching FT-NMR spectrometer utilizing a permanent magnet with a cost below $100,000. This would make possible a full and appropriate inclusion of this important element in the chemistry curriculum at many more smaller colleges than is presently the case.

C. In the absence of an FT-NMR spectrometer, it is feasible to make at least a partial inclusion of the method through use of FID's previously accumulated at an off-campus site where the greater power of a high field spectrometer is available. These FID's can be used effectively through the use of inexpensive personal computers and plotters equipped with currently available software packages.

D. FT-NMR methods can be incorporated into the existing curricula in the following areas:

1. Sophomore organic chemistry, through interpretation of ^{1}H-n.m.r. and ^{13}C-n.m.r. spectra.

2. Junior and Senior level courses, where theory and 2-D interpretation may be included.

3. Instrumental analysis and other specialized courses.

4. Undergraduate and Research, where hands-on application is almost essential although use of an off-campus spectrometer becomes more feasible because of the recently introduced microcomputer software noted in section III.B. above.

Report of the Molecular Modeling NSF Workshop
April 30, 1990

Overall. Molecular modeling is growing to be an important tool in teaching and research in many ways. First, it is very useful in presenting stereochemical concepts to the students. This benefit is seen primarily in organic chemistry; participants had also had some experience using the program in inorganic chemistry. Second, molecular modeling allows students to develop a feeling for certain aspects of the energetics of molecules. Examples include the torsional energy in carbocyclic rings and the energy needed to rotate around a given carbon-carbon bond.

Molecular modeling presents a number of technical advantages. First, the students enjoy seeing the molecules and are motivated to study certain aspects of chemistry further. Second, although it takes about two hours to introduce a student to the programs, thereafter the student can work without supervision. Third, faculty with schedules which allow little uninterrupted time enjoyed being able to work on molecular modeling projects, which are ideally suited to short blocks of time. The main disadvantage of the technique is that it has substantial hardware requirements, although most small schools can now afford at least one appropriate computer.

Teaching. The participants had developed a variety of laboratories at the undergraduate level which incorporated molecular modeling. These included:

1. Modeling of a complicated cage-compound rearrangement involving numerous carbocation intermediates. Starting material and product are both commercially available and the experimental portion of this exercise, involving experimental analysis of the rearrangement, is under development (Advanced organic).

2. Modeling of the torsional barrier to rotation in a series of substituted ethanes (Sophomore organic).

3. Modeling of the stereochemistry and calculation of the dimerization of fatty acids (Biochemistry).

4. Modeling of various three to six-membered carbocyclic rings to show the correlations between conformation and torsional strain (Sophomore organic).

5. Modeling of various isomers of an inorganic complex (Inorganic).

6. Making a videotape (any level).

Research. In research, participants ha used molecular modeling to investigate the structures of morphine analogs and dopamine agonists, to predict the stereochemistry of cyclopropane derivatives, to decide between various possible structures arising from a rearrangement and to investigate carbocation rearrangements.

Instrument Interfacing Group Report

Colleague Acceptance and Incorporation into Teaching Activities

Acceptance of the value of the workshop at the administrative level is demonstrated by the fact that seven of the participants have obtained funding to acquire interfacing systems during the past year. The reunion was beneficial in allowing participants to discuss and compare the characteristics of these systems. Several of the participants have worked with departmental colleagues in designing interface configurations and developing experiments using interfaces. The general applicability and importance of computer interfacing in modern science and engineering will doubtless foster further cooperation among workshop participants and their colleagues in the future.

Participation in the workshop has stimulated a great deal of activity in designing and modifying experiments used in education. These projects are reported in the individual reports prepared for the workshop reunion.

The process of titrations can be accurately and rapidly monitored, displayed, and analyzed using interfaces. The complexation process can be demonstrated by monitoring pH, conductance, and selected ions during compleximetric titration. For example, the titration of Cl^- with Ag^+ can be monitored to show complexation and the determination of K_{sp}. Further titration with a solubilizing ligand, such as NH_3, allows computation of K_f. Having the data in a computer file greatly facilitates demonstration of refined data processing operations such as analysis by the first or second derivative of the analytical curves. Systems for demonstrating thermometric and spectrophotometric titrations have also been developed. Instruction in computer programming can be incorporated into these experiments by having students write segments of the necessary programs. These activities can be incorporated in the laboratories of general, analytical, and inorganic chemistry courses.

Computerized titration can also be useful in the classroom. One participant described the demonstration of buffering through titration of a weak acid while monitoring titrant volume, pH, and salt concentration. Rapid data analysis using the computer makes such classroom demonstrations time efficient and instructive.

A number of physical chemistry experiments can be augmented by computer interfacing. Accurate heating and cooling curves can be obtained using simple and inexpensive systems. The accuracy of computerized data acquisition facilitates experimental demonstration of the phenomenon of supercooling. The relationship between pressure and temperature of gases can be easily demonstrated with computerized data acquisition. One participant has developed an apparatus for obtaining pressure-temperature measurements during adiabatic expansion of gases. This apparatus can be used to measure Joule-Thomson coefficients of gases. An experiment for obtaining second virial coefficients of real gases was also described.

Reaction kinetics can be studied using computerized data acquisition. The interfacing of spectrophotometers, demonstrated in the workshop, is being utilized by two participants in kinetics experiments. One participant described the interfacing of a flash kinetic spectrometer. This application demonstrates the advantage of the rapid data acquisition possible through interfacing.

One participant is involved in development of an experiment to demonstrate the laws of motion in a physics course. This experiment utilizes an ultrasonic measurement system to monitor the motion of objects on air tracks.

Knowledge gained through the workshop has helped a number of participants in efforts to upgrade analytical instrumentation used in teaching. Instruments which have been or will be upgraded include various UV-visible spectrophotometers, a spectrofluorometer, an atomic absorption spectrophotometer, multichannel analyzers, a polarographic analyzer, and two chromatographs. Such upgrading not only increases the usefulness of the instruments, but demonstrates the mechanics of interfacing to students who use the instruments.

The subject of instructing students on interfacing was discussed at the reunion. The importance and variety of applications of computerized data acquisition and instrument control makes this an important subject for science and engineering students. One participant plans to demonstrate the process of data acquisition and processing by having students in an instrumental analysis course use a general purpose system to acquire and manipulate chromatographic data. The system will also be used in an advanced analytical chemistry course to demonstrate electronic and statistical signal processing. The possible benefit of including the topic of computerized systems in industrial process monitoring in analytical courses was discussed.

The above applications of knowledge gained at the instrument interfacing workshop clearly demonstrate the value of the course in stimulating and facilitating improvement of educational experiments among participants. Several participants also noted the value of the workshop in improving the depth of lecture discussions of computer interfacing and electronics.

Report of the Reunion Meeting
of the
Chromatography Workshop
held at
Georgia State
April 26 and April 27, 1991

Introduction:

A combination of theory, technology and teaching is basic to meeting the needs of society. While technical advances may precede theoretical explanation or theory may exist long before the technology needed for practical applications, teaching always follows the evolution of technology and theory and in turn fuels future cycles of progress. The NSF Workshops at Georgia State are playing a vital role in bringing the knowledge of regional faculty at undergraduate institutions up to date in areas of vital importance to future development.

Chromatography is a twentieth century phenomenon. In 1978 a review of the Pittsburgh Conference stated that the dollar amount spent on separations instrumentation (especially chromatography) had surpassed that of the former leader, spectroscopy. Clearly the twin messages were both of the great importance and of the great expense of this technology. Chromatography had arrived at this paramount point by major developmental milestones which have been occurring at an accelerated pace since 1940. Theoretical and technical innovations have produced a myriad of techniques. Unfortunately, the fundamental similarity of various chromatographic techniques is often unrecognized. Applications are found in nearly all areas of scientific endeavors but are often used in an empirical fashion and viewed only as a means to an end. This narrow orientation negates the possibility of seeing chromatography as a collection of interrelated and powerful tools that must be well understood to be used effectively. One result is that chromatographic methods are often found scattered and isolated in various pockets within the chemistry curriculum and elsewhere.

The Chromatography Workshops:

Mirroring the diversity of the relevance of chromatography, the twenty participants selected for the June and December 1990 Chromatography Workshops held at Georgia State came from as wide a range of backgrounds as chemistry itself. Represented were individuals whose primary discipline was Analytical, Biochemistry, Inorganic, Organic and Physical Chemistry. Most were in mid-career and from institutions with very limited funding available for support of teaching chromatography.

An excellent means of reducing the general confusion associated with chromatography and meeting the individual needs of participants was found in the person of Gabor Patonay. Here was a young instructor who had matured as a scientist while chromatographic methods were gaining importance. As the developer of the Chromatography course for graduate and undergraduate students of Georgia State he had the experience needed to present clearly the many details of this complex subject. As the head of a large research group active in chromatography he had the experimental skill necessary to be effective in guiding solutions to problems for workshop participants. Among these issues was the repair of pieces of instrumentation brought from the home institutions of several participants.

Results of the workshop:

Activities reported on at the reunion meeting cut across the chemistry curriculum. What follows is a listing of individual highlights.

Vincent Anigbogu of Austin Peay State University reported that thanks to technical assistance provided by Gabor Patonay he was able to get the HPLC borrowed from Emory University to work. As a result students of his had made **six** presentations at a meeting of the Tennessee Academy of science. These papers reported the results of research on the effects of cyclodexins on separations, which was one of the advanced topics covered by both the laboratory and lecture sessions of the workshop.

David Hartman of Western Kentucky University reported on plans to incorporate gas chomatographic determination of the methylated saponification products of fats into his Biochemistry course. TLC will also be used in this course for monitoring fatty acids and triglycerols.

David Hawkes of Lambuth College reported on the establishment of an interface between his GC instrument and a microcomputer. As a result his students were able to shift their attention from dealing with the mechanics of extracting data from a chart to the experimentally important variables. He also reported on the difficulties associated with trying to get an obsolete HPLC apparatus to work.

Hsin Hsieh of Southern University reported on incorporating a GC experiment on optimizing the separations of linear alkanes into his Organic Chemistry course. He also reported on adaptation of the workshop exercise on TLC separation of benzoic acids for use in this laboratory.

George Hung of the University of Montevallo reported on addition of both a GC determination of the components of analgesic tablets and a TLC determination of amino acids to his Biochemistry course.

Joe Jeffers of Ouachita Baptist University reported on the use of GCMS to solve environmental problems involving distinguishing between polychlorinated biphenyls, PCB's, and polynuclear aromatic hydrocarbons, PHA's. He also reported on plans for expanded use of various chromatographic methods in the curriculum at Ouachita.

Jothi Kumar of North Carolina A&M State University delighted reunion participants with her demonstration of the use of Sep-Pak C18 cartridges to separate the component dyes of Kool-Aid. Using **very inexpensive** and safe materials she was able to have large numbers of students perform the separation and calculate fundamental parameters such as the number of theoretical plates.

John Lynch of the University of Tennessee at Chattanooga gave a demonstration of the instructional program on chromatography he is developing with Eric Lane. He reported that he had used this extensively in his Analytical Methods class and that workshop participants with an Apple Computer who are willing to return a critique of the program within two weeks of it receipts are invited to write him requesting a test copy.

John Manock of the University of North Carolina at Wilmington reported on his development of a student experiment using GC to monitor pesticide runoff and to measure its uptake in grass shrimp.

Manchery Menon of Savannah State College reported on the use of GC for a study of methanol, ethanol and n-butanol in which reassuringly linear plots of $\log(t_R)$ versus 1/T were obtained.

Jack Steel of Albany State College probably teaches a wider variety of courses than anyone else at the workshop. As a result of the workshop he has added TLC and HPLC experiments to a variety of courses including a graduate Analytical Chemistry course and a Criminalistics course.

W. J. Wysochansky of Georgia Southwestern College has had great difficulties working with obsolete equipment but has recently acquired a new gas chromatograph. He plans to introduce new experiments involving column characterization into Organic Chemistry Laboratory.

Royce Woosley of Western Carolina University has introduced GC and HPLC into Organic Chemistry as a means of characterizing reaction products. He is also planning a research project involving students in the chromatographic separation and characterization of isomers of citral, which is known to function as a pheromone.

Current Prospectus:

Industrial chemists talk frequently about chemists in terms of the need to "Grow-their-Own." Obviously their practical task-at-hand orientation often dictates a narrowing of individual focus from the typical academic presentation of chemistry as a basic science. Clearly in chromatography the applied and the fundamental cross paths. With a plethora of variations along the same theme, chromatography provides many options for getting a job done. Having so many choices necessitates an overview of the method based on its fundamental unifying qualities. This was the essential orientation provided participants in the Chromatography Workshop. From the participants' reports presented at the reunion meeting it is clear that the scope of the real and simulated applications brought to students as a result of the workshop is very impressive. Quite likely increased activity in this important area has been stimulated for years to come.

All participants are very grateful to the NSF, Georgia State and especially Gabor Patonay for their new confidence and competence in dealing with the complex subject of chromatography. It is hoped that this program, and others like it, will continue.

Final Report: Computer Interfacing Workshop
By: Sam Anderson, Roger Bacon, Peter Fichte, Ed Gouge
Date: April 27, 1991

INSTRUMENT ACCESS

One member purchased a multipurpose lab interface: an IBM Model 30 and two AT compatibles.

One member has three AT compatibles and has acquired the Unkelscope Data Acquisition Software Package as well as a DAS-8 Data Acquisition Board for the IBM PC. The DAS-8 is an 8-channel, 12-bit A/D converter and timer/counter board. Utility software is provided for the I/O driver for control of A/D functions via BASIC CALL.

One member has on order an 8-channel, 12-bit A/D I/O board. The department has a local area network. Each member of the faculty has a computer in the office. The laboratory is wired for computers, and one will be installed in the near future.

One member of the group has available six multipurpose lab interfacing boards and six IBM clone computers. An Apple II GS computer has been used to control experiments performed using an automatic titrator. An Apple IIe has been equipped with an Interactive Microware Inc. ADALAB Data Acquisition System and Control Board. This system is contained on a mobile cart. The laboratory has two Macintoshs, three Apple II GS, and ten Apple IIe,s.

TEACHING ACTIVITIES

A variety of applications of instrument interfacing have already been incorporated in teaching activities at the at the workshop participants' institutions. At Norfolk State University, students in the interdisciplinary course, Scientific Instrumentation, have utilized an IBM-AT to control a Spectronic 301 Spectrophotometer. An "in-house" Microsoft Quick BASIC program was used to calibrate and control the instrument as well as obtain data. At Western Carolina University a Computer Interfacing course is offered every third semester. In Fall, 1991, the course will be offered again with a switch from use of Apple-based products to IBM. Specifically, Vernier Software MPLI interface boards and IBM clones will be utilized to teach such topics as data acquisition, instrument control, Fourier transform analysis, digital filtering, and graphical presentation of results. An Apple IIe microcomputer is being used at Presbyterian College to digitalize time independent signals from analog pH meters and spectrophotometers. Since the workshop the same system has been used to acquire a time-dependent signal produced by a recording spectrophotometer, a first step in a program that will eventually have students in General Chemistry and Instrumental Analysis courses use the microcomputer rather than strip chart recorders to acquire and process data.

Two participants have not yet incorporated the workshop contents in their chemistry courses but have made the necessary preparation to do so. At Coker College a PCL-711S Lab and Industrial Interface will be purchased and used to take thermochemical data in the Physical Chemistry Laboratory as well as to interface laboratory instrumentation with serial and parallel ports. The same MPLI Package used at Western Carolina University has been purchased by the Chemistry Department at the University of Puerto Rico. Plans call for using the package in the fall of 1991 in the Instrumental Analysis Laboratory for acquisition and processing data from an interfaced Gow Mac GC and a P-E Lambda 1 Spectrophotometer.

RESEARCH ACTIVITIES

Research applications of computer interfacing have been fairly limited since most of us come from small non-research oriented schools. Of the four faculty members returning to the reunion, only two came from schools that have an active undergraduate research program. Only one was from a school with MS-level research. Two undergraduate research projects resulted directly from the workshop. One involved communication between a Milton Roy Spectronic 301 spectrophotometer and an IBM clone, via the built-in serial ports. The research involved acquiring spectra for a biochemical research project.

A second project involves acquiring data from two HPLC detectors. The detectors were spectrophotometric and electrochemical. One MS project which was in progress was continued. This involved automating titration under control of an Apple computer.

At the personal level three of the four participants have worked on research involving computer interfacing. All have written programs of some sort that involved computer control or data acquisition.

ACCEPTANCE BY COLLEAGUES

Colleague acceptance of establishing and supporting computer interfacing in their departments is not overwhelming, in the sense that the use or non-use of computer interfacing has been at the discretion of the individual faculty member. With the exception of one department head who insisted that all of the data generated in his department that can, must be able to be digitized, no administrator insistence that his or her departments upgrade their data acquisition and control approaches has occurred. As a result, most faculty continue to use computers for word processing, calculation, data presentation, and the like.

NSFUFE FTNMR WORKSHOP REUNION

Introduction

Twelve participants returned for the NSF FT-NMR Workshop Reunion at Georgia State University 26-27 April 1991. Accomplishments since the December 1990 workshop were categorized into software purchase and development, acquisition or attempts at acquisition of instrumentation, and specific applications. Several schools were represented which have access to or are now in the process of being funded to purchase instruments. A considerable amount of time was spent discussing funding options for those institutions that currently do not have instruments. Some faculty members from those institutions focused on availability of software and how it might be used to augment text materials in lecture or laboratory activities. Others who had gained instruments or software at their institutions reported progress in developing workshops, special topic courses and NMR components for regular courses in analytical, physical and organic chemistry. The following is a more detailed report of the various accomplishments and plans of the participants.

NMR Instruments and Acquisition

The universal problem for small universities and colleges in acquiring FT NMR instrumentation is the high cost. Furthermore, the success rate in obtaining funds from nationally competitive grants programs is low. A specific problem is typical of that experienced by Professor Hoffman Chen (Grambling State U.). As a result of attending the NSF Workshop, he was able to obtain a commitment for $ 30,000 from his local institution. However, this amount is far too small to purchase a FT NMR instrument, and since the seed money will be available for a finite time, it might become unavailable before he is able to obtain funding outside his institution.

In the absence of actual FT NMR instrumentation and as a result of attendance at the NSF workshop, Professors Jim Beal (University of Alabama - Montevallo) and Paul Hunt (Frostburg State University) have purchased workstation software that allows students and faculty to perform Fourier transformations and other processing of FID data files obtained from off campus spectrometers.

A reasonable approach to solving the financial problem is the collaborative acquisition of instruments by neighboring institutions. Attendance at the NSF FT NMR workshop by individuals from several institutions has prompted and made possible such collaborative efforts. Specifically, Professors Charles Harding (U. of Tennessee-Martin) and David Owen (Murray State University) are planning to work out an arrangement whereby Murray State runs NMR spectra for faculty members at the U. of Tennessee at Martin, who then interpret the spectra on the local computers with software package entitled PCNMR+. Professors Cliff Carlin and Doug Brower are beginning discussions aimed at submitting a proposal to establish a regional FT NMR instrument facility involving their institutions (U. of N. Carolina-Charlotte and Catawba College) and other small colleges in the Charlotte.

Several of the institutions represented at the reunion have submitted proposals, are planning proposals or have had proposals funded as a result of their attendance at the NSF workshop. The table on the final page of this report summarizes the availability of instrumentation, the current status of funding, and pending proposals for instrumentation sought as result of attendance at the NSF workshop.

Incorporation of FT-NMR into courses and workshops

Workshop participants favor the following courses and activities as means of incorporating FT-NMR materials into the curriculum and for the general disseminating information about the subject:

A short course (1 credit hour) for advanced graduate and undergraduate students.

A junior level course on overview of instrumentation could include FT-NMR

Incorporation of FT-NMR into the areas of physical chemistry laboratory and modern analytical chemistry.

Workshops for local high school teachers, interested personal from industries and other academicians for familiarization with modern FT-NMR techniques.

The following suggestions have been made for increasing the availability of FT-NMR.

Field trips could be arranged for institutions without instruments to nearby campuses with available facilities.

It is suggested to develop a simplified manual intended for users to obtain spectra at institutions with instruments.

It is recommended that workshop materials and experiences should be used as basis for writing proposals and grant applications for the acquisition of computers and software through on-campus funding.

TABLE. Summary of NMR Instrumentation at Institutions Represented at the December 1990 FT-NMR Workshop

Institution	Instrumentation		Grant Proposal Status	
	Present	Planned	Pending	Response
Asheville-Buncombe Technical C.C. Asheville, NC				
Catawba College Salisbury, NC	c			
Cleveland State Community College Cleveland, TN	b			
Davidson College Davidson, NC	60 Mhz	300 Mhz		Funded 4/91: NSF and Keck Foundation
Elizabeth City State University Elizabeth City, NC	a	60 MHz	Submitted to NSF	
Fayetteville State University Fayetteville, NC		Undecided		
Frostburg State University Frostburg, MD	a			
Grambling University Grambling, LA	60 MHz	200 MHz		
Murray State University Murray, KY	200 MHz a,e			
Saint Paul's College Lawrenceville, VA				
University of Arkansas at Little Rock Little Rock, AR	200 MHz			
University of Montevallo Montevallo, AL	60 MHz a	270 MHz	Submitted to NSF	
University of North Carolina-Charlotte Charlotte, NC	300 MHz d			
University of North Florida Jacksonville, FL	200 MHz e			
University of Tennessee-Martin Martin, TN	60 MHz a,e	200 MHz	Submitted to NSF	
University of Western Kentucky Bowling Green, KY	60 MHz 270 MHz a			

a Use or plan to use PCNMR+, FELIX, or FTNMR.
b Use EM360 Simulator software.
c Plans to develop software.
d Uses Spectracalc plus in conjunction with shimming correction program.
e Plans collaborative work with nearby institutions.

Mass Spectroscopy

Progress Report

Mass Spectroscopy Workshop Reunion

April 26-27, 1991

The reunion group consisted of five of the ten participants and the instructor (Tom Moran) in the August 1990 Workshop in Mass Spectroscopy.

The discussions within the group centered on four areas:

1. Instrument availability, acquisition and maintenance
2. Curriculum development
3. Research opportunities
4. College-high school interfacing

1. Instrumentation: (Availability and Acquisition.) The group discussed the various mass spectrometers available in the home institutions. Three of the five reunion participants have HP GC/MS systems that provide faculty and students hands-on experience in both academic laboratory and research experiences. Two workshop participants (not reunion) have applied for funding to purchase HP benchtop mass spectrometers.

   The reunion group discussed the need for some faculty to find non-matching programs since the home institutions are not always willing to provide the 50% match required by NSF-ILI. Discussion centered on other federal programs such as those in the Department of Education and the Department of Energy as well as private sources; e.g., Kresge, Keck, Frausaff, Booth-Ferris, and Dreyfus. Many of these foundations, although providing full-funding, may require a more broad application of the instrument.

Instrument Maintenance: Beyond the initial cost of the instrument, there is a continued need for money to support purchase of expendables (He, syringes), as well as repairs or maintenance. There is general agreement that a maintenance contract is an absolute necessity for mass spectrometers in institutions such as those represented in the workshop.

One suggestion that received unanimous support is the training of sophomore and junior chemistry majors to assist faculty in the use and upkeep of the mass spectrometer.

2. Curriculum Development: Influence on Curriculum. Participants in the NSF Workshop on Mass Spectroscopy expressed that the workshop had a very positive influence on their curriculum. Specifically the workshop enhanced what they taught and how they taught. First and foremost the knowledge they gained from the workshop made them more comfortable with teaching mass spectrometry. They were better able to interpret spectra and explain the spectral data to their students. They were also able to expand their lecture material on mass spectrometry to include information learned during the workshop.

   Some participants saw the workshop influence on their lab curriculum as well. New experiments were developed that incorporated the use of the mass spectrometer. Again, the knowledge gained through the workshop on the use and maintenance of the instruments seemed to help a great deal.

3. Research Opportunities: The mass spectroscopy workshop has increased the existing

knowledge of faculty at various institutions. Interpretations have enhanced, supported, and developed research projects. Examples of these are briefly characterized below:

a. Development of a purge and trap procedure with capillary GC/MS for volatile organics in drinking water.

b. Development of research projects to be incorporated into environmental science courses with GC/MS analysis of pesticide.

c. Analysis of electrolyzed mycotoxin products.

d. Identification of products after synthesis by molecular weight determination.

4. College - High School Interface: Opportunities for high school students to obtain experience with mass spectrometers have developed from the training received at the NSF-mass spectroscopy workshop.

One institution has developed a program that allows high school students to perform experiments on the mass spectrometer. Another institution is developing a program which would bring high school students to campus to use the mass spectrometer and other computer-driven instruments to perform experiments.

High school teachers and students have therefore reaped the benefits of the workshop. It is hoped that the high school students will thereby acquire an interest in chemistry and pursue chemistry as a college major and career.

NSF Workshop Reunion, Georgia State University
Atlanta, Georgia, April 26-27, 1991

Molecular Modeling

Participation

Of the ten participants in the workshop, five attended the reunion: Ken R. Fountain, Northeast Missouri State University, Kirksville, MO; Charles H. Hendrickson, Western Kentucky University, Bowling Green, KY; Robert H. Higgins, Fayetteville State University, Fayetteville, NC; Glen M. Kauffman, Eastern Mennonite College, Harrisonburg, VA; and Jimmie M. Purser, Millsaps College, Jackson, MS. Also attending and serving as group facilitator was Dwight Kinzer, Berry College, Mount Berry, GA, a participant in the August 1989 workshop.

Software

All present have obtained PCMODEL. Some are also using ALCHEMY, CHEM3DPLUS, CHEM DRAFT II, and MOPAC, as well as various spreadsheets, word processors, and computational and graphics packages in conjunction with PCMODEL.

Hardware

One participant is using Macintosh. All others have acquired either 286 or 287 based MSDOS machines. These acquisitions have been funded in part by grants from outside sources. One participant is hoping to develop a UNIX based network for a computational chemistry laboratory.

Curriculum

The most common points of introduction for molecular modeling has been the organic and/or physical chemistry courses; however, applications in biochemistry and inorganic are also being examined. There is general agreement that molecular modeling should be introduced into the freshman course but there has been less progress in that area but plans are taking shape. One participant has established a separate course in computational chemistry with molecular modeling as one of several components. In this case, PCMODEL is being used for investigation of energy relationships and steric effects as well as to construct input files for molecular orbital calculations using MOPAC.

Three participants have established "computational chemistry laboratories" or "molecular graphics centers" within their departments. Some have conducted workshops for both faculty and students. These workshops should aid in the spread of the technique across the chemistry curriculum.

Manuals on the use of molecular modeling have been prepared or are in progress for use in various courses and workshops.

Research

All have research programs involving molecular modeling either in progress or planned. One research proposal has received foundation funding. Two papers on undergraduate research have been presented at meetings and both are in preparation for publication.

Topics under investigation include epoxidation of alkylcyclopentanes, conformational energies of N-H and N-alkyl azetidines and azetidinols and the effects upon internal bond angles as a function of rotation about the N-alkyl bond, the regiochemistry and stereochemistry of ring opening of azetidinols by phenols, aromatic substitution and the ipso effect, boron-nitrogen compounds and possible improvement of force field constants, and mechanisms of some directed metalation reactions.

Examples

Correlations with NMR data: In the course of a research project, the HNMR spectrum of C_6H_5-N(OH)-CO-O-CH_3 was found to contain a complex pattern for the methyl group. Molecular modeling showed this compound to have three conformations within 1-3 kcal of each other. The resulting calculation of conformation distribution seems to be in agreement with the observed NMR data.

Potential energy surfaces: An investigation of the rotational energy of methyl aceto-α-hydroxyacetate about the C1-C2 and C2-C3 bonds was conducted. This was accomplished by manually rotating one bond by an increment, fixing it and using the ROT-E option to then rotate the second bond. A 3-dimensional plot of the data was then constructed using the program, SURFER. From the result it is seen that what would appear to be the minimum from the two individual rotations is not the global minimum but is a saddle point. The global minimum is not reflected in either of the rotations alone but must result from a combination of the two.

Correlations with IR and X-ray data: An examination of nitrogen-boron bonds such as the one in H_3N^+-B^-H_3 by molecular modeling does not give satisfactory correlations with infrared vibrational frequencies or X-ray diffraction data. It has been concluded that the force field needs improvement with respect to this bond. Additional work toward that goal is planned.

Plans for the immediate future

There is a consensus that molecular modeling should be combined with molecular orbital calculations in order to make best use of both methods. All of the participants will be undertaking additional study of molecular modeling and molecular orbital theory this summer either on their own or by attending an NSF sponsored workshop on molecular orbital theory. The acquisition of additional hardware and software to allow more widespread use of computational techniques is also of high priority. Considerable information was exchanged at this reunion concerning improved software that was presented at last week's national A.C.S. meeting. Much of this requires some expansion of memory on existing systems.

There is a strong commitment to the idea of increasing the involvement of computational chemistry in the chemistry curriculum. In order to maintain momentum in this direction, another reunion of the members of this group has been tentatively scheduled for this fall at Western Kentucky University, Bowling Green, KY. An invitation may be extended to participants in the other two NSF sponsored molecular modeling workshops.