

11:19:14

OCA PAD INITIATION - PROJECT HEADER INFORMATION

04/18/94

Active

Project #: B-10-F66 Cost share #: B-10-381 Rev #: 0
Center # : 10/24-6-R8115-0A0 Center shr #: 10/22-1-F8115-0A0 OCA file #:
Contract#: BIR-9306392 Mod #: Work type : RES
Prime # : Document : GRANT
Contract entity: GTRC

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

Project unit: OIP Unit code: 03.010.200
Project director(s):
 GELBAUM L T OIP (404)894-8417

Sponsor/division names: NATL SCIENCE FOUNDATION / GENERAL
Sponsor/division codes: 107 / 000

Award period: 940501 to 961031 (performance) 970131 (reports)

| Sponsor amount | New this change | Total to date |
|---------------------|-----------------|---------------|
| Contract value | 150,000.00 | 150,000.00 |
| Funded | 150,000.00 | 150,000.00 |
| Cost sharing amount | | 150,000.00 |

Does subcontracting plan apply ?: N

Title: UPGRADE OF 400MHZ NMR SPECTROMETER

PROJECT ADMINISTRATION DATA

OCA contact: Jacquelyn L. Tyndall 894-4820

Sponsor technical contact

Sponsor issuing office

CHARLES H. KEITH
(703)306-1472

JOHN CRUICKSHANK
(703)306-1217

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4201 WILSON BLVD.
ARLINGTON, VA 22230

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ARLINGTON, VA 22230

Security class (U,C,S,TS) : U

ONR resident rep. is ACO (Y/N): N

Defense priority rating : N/A

NSF supplemental sheet

Equipment title vests with: Sponsor

GIT X

Administrative comments -

INITIATION OF PROJECT. THIS IS AN EQUIPMENT GRANT WHICH BEARS NO OVERHEAD.
GIT MUST MEET THE COST SHARING OBLIGATION OF \$150,000.

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 01/29/97

Project No. B-10-F66

Center No. 10/24-6-R8115-OA0

Project Director GELBAUM L T

School/Lab OIP

Sponsor NATL SCIENCE FOUNDATION/GENERAL

Contract/Grant No. BIR-9306392

Contract Entity GTRC

Prime Contract No.

Title UPGRADE OF 400MHZ NMR SPECTROMETER

Effective Completion Date 961031 (Performance) 970131 (Reports)

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

Comments
LETTER OF CREDIT APPLIES. 98A SATISFIES PATENT REPORT.

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 Management | Y |
| Research Security Services | N |
| Reports Coordinator (OCA) | Y |
| GTRC | Y |
| Project File | Y |
| Other | N |
| | N |

Annual Progress Report
Upgrade of 400 MHz NMR Spectrometer
National Science Foundation BIR-9306392

During the period ending Jan 1, 1996 demonstration trips were taken to Varian Associates in Palo Alto, CA on January 18, and 19, 1995 and to Bruker Instruments in Billerica MA on February 14, and 15, 1995. It was decided not to go to Chemagnetics in Fort Collins, CO since this company has only recently begun selling solutions instruments so there would be only a very limited user base.

Based on the above trips it was decided that NMR spectrometers from either company would be acceptable. We began negotiations with the above companies for the purchase of the instrument upgrade. During this process it was learned that Varian Instruments was going to introduce an new instrument. We decided to wait until the new instrument was available to continue with the negotiations.

During the negotiations with Varian and Bruker, Georgia Tech decided to consolidate their NMR Facility into one Campus wide center to be housed in the School of Chemistry and Biochemistry. This was in response to a grant received by the College of Engineering for a solid state and imaging NMR instrument. Renegotiations were begun on a combined purchase.

As part of the negotiations it was decided that the College of Engineering would use our existing 9.4 Tesla widebore magnet for the solids and imaging instrument and purchase an 11.75 Tesla narrow bore magnet for the solutions instrument. This meant that we were able to purchase a 500 MHz console for our upgrade. We have decided to purchase a Bruker DRX 500 NMR three channel console. Along with the console will be three axis gradients and ^1H , ^{13}C , X triple resonance triple gradient probe for biological samples and a proton only probe which has an extended temperature range.

The purchase process is now implemented and we hope to have delivery by May 1, 1996. from Bruker Instruments.

NATIONAL SCIENCE FOUNDATION

4201 Wilson Blvd.,
Arlington, VA 22230BULK RATE
POSTAGE & FEES PAID
National Science Foundation
Permit No. G-69

PI/PD Name and Address

Leslie Gelbaum

~~GA Tech Res Corp - DBI~~

Atlanta

GA 30332

01P0230

NATIONAL SCIENCE FOUNDATION
FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION

- | | | |
|----------------------------|--|-----------|
| 1. Program Official/Org. | Karl A. Koehler - DBI | |
| 2. Program Name | INSTRUMENT DEVELOPMENT | |
| 3. Award Dates (MM/YY) | From: 05/94 | To: 10/96 |
| 4. Institution and Address | GA Tech Res Corp - DBI Administration Building Atlanta GA 30332 | |
| 5. Award Number | 9306392 | |
| 6. Project Title | Upgrade of 400 MHz NMR Spectrometer | |

** You are encouraged to submit your Final Project Report electronically
 ** through the NSF FastLane home page (www.fastlane.nsf.gov).

This Packet Contains
 NSF Form 98A
 And 1 Return Envelope

ISF Grant Conditions (Article 17, GC-1, and Article 9, FDP-11) 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 Grants Policy Manual Section 677).

Below, or on a separate page attached to this form, provide a summary of the completed projects 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.

I certify to the best of my knowledge (1) the statements herein (excluding scientific hypotheses and scientific opinion) are true and complete, and (2) the text and graphics in this report as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or of individuals working under their supervision. I understand that willfully making a false statement or concealing a material fact in this report or any other communication submitted to NSF is a criminal offense (U.S. Code, Title 18, Section 1001).

| | |
|---|----------------|
|  | <i>1/27/97</i> |
| 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. |
| <i>see attached report</i> | | | | | | | | | | |
| A. Total, U.S. Citizens | | | | | | | | | | |
| 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 | | | | | | | | | | |
| C. Total, Other Non-U.S. Citizens | | | | | | | | | | |
| Specify Country | | | | | | | | | | |
| 1. | | | | | | | | | | |
| 2. | | | | | | | | | | |
| 3. | | | | | | | | | | |
| D. Total, All participants (A + B + C) | | | | | | | | | | |
| Disabled³ | | | | | | | | | | |

☐ 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 maintains cultural identification through tribal affiliation or community recognition.

ASIAN: A person having origins in any of the original peoples of East Asia, Southeast Asia or 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, and the Northern Marianas; the U.S. Trust Territory of Palau; the islands of Micronesia and 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.

Upgrade of 400 MHZ NMR Spectrometer

Grant No. BIR-9306392

Final Report

Leslie T. Gelbaum

School of Chemistry and Biochemistry
Georgia Institute of Technology
Atlanta, Georgia 30332-0400

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404-894-4079
fax 404-894-7452

Summary

The purpose of this grant was to upgrade our existing NMR instrument so that it could be used to obtain data on biological samples in water and to give it the capabilities to carry out the newest NMR experiments. After an evaluation of the available instruments a Bruker DRX 500 NMR with three channels and triple axis gradients and a used Bruker AMX 400 NMR instruments were purchased. In an effort to increase the availability of NMR services the College of Sciences at the Georgia Institute of Technology consolidated a number of facilities and created an NMR Center. The instrument upgrade was included in this Center. The Bruker AMX 400 was purchased to take over the duties of our previous Varian XL 400 to carry our multinuclear NMR experiments and the Bruker DRX 500 is a state of the art instrument capable of carrying out the most demanding experiments on biological samples.

Technical Information

The Bruker AMX 400 and DRX 500 NMR instruments were very recently installed. The DRX 500 is equipped with three channels and a triple axis gradient accessory. We purchased two probes for this instrument a triple resonance ^1H , ^{13}C , X triple axis gradient probe designed for biological work and a ^1H only probe for extended range variable temperature experiments. The AMX 400 is a two channel instrument with 5mm and 10mm broadband probes. These instruments were accepted on November 27, 1996. Because of this the amount of data that has been collected is limited.

Some research was done using the instruments during the installation. Twelve research groups in four departments were able to collect data. This research included the structure of a 10 mer DNA and its interactions with TMPyP_4 and an 18 mer DNA containing a hairpin loop to determine the binding of single strand selective molecules. Georgia Tech is now in the process of hiring a faculty member with an expertise in the area of biological NMR. The usage of the Bruker DSX 500 should increase drastically when this person begins their research. The structure of new steroid molecules for use in AIDS treatments were also determined. The instrument was also used in material science work to determine the formation of new polymers.

In addition a number of projects have been carried out using the multinuclear instrument looking at nuclei other than ^1H , and ^{13}C . These include ^{113}Cd studies of humic acids to understand metal ion transport in streams and ^{87}Sr , ^{207}Pb , ^{43}Ca , ^{14}N , ^{31}P and ^{29}Si of new materials as potential precursors of OMVPE doping of zinc selenide.

As indicated in the summary section Georgia Tech has created an NMR Center for the housing of all NMR instruments on campus. Georgia Tech paid for renovation furnishing and upgrade of computer facility for this Center. Attached is a description of the facility, management and user fees.

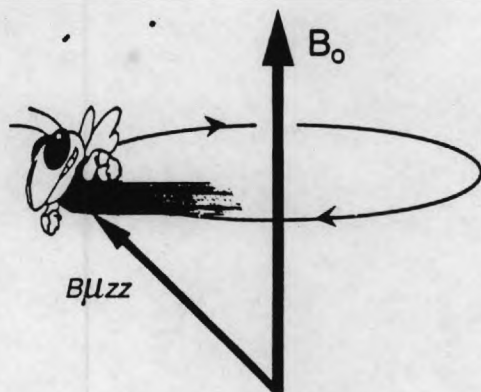
Part IV Summary Data on Project Personnel

The NMR instrument is located in a campus wide facility. Because of this the users come from many departments of Georgia Tech making it difficult to fill out the Project Personnel data form as given. I have compiled some statistics about the departments that are the major users of the instruments purchased using this grant.

The senior staff is 86% male and 14% female. Of the male staff 80% are white, 3% are black and 17% are other. Of the female staff 86% are white, 2% are black and 12% are others.

The users of the facility are primarily graduate students and postdoctoral research associates. Since the facility is just becoming available I am listing the numbers of students in the departments most used by the facility. Not all of these students will be using the facility but a large number of them have acquired NMR data in our previous facility, therefore, I believe it is an adequate representation of the facility usage. The combined data is listed below:

| | Male | Female |
|-----------------|------|--------|
| Asian | 62 | 35 |
| Black | 15 | 17 |
| Hispanic | 5 | 5 |
| American Indian | 1 | 1 |
| White | 143 | 65 |



Georgia Tech NMR Center

NEW NUCLEAR MAGNETIC RESONANCE CENTER IS OPEN!

Facility Description

The Georgia Tech NMR Center has been established as a campus-wide multiuser facility to support a wide variety of materials and chemical synthesis and characterization. Located in Boggs B-46 and B-47, the Center houses the following nuclear magnetic resonance instrumentation:

500-MHz Bruker DRX for high-resolution liquids, intended for multidimensional spectral acquisition of complex samples. Used for ^1H NMR when sensitivity or spectral dispersion are important. Includes triple resonance and pulsed gradient capabilities.

400-MHz Bruker DSX for solids and micro-imaging, high-resolution spectra of solids containing quadrupolar nuclei, and NMR imaging studies of liquids in solid substrates.

300-MHz Bruker DSX for solids, high-resolution solids acquisition, wideline NMR studies of molecular dynamics and orientation.

400-MHz Bruker AMX for high-resolution liquids, totally multinuclear but intended for nuclei other than ^1H and ^{13}C . Equipped with a 10-mm probe for samples where solubility is limited. An automatic sample changer allows for overnight acquisitions of multiple samples.

300-MHz Varian Gemini for routine ^1H and ^{13}C liquids acquisitions. This spectrometer supports campus-wide research involving chemical syntheses. The system is being upgraded.

The four Bruker spectrometers are completely multinuclear and include variable temperature capabilities. As of 8/26/96, all instruments are operational with the exception of the DSX 400.

Management

The Center will be managed by Leslie T. Gelbaum (894-4079, 894-1827, lg2@prism.gatech.edu) with the assistance of a Users Advisory Group. The Users Advisory Group will consist of primary users, appointed by the Dean of the College of Sciences and representing each unit in which users reside. The Center Manager will be responsible for scheduling and maintenance of the spectrometers, user training, and for providing NMR spectroscopy services. The Users Advisory Group will assist the Center Manager in establishment and evolution of Center policies and operation. Current members of the Users Advisory Group include: Mike Perdue (EAS), Mark

White (CHE), Rob Whetten (PHYS), Leon Zalkow (CH), Will Rees (MSE), Bob Schwerzel (GTRI), Kent Barefield (COS, ex-officio) and Haskell Beckham (TFE, chair).

Scheduling

The instruments will be divided up into two scheduling groups:

(1) Time on the DRX 500, DSX 400, DSX 300, and AMX 400 will be assigned at weekly booking meetings in order to facilitate equal and fair access. Initially, these meetings will take place at 12 noon on Thursdays for time beginning the following Monday morning. One representative from each research group should be present to request time for all members of that group. Request conflicts will be arbitrated by the Center manager. Whatever time remains after these meetings can be had on a first-come, first-served basis. If one cannot be present at these meetings, requests can be submitted via e-mail (lg2@prism.gatech.edu), but must be received before noon on Thursdays. Booking meetings begin 8/29/96.

(2) The Varian Gemini 300 will remain an open access instrument to all individuals who have been trained. Access is first-come, first-served on a weekly time sheet that is put up every Monday morning. Internet sign-up software is currently being evaluated.

The Center Manager reserves time for user training, instrument maintenance, and operator-acquired spectra. One SGI work station exists in the Center for dedicated offline data processing.

Costs

The NMR Center will operate as a cost center. Charges will be made directly to Georgia Tech accounts which have already been created. Funds collected will be used for the daily operation of the center. Hourly fees are set as follows:

| | | |
|--------------------|-------|--------------------------|
| spectrometer usage | \$7. | 9 am to 6 pm on weekdays |
| | \$4. | 6 pm to 9 am on weekdays |
| | | weekends and holidays |
| operator-assisted | \$20. | including user training |
| non-academic users | \$71. | |

Time between quarters is not considered holidays. Operator-assisted charges include time for set-up and instrument time. This charge structure is based on current and projected usage of the spectrometers. It will be periodically updated as actual usage data are collected. In order to encourage the development of a users' facility, the operator-assisted rate will possibly increase.

Funding for the Georgia Tech NMR Center has come from a variety of sources:

National Science Foundation
College of Sciences
School of Textile and Fiber Engineering
Molecular Design Institute

State of Georgia
College of Engineering
School of Chemistry and Biochemistry
Polymer Education and Research Center