

13:27:59

OCA PAD AMENDMENT - PROJECT HEADER INFORMATION

05/22/90

Active

Project #: G-33-636                      Cost share #: G-33-332                      Rev #: 6  
Center # : R6498-OA0                      Center shr #: F6498-OA0                      OCA file #:  
Contract#: CHE-8805577                      Mod #: AMENDMENT 02                      Work type : RES  
Prime # :    Document : GRANT  
Contract entity: GTRC

Subprojects ? : N  
Main project #:

Project unit:                      CHEM                      Unit code: 02.010.136  
Project director(s):  
TOLBERT L M                      CHEM                      (404)894-4043

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

Award period:                      880601                      to                      911130 (performance)                      920228 (reports)

Sponsor amount	New this change	Total to date
Contract value	71,540.00	222,540.00
Funded	71,540.00	222,540.00
Cost sharing amount		2,225.00

Does subcontracting plan apply ? : N

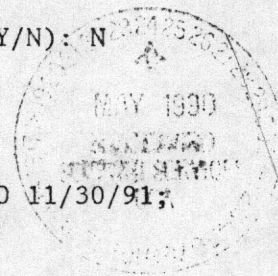
Title: CHARGE DISTRIBUTION IN PHOTOEXCITED MOLECULES / CHE-8513666

PROJECT ADMINISTRATION DATA

OCA contact: David B. Bridges	894-4820
Sponsor technical contact	Sponsor issuing office
DOUGLAS J. RABER (202)357-7956	STEPHEN G. BURNISKY (202)357-9653
NATIONAL SCIENCE FOUNDATION 1800 G STREET, N.W. WASHINGTON, D.C 20550	NATIONAL SCIENCE FOUNDATION 1800 G STREET, N.W. WASHINGTON, D.C. 20550

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 -  
AMENDMENT 02 ADDS FUNDS IAO \$71540 AND EXTENDS TERMINATION DATE TO 11/30/91;  
3RD YEAR OF 3 YEAR CONTINUATION GRANT, FINAL RPT DUE 2/28/92;



2-48  
SR627

GEORGIA INSTITUTE OF TECHNOLOGY  
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 03/09/92

Project No. G-33-636 \_\_\_\_\_ Center No. R6498-0A0 \_\_\_\_\_

Project Director TOLBERT L M \_\_\_\_\_ School/Lab CHEMISTRY \_\_\_\_\_

Sponsor NATL SCIENCE FOUNDATION/GENERAL \_\_\_\_\_

Contract/Grant No. CHE-8805577 \_\_\_\_\_ Contract Entity GTRC

Prime Contract No. \_\_\_\_\_

Title CHARGE DISTRIBUTION IN PHOTOEXCITED MOLECULES / CHE-8513666 \_\_\_\_\_

Effective Completion Date 911130 (Performance) 920228 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	N	_____
Final Report of Inventions and/or Subcontracts	Y	920225
Government Property Inventory & Related Certificate	N	_____
Classified Material Certificate	N	_____
Release and Assignment	N	_____
Other _____	N	_____

Comments BILLING VIA LOC; "PATENT REPORT" VIA 98A. \_\_\_\_\_

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

NOTE: Final Patent Questionnaire sent to PDPI.

G-33-636

**GEORGIA TECH RESEARCH CORPORATION**

GEORGIA INSTITUTE OF TECHNOLOGY  
ATLANTA, GEORGIA 30332-0420

Telex: 542507 GTRCOCAATL  
Fax: (404) 894-3120

Phone: (404) 894-

Refer to: LB/G-33-636

February 28, 1989

PROPOSAL NO. CHE-8805577

National Science Foundation  
Chemistry Division  
1800 G Street N.W.  
Washington, D.C. 20550

Attention: Dr. Seymour Lapporte


Subject: Request for Year 2 Funding and Progress Report for  
Research Project Entitled, "Charge Redistribution  
in Photoexcited Molecules NSF Grant No.  
CHE-8805577"

Dear Dr. Lapporte:

The GEORGIA TECH RESEARCH CORPORATION is pleased to submit the annual progress report for the subject grant and budget for year 2 funding prepared by Dr. Laren M. Tolbert, Georgia Institute of Technology. Should additional information be desired, please do not hesitate to contact Dr. Tolbert at 404/894-4043 regarding technical matters or the undersigned at 404/894-4817 for administrative concerns.

Thank you for your support.

Sincerely,

  
Lynn Boyd  
Contracting Officer

LB/kal

Addressee: Two copies  
Enclosure: Proposal - Two copies  
Progress Report

Progress Report  
NSF Grant CHE-8805577

Submitted by: Laren M. Tolbert  
School of Chemistry  
Georgia Institute of Technology  
Atlanta, GA 30332

**Progress.**

The current NSF grant has supported the efforts of Jeanne Haubrich, a postdoctoral fellow from the University of California-Berkeley, Nurul Islam, a graduate student from the University of Kentucky, and Susan M. Fitzwater, a graduate student at Georgia Tech. After finishing a project on substituent effects on carbanion photoexcited decay pathways, Ms. Fitzwater has made significant progress in developing model compounds for studying proton transfer reactions in non-aqueous media. She has synthesized a number of 1-naphthol derivatives which contain proton acceptors within defined proton-transfer geometries, including 2-(hydroxymethyl)- and 2-(2-hydroxyethyl)-, and 2-(dimethylaminomethyl)-1-naphthol. Mr. Islam has synthesized 1,3-diphenyl-1,2-cyclohexadiene, a strained allene, as well as the monophenyl derivative, through our novel carbanion photochemistry route. He has characterized adducts with furan, 2,3-dimethylbutadiene, and isoprene. This work will be shortly submitted for publication, and Mr. Islam will receive his Ph. D. in June. Dr. Haubrich has synthesized a number of cyanonaphthols and one methylsulfinylnaphthol. These naphthols are characterized by enhanced excited state acidities in ways that are rationalized by an appeal to molecular orbital theory. Two of these naphthols are strong enough photoacids to protonate organic substrates, e. g., dimethyl sulfoxide and alcohols. We are currently investigating their utility both as photopolymerization initiators and as monitors for polymer curing processes.

Expenditures and encumbrances as of 2-20-89 total \$67,458, with a current balance of \$10,542. At the current rate, the remaining \$5,981 in direct costs will be expended by May 31, 1989.

**Active and Pending Grants.**

(1) National Science Foundation, "Charge Redistribution in Photoexcited Molecules," 8-1-88 to 1-31-92, \$234,000.

(2) U. S. Department of Energy, "The Organic Chemistry of Conducting Polymers," 7-1-88 to 6-31-91, \$315,000.

(3) National Institutes of Health, "Biooxidation of Arylalkyl Hydrocarbons," 7-1-87 to 6-31-90, \$236,000 approximate direct costs.

(4) Sandoz Foundation, "New Materials for Molecular Electronics", 1-1-87 to 12-31-89, \$39,000.

Publications (1987- ). NSF acknowledgment marked by \*.

\*L. M. Tolbert, in "Handbook of Organic Photochemistry", "Spectroscopic Properties of Radical-Ions and Short-Lived Carbocations and Anions," J. C. Scaiano, ed., CRC Press, in press.

Joseph A. Schomaker and Laren M. Tolbert, "Deprotonation of Poly(acetylen-co-1,3-butadiene). An Alternate Approach to N-heped Polyacetylene", Polym. Preprints (American Chemical Soc. Div. Polym. Chem.) 29, 267 (1988).

Laren M. Tolbert and Rajive K. Khanna, "Dramatic Solvent and Stereoelectronic Effects in a Biomimetic Oxidation: 9,10-Dialkylanthracenes", J. Amer. Chem. Soc., 1987, 109, 3477.

\*A. Rajca and L. M. Tolbert, "How Does an Allene Distort to Accommodate Excess Negative Charge." J. Am. Chem. Soc., 109, 1782 (1987).

\*A. Rajca, A. Streitwieser, Jr., and L. M. Tolbert, "Ab Initio Study of 2,3-Dilithiopropene", J. Am. Chem. Soc., 109, 1790 (1987).

\*L. M. Tolbert, "The Excited States of Resonance-Stabilized Anions," in Comprehensive Carbanion Chemistry, Part C, E. Buncl, Ed., Elsevier, pp. 223-270 (1987).

\*Laren M. Tolbert, Susan M. Fitzwater, Narciso Raya, and Michael Stapleton, "Substituent Effects on Carbanion Photophysics. An Application of The Energy Gap Law," J. Am. Chem. Soc., submitted.

Laren M. Tolbert, Rajive K. Khanna, Sarath E. Sirimanne, Ann E. Popp, and Larry A. Bottomley, "The Effect of Water on Radical Cation Deprotonations: 9,10-Dimethylanthracene", J. Amer. Chem. Soc., submitted.

Laren M. Tolbert, Rajive K. Khanna, Leslie A. Gelbaum, Ann E. Popp, and Larry A. Bottomley, "Stereoelectronic Effects in the Deprotonation of Arylalkyl Radical Cations: meso-Ethylanthracenes", J. Amer. Chem. Soc., submitted.

Laren. M. Tolbert and N. Islam, "1-Phenyl-1,2-cyclohexadiene." J. Am. Chem. Soc., to be submitted.

Laren M. Tolbert and J. Kowalik, "ortho-Metallation of Diphenylacetylene. Triple-bond-assisted Deprotonation", J. Org. Chem., to be submitted.

#### Meetings and Symposia:

"Novel Charge-Transfer Polymers", 40th Southeast Regional Meeting, American Chemical Society, Atlanta, GA, September 10, 1988.

"Deprotonation and Conductivity Studies of  $sp^3$ -Interrupted Polyacetylene", 40th Southeast Regional Meeting, American Chemical Society, Atlanta, GA, September 10, 1988.

\*"1-Phenyl-1,2-cyclohexadiene". 40th Southeast Regional Meeting, American Chemical Society, Atlanta, GA, September 9, 1988.

- \*"Structural Constraints in Proton Transfer of Photoexcited Naphthols",  
40th Southeast Regional Meeting, American Chemical Society, Atlanta,  
GA, September 9, 1988.
- "Regioselectivity in 1,4-Dialkylnaphthalene", 40th Southeast Regional  
Meeting, American Chemical Society, Atlanta, GA, September 9, 1988.
- "<sup>13</sup>C-Magnetic Resonance Studies of Charge Densities in alpha,omega-  
Diphenylpolyenyl Anions", 40th Southeast Regional Meeting, American  
Chemical Society, Atlanta, GA, September 11, 1988.
- \*"The Excited-State Acidities of Substituted Cyano-2-naphthols", 196th National  
Meeting, American Chemical Society, Los Angeles, California, September 26,  
1988.
- \*"Substituent Effects on Carbanion Photophysics. 9-Arylfluorenyl Anions", XI.  
IUPAC Conference on Organic Photochemistry, Bologna, Italy, July 20, 1988.
- \*"The Excited-State Acidities of Substituted Cyano-2-naphthols", 196th National  
Meeting, American Chemical Society, Los Angeles, California, September 26,  
1988.
- \*"Substituent Effects on Carbanion Photophysics. An Application of the Energy  
Gap Law", Third Chemical Congress of North America, Toronto, Canada, June  
6, 1988.
- "The Effect of Water on Radical Cation Deprotonations: 9,10-Dimethylanthracene",  
Third Chemical Congress of North America, Toronto, Canada, June 9, 1988.
- \*"Aromaticity and Resonance Stabilization in Hydrocarbon Anions", Third Chemical  
Congress of North America, Toronto, Canada, June 8, 1988.
- "Reactions Following Electron Transfer: Deprotonation of Arylalkyl Radical  
Cations", Gordon Research Conference on Radical Ions, New Hampshire, July  
1, 1988.
- "Reactions Following Electron Transfer: Deprotonation of Arylalkyl Radical  
Cations", Northeast Regional Meeting, American Chemical Society,  
Rochester, NY, November 11, 1987.
- "A Dramatic Solvent and Stereoelectronic Effect in a Biomimetic Oxidation,"  
National Meeting, American Chemical Society, New Orleans, Louisiana,  
September 5, 1987.

6-33-636



School of Chemistry  
(404) 894-4002 (Tel.)  
(404) 894-7452 (Fax)

**Georgia Institute of Technology**  
Atlanta, Georgia 30332  
A Unit of the University System of Georgia

March 1, 1990

NSF Grant:  
CHE-8805577

Dr. Douglas J. Raber  
Organic Chemical Dynamics  
Division of Chemistry  
National Science Foundation  
Washington, D. C. 20550

Dear Dr. Raber:

Enclosed is my report and third year budget request for my NSF grant, based upon the previously agreed-upon level of \$73,000. Please contact me at (404)-894-4043 if there are any questions.

With kind regards,

[Redacted Signature]  
Laren M. Tolbert  
Professor of Chemistry

cc. Mary Wolff, OCA

Progress Report  
NSF Grant CHE-8805577

Submitted by: Laren M. Tolbert  
School of Chemistry  
Georgia Institute of Technology  
Atlanta, GA 30332

**Progress.**

The current NSF grant has supported the efforts of Jeanne Haubrich, a postdoctoral fellow from the University of California-Berkeley, as well as graduate students Nurul Islam and Susan M. Fitzwater. Dr. Islam received his Ph. D. in August 1989 after completing a project on a novel photochemical approach to strained allenes, including 1,3-diphenyl-, 1-phenyl-, and 1-carboethoxy-1,2-cyclohexadiene, which was trapped with a number of dienes. Portions of this work have been submitted for publication in the Journal of the American Chemical Society. In addition to synthesizing a number of 1-naphthol derivatives which contain proton acceptors within defined proton-transfer geometries, including 2-(hydroxymethyl)- and 2-(2-hydroxyethyl)-, and 2-(dimethylaminomethyl)-1-naphthol, Ms. Fitzwater has synthesized 5-cyano-1-hydroxymethyl-2-naphthol, which demonstrates efficient intramolecular proton transfer to the weakly basic hydroxymethyl group. Dr. Haubrich has synthesized a number of cyanonaphthols and one methylsulfinylnaphthol which are characterized by enhanced excited state acidities. One of these, 5,8-dicyano-2-naphthol has an excited state  $pK_a$  of -6, approaching that of mineral acids! Up to this point, we have not been able to use these as polymerization or depolymerization initiators, since the proton flux is apparently still not sufficient to compete with excited state decay. However, we have demonstrated that proton transfer to water monomer can be induced, thus providing a new substrate for theories on proton transfer which require clustering for efficient proton transfer.

Expenditures and encumbrances as of 2-26-90 total \$140,592 for years 1 and 2, with a current balance of \$10,408. At the current rate, the remaining amount in direct costs will be expended by May 31, 1990.

**Active and Pending Grants.**

(1) National Science Foundation, "Charge Redistribution in Photoexcited Molecules." 8-1-88 to 1-31-92, \$234,000.

(2) U. S. Department of Energy, "The Organic Chemistry of Conducting Polymers." 7-1-88 to 6-31-91, \$315,000.

(3) National Institutes of Health, "Biooxidation of Arylalkyl Hydrocarbons." 7-1-87 to 6-31-90, \$236,000 approximate direct costs. A renewal of this grant is pending.

(4) Sandoz Foundation, "New Materials for Molecular Electronics". 1-1-87 to 7-1-90, \$39,000.



**Publications (1988- )**. NSF acknowledgment marked by \*.

\*L. M. Tolbert, in "Handbook of Organic Photochemistry", "Spectroscopic Properties of Radical-Ions and Short-Lived Carbocations and Anions," J. C. Scaiano, ed., CRC Press, 1989, 0000.

Laren M. Tolbert and Mark E. Ogle, "<sup>13</sup>C-NMR Spectroscopy of  $\alpha,\omega$ -Diphenylpolyenyl Anions. Confirmation of Charge Localization in Soliton Model Compounds", J. Am. Chem. Soc., 1989, 111, 5958.

\*Laren M. Tolbert, Susan M. Fitzwater, Narciso Raya, and Michael Stapleton, "Substituent Effects on Carbanion Photophysics. An Application of The Energy Gap Law," J. Am. Chem. Soc., submitted.

Laren M. Tolbert, Rajive K. Khanna, Sarath E. Sirimanne, Ann E. Popp, and Larry A. Bottomley, "The Effect of Water on Radical Cation Deprotonations: 9,10-Dimethylanthracene", J. Amer. Chem. Soc., submitted.

Laren M. Tolbert, Rajive K. Khanna, Leslie A. Gelbaum, Ann E. Popp, and Larry A. Bottomley, "Stereo-electronic Effects in the Deprotonation of Arylalkyl Radical Cations: meso-Ethylanthracenes". J. Amer. Chem. Soc., in press.

\*Laren. M. Tolbert, N. Islam, W. Shakespeare, and R. P. Johnson, "Carbanion Photochemistry. A New Route to Strained Allenes." J. Am. Chem. Soc., submitted.

Sarath Sirimanne and Laren M. Tolbert, "Reversal of Cation Radical Selectivity by the Trimethylsilyl Group." J. Am. Chem. Soc., submitted.

**Meetings and Symposia (1989):**

\*" <sup>13</sup>C-NMR and Resonance Stabilization in Hydrocarbon Anions", Gordon Conference on Physical Organic Chemistry, Holderness, New Hampshire, June 14, 1989.

"The Carbanion Chemistry of Conducting Polymers." Biannual Symposium on Carbanion Chemistry, Canadian Society for Chemistry, Ottawa, Canada July 24, 1989.

\*"Intra- vs. Intermolecular Proton Transfer in Photoexcited Naphthols," 198th National Meeting, American Chemical Society, Miami Beach, September 10, 1989.

\*"Fluorescent Probes for Solvent Basicities". 40th Pittsburgh Conference and Exposition, Atlanta, Georgia, March 7, 1989.

"New Fluorophores for Chemiluminescent Assays". 40th Pittsburgh Conference and Exposition, Atlanta, Georgia, March 9, 1989.

\*"Proton Transfer by New Organic Photoacids." International Conference of Pacific Basin Societies, Honolulu, Hawaii, December 21, 1989.

**Budget.**

A. Personnel

1. Laren M. Tolbert, Principal Investigator  
12.5% AYS \$ 9,750

B. Other Professional personnel

1. Visiting Scholar Prof. Pili-Hoon Bong  
12 months @ \$600 (supplement) 7,200

2. Graduate Assistant, L. Cuesta  
12 months @ \$1000 12,000

3. Graduate Assistant, Z. He  
6 months @1000 6,000

Total Salary and Wages 34,950

C. Fringe Benefits

@26.3% of Category A personnel 2,564

Total Salary, Wages, and Fringe Benefits 37,514

E. Travel (1.5 meetings) 1,000

G. Other Direct Costs

1. Supplies 5,409

2. Publication costs 1,000

Total other direct costs 6,409

H. Total direct costs \$44,923

I. Indirect costs (62.5% of modified direct costs) \$28,077

J. Total \$73,000

(SEE INSTRUCTIONS ON REVERSE BEFORE COMPLETING)

**SUMMARY PROPOSAL BUDGET**

**APPENDIX**

		FOR NSF USE ONLY			
ORGANIZATION		PROPOSAL NO.		DURATION (MONTHS)	
Georgia Tech Research Corporation				Proposed	Granted
PRINCIPAL INVESTIGATOR/PROJECT DIRECTOR		AWARD NO.			
Laren M. Tolbert					
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title; A.6. show number in brackets)		NSF FUNDED PERSON-MOS.		FUNDS REQUESTED BY PROPOSER	FUNDS GRANTED BY (IF DIFFERENT)
		CAL.	ACAD	SUMR	
1.	L. M. Tolbert, Principal Investigator	1.5			\$ 9,750
2.					
3.					
4.					
5.	( ) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION PAGE)				
6.	( ) TOTAL SENIOR PERSONNEL (1-5)				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1.	( 1 ) POST DOCTORAL ASSOCIATES (supplement)	12			7,200
2.	( ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				
3.	( 1, 5 ) GRADUATE STUDENTS				18,000
4.	( ) UNDERGRADUATE STUDENTS				
5.	( ) SECRETARIAL-CLERICAL				
6.	( ) OTHER				
TOTAL SALARIES AND WAGES (A+B)					34,950
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS) 26.3% of A					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					37,514
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$1,000:)					
TOTAL PERMANENT EQUIPMENT					
E. TRAVEL 1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					1000
2. FOREIGN					
F. PARTICIPANT SUPPORT COSTS					
1.	STIPENDS \$ _____				
2.	TRAVEL _____				
3.	SUBSISTENCE _____				
4.	OTHER _____				
TOTAL PARTICIPANT COSTS					
G. OTHER DIRECT COSTS					
1.	MATERIALS AND SUPPLIES				5,409
2.	PUBLICATION COSTS/PAGE CHARGES				1,000
3.	CONSULTANT SERVICES				
4.	COMPUTER (ADPE) SERVICES				
5.	SUBCONTRACTS				
6.	OTHER				
TOTAL OTHER DIRECT COSTS					6,409
H. TOTAL DIRECT COSTS (A THROUGH G)					44,923
I. INDIRECT COSTS (SPECIFY)					
TOTAL INDIRECT COSTS 62,5% of MTDC					28,077
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					73,000
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPM 252 AND 253)					0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					\$ 73,000
PI/PD TYPED NAME & SIGNATURE _____		DATE _____		FOR NSF USE ONLY	
INST. REP. TYPED NAME & SIGNATURE _____		DATE _____		INDIRECT COST RATE VERIFICATION	
		Date Checked	Date of Rate Sheet	Initials - DGC	

\*SIGNATURES REQUIRED ONLY FOR REVISED

IND 11

633-636

**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**

Laren M. Tolbert  
School of Chemistry  
GA Tech Res Corp - GTRI  
Atlanta GA 30332

# NATIONAL SCIENCE FOUNDATION FINAL PROJECT REPORT

PART I - PROJECT IDENTIFICATION INFORMATION	
1. Program Official/Org.	Charles E. Hoyle - CHE
2. Program Name	ORGANIC & MACROMOLECULAR CHEMISTRY PROGR
3. Award Dates (MM/YY)	From: 06/88 To: 11/91
4. Institution and Address	GA Tech Res Corp - GTRI Atlanta GA 30332
5. Award Number	8805577
6. Project Title	Charge Distribution in Photoexcited Molecules



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.

	2-25-92
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.

Laren M. Tolbert  
Project Summary - NSF CHE-8805577  
"Charge Distribution in Photoexcited Molecules"

*Part II. Summary.*

The goal of this research is to define the proton transfer kinetics and related properties of certain organic molecules which, as a result of electron redistribution upon photoexcitation, become very strong transient acids. By strategic design and directed synthesis, organic photoacids (naphthols) with specifically designed internal proton acceptors or with greatly enhanced photoacidity have been prepared. By a combination of time-resolved fluorescence and other kinetic techniques, these substrates have allowed testing of various theories of excited-state proton transfer (ESPT), provided new methods for studies of proton-transfer-initiated reactions, and yielded novel structures unattainable by ground-state methods. Important discoveries include the observation that, in mixed aqueous solutions, water clustering of a lower order is required if "superacids" or molecules with internal proton acceptors are employed. Thus these studies provide critical information on the transition-state structure of that most important of chemical reactions, proton transfer.

In related studies, time-resolved fluorescence and absorption experiments have, for the first time, provided information on the excited-state structure of a resonance-stabilized carbanion, namely, 9-phenylfluorenyl anion. Curiously, the conjugate acid, 9-phenylfluorene, has an enormous thermodynamic excited-state acidity which is kinetically inaccessible. Finally, irradiation of other resonance-stabilized carbanions, namely, 2-chloroallyl anions, leads to formation of allenes which, if constrained in a ring, are reactive synthetic intermediates.

Laren M. Tolbert  
Project Summary - NSF CHE-8805577  
"Charge Distribution in Photoexcited Molecules"

*Part III. Technical Information.*

D. L. Tomasko, B. L. Knutson, C. A. Eckert, J. E. Haubrich, and L. M. Tolbert, "Fluorescence Investigation of Cosolvent/Solute Interactions in Supercritical Fluid Solutions, ACS Symp. Ser., in press.

Laren M. Tolbert, Susan M. Fitzwater, Narciso Raya, and Michael Stapleton, "Substituent Effects on Carbanion Photophysics. An Application of The Energy Gap Law," J. Phys. Chem., in press.

Laren M. Tolbert and Susan M. Nesselroth, "Proton Transfer in the Inter- vs. Intramolecular Quenching of Naphthol Fluorescence by Amines, *J. Phys. Chem.*, **95**, 10331 (1991).

L. M. Tolbert and Jeanne E. Haubrich, "Enhanced Photoacidities of Cyanonaphthols", J. Am. Chem. Soc., **112**, 8163 (1990).

Laren M. Tolbert, Md. Nurul Islam, Richard P. Johnson\*, Paul M. Loisel and William C. Shakespeare, "Carbanion Photochemistry: A New Route to Strained Allenes", J. Am. Chem. Soc., **112**, 6416 (1990).

L. M. Tolbert, in "Handbook of Organic Photochemistry", "Spectroscopic Properties of Radical-Ions and Short-Lived Carbocations and Anions," J. C. Scaiano, ed., CRC Press, p. 23 (1989).

Andrzej J. Rajca and Laren M. Tolbert, "Y-Conjugated Dianions. A <sup>13</sup>C Nuclear Magnetic Resonance Study", J. Am. Chem. Soc., **110**, 871 (1988).

The primary data for this work consists of computer calculations, organic synthesis of target molecules with associated physical measurements, bulk photochemistry of the target molecules, and time-resolved studies of their photophysics and photochemistry. The primary means of dissemination is through the open literature. However, samples of the compounds prepared have been made available to other researchers for their own studies upon request.

**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 <sup>1</sup>	
	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.	Male	Fem.
<b>A. Total, U.S. Citizens</b>	1			1		2		1		
<b>B. Total, Permanent Residents</b>										
U.S. Citizens or Permanent Residents <sup>2</sup> :										
American Indian or Alaskan Native . . . . .										
Asian . . . . .										
Black, Not of Hispanic Origin . . . . .										
Hispanic . . . . .						1				
Pacific Islander . . . . .										
White, Not of Hispanic Origin . . . . .	1			1		1		1		
<b>C. Total, Other Non-U.S. Citizens</b>										
Specify Country										
1. <i>Korea</i>	1									
2.										
3.										
<b>D. Total, All participants (A + B + C)</b>	2			1		2		1		
<b>Disabled<sup>3</sup></b>										

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).

<sup>1</sup>Category includes, for example, college and precollege teachers, conference and workshop participants.

<sup>2</sup>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.)

<sup>3</sup>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.