

PROJECT ADMINISTRATION DATA SHEET

ORIGINAL  REVISION NO. \_\_\_\_\_

Project No. G-41-672 (R5980-OAO) GTRC/~~XXX~~ DATE 7 / 16 / 85

Project Director: W. G. Harter School/~~XXX~~ Physics

Sponsor: National Science Foundation

Type Agreement: Grant No. PHY-8421210

Award Period: From 6/15/85 To 12/4/85 ~~11/30/87\*~~ (Performance) 3/4/86 ~~2/28/88~~ (Reports)

Sponsor Amount: This Change Total to Date

Estimated: \$ \_\_\_\_\_ \$ 111,000

Funded: \$ \_\_\_\_\_ \$ 71,000

Cost Sharing Amount: \$ 7,108 Cost Sharing No: G-41-350

Title: Molecular Rotational Dynamics (Physics)

ADMINISTRATIVE DATA

OCA Contact John B. Schon x-4820

1) Sponsor Technical Contact:

2) Sponsor Admin/Contractual Matters:

J. Norman Bardsley

Stephen G. Burnisky

National Science Foundation

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Defense Priority Rating: N/A Military Security Classification: N/A

(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached NSF Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval - Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of \$500 or 125% of approved proposal budget category.

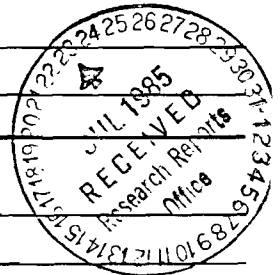
Equipment: Title vests with GIT.

COMMENTS:

No funds may be expended after 11/30/87.

\* A six month unfunded flexibility period is included.

Initial support for the project is 2 years, a third year of support is anticipated.



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Accounting Research Communications (2) Other A. Jones

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 5/14/86

Project No. G-41-672 School/~~EES~~ Physics

Includes Subproject No.(s) N/A

Project Director(s) W. G. Harter ~~GTRI~~ GTRC/GT

Sponsor National Science Foundation

Title- Molecular Rotational Dynamics

Effective Completion Date: 12/14/85 (Performance) 3/14/86 (Reports)

Grant/Contract Closeout Actions Remaining:

- None
- Final Invoice or Final Fiscal Report
- Closing Documents
- Final Report of Inventions      Questionnaire sent to P.I.
- Govt. Property Inventory & Related Certificate
- Classified Material Certificate
- Other \_\_\_\_\_

Continues Project No. \_\_\_\_\_

Continued by Project No. \_\_\_\_\_

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R. Embry

Final Report

"Molecular Rotational Dynamics (Physics)"

JAN 21 9 40 AM '86

NSF  
DIVISION OF  
PHYSICS

Progress has been made on the principal problem stated in the proposal for grant PHY-8421210. This concerns the development and understanding of multiple rotational energy (RE) surface dynamics and the related quantum and semiclassical mechanics of molecules. A model system which requires just two adiabatic RE surfaces has been constructed and partially analyzed. The model consists of an asymmetric rotor carrying a two state spin-1/2 or vibrational two level quasi-spin system. The classical version of the model is capable of exhibiting classical chaos while the purely quantum version of the model is conveniently solved numerically for any physically reasonable value of the angular quantum number ( $J$ ). Therefore, the model provides an excellent test for semi-classical approaches to its solutions.

The semiclassical solutions will involve a combination of adiabatic motions on RE surfaces and diabatic motions through or between these surfaces. A continuum of surfaces may be defined to trace the motion. This study should provide information about the detailed nature of coriolis interaction in the presence of angularly anisotropic rotational dynamics. This is important for understanding modern high resolution laser spectroscopy, dynamics, and chemical physics of molecules.

Prof. William G. Harter  
Principal Investigator

G-41692

NATIONAL SCIENCE FOUNDATION  
Washington, D.C. 20550FINAL PROJECT REPORT  
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

## PART I-PROJECT IDENTIFICATION INFORMATION

1. Institution and Address Georgia Tech Research Corporation Georgia Institute of Technology Atlanta, Georgia 30332	2. NSF Program	3. NSF Award Number PHY-8421210
	4. Award Period From 6/15/85 To 12/14/85	5. Cumulative Award Amount \$21,394

6. Project Title  
Molecular Rotational Dynamics (Physics)

## PART II-SUMMARY OF COMPLETED PROJECT (FOR PUBLIC USE)

This project concerns the development and understanding of multiple rotational energy (RE) surface dynamics and the related quantum and semiclassical mechanics of molecules. A model system which requires just two adiabatic RE surfaces has been constructed and partially analyzed. The model consists of an asymmetric rotor carrying a two state spin-1/2 or vibrational two level quasi-spin system. The classical version of the model is capable of exhibiting classical chaos while the purely quantum version of the model is conveniently solved numerically for any physically reasonable value of the angular quantum number (J). Therefore, the model provides an excellent test for semi-classical approaches to its solutions.

## PART III-TECHNICAL INFORMATION (FOR PROGRAM MANAGEMENT USES)

1. ITEM (Check appropriate blocks)	NONL	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM	
				Check (✓)	Approx. Date
a. Abstracts of Theses	X				
b. Publication Citations	X				
c. Data on Scientific Collaborators	X				
d. Information on Inventions	X				
e. Technical Description of Project and Results			X		
f. Other (specify)					
2. Principal Investigator/Project Director Name (Typed) William G. Harter	3. Principal Investigator/Project Director Signature			4. Date 3/25/86	