NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT

NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I–PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
School of Physics Georgia Institute of Technology	Theoretical Physics	PHY-7927098
	4. Award Period From Sept. 81 To June 83	5. Cumulative Award Amount 27,758

6. Project Title

Theory of High Resolution Molecular Spectra

PART II–SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

The objective of this project was to understand the quantum mechanics of rotating vibrating molecules and their high resolution-laser spectra. In particular, understanding and implications were sought for the spectral clusters which appear in 10μm and 16μm infrared spectra of SF_6. The clustering permits nuclear spin moments to have an unexpectedly large effect on the molecular wavefunction, and we predicted that the nuclear spin symmetry species would be mixed. Mixing of species had been ruled out in texts on molecular spectroscopy such as Herzberg's famous works, but it has recently been observed by Bordé and coworkers in Paris. Detailed theories and formulas for the mixing effects was worked out in this project using unitary and permutation operator analysis. New mathematical techniques including tableau hook algebra were developed, and a new type of energy surface called the rotational energy (RE) surface was invented. The latter invention lead to the extending the scope of investigation to other molecules besides SF_6, it was discovered that spectral clustering is a universal effect which occurs in virtually all polyatomic molecules. It happens in even the lowest symmetry complexes such as H_2O, and its presence and implications have been almost completely ignored. Knowledge of these new effects should lead to new physical and chemical phenomena and applications.

PART III–TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	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)*	3. Principal Investigator/Project Director Signature	4. Date
William G. Harter		3/28/83