OFFICE OF NAVAL RESEARCH
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Task No. NR 056-607

FINAL REPORT

"LASER SPECTROSCOPIC STUDIES OF MOLECULAR CRYSTALS"

1 June 1975 - 30 November 1979

E. R. Bernstein, Principal Investigator
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March 1980

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This report summarizes the work performed under the contract from 1 June 1975 to 30 November 1979. It includes a summary of new results, a list of all technical reports generated during the life of the contract, and a listing of personnel associated with the project.
I. PERSONNEL WHO PARTICIPATED IN THE RESEARCH

1. Elliot R. Bernstein, Principal Investigator.
2. Daniel L. Michalopoulos, Graduate Student - Electronic Raman scattering and inorganic molecular vibronic coupling.
3. Gerald R. Meredith, Graduate Student - ReF₆ magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
4. John D. Webb, Graduate Student - IrF₆ magnetic properties, vibronic coupling, electronic Raman scattering and crystal vibrational levels.
6. Kerry M. Swift, Graduate Student - Nonlinear optical phenomena - multiphoton photochemistry and spectroscopy of OsO₄, C₃N₃H₃.
7. Philip M. Kennedy, Graduate Student - Nonlinear optical phenomena - multiphoton photochemistry and spectroscopy of transition metal hexafluorides.
8. K. M. Chen, Graduate Student - Spectroscopy of rare earth borohydrides, vibronic transitions in rare earth compounds.

II. TECHNICAL REPORTS GENERATED

II. (Continued)

15. "On the Jahn Teller Effect in IrF₆: The $\Gamma_{8g} (t_{2g})^3$ State at 6800 Å," E. R. Bernstein and J. D. Webb.


17. "Absorption and Electronic Raman Scattering Spectra of the $\Gamma_{8g} (T_{1g})$ State of IrF₆ at 1.6μ - A Resolution of the Jahn Teller Problem," E. R. Bernstein and J. D. Webb.


21. "A Ligand Field Theory Analysis of the Spectra of the $t_{2g}^3$ Levels of IrF₆," J. D. Webb and E. R. Bernstein.


III. ACCOMPLISHMENTS

New results and new work our research has led to includes the following:

a) Electronic Raman scattering in molecules.

b) Magnetic phase transition in molecular solids (ReF₆, IrF₆).

c) Elucidation of quadratic vibronic coupling (intra- and interstate) - MF₆, C₃N₃H₃.

d) New insight into photochemical vs. fluorescence yields of excited states (C₃N₃H₃, C₄N₂H₄, OsO₄).

e) Spectroscopy of cryogenic liquid solutions and energy transfer.

f) Phase transition studies in molecular solids.

g) Polariton behavior in molecular solids.

h) Elucidation of vibrational mixing (normal mode breakdown) in degenerate electronic states (MF₆ systems).
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