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6 OPTICAL AND MAGNETIC RESONANCE STUDIES
OF ENERGY TRANSFER IN INORGANIC MOLECULAR SOLIDS

9 FINAL REPORT, 1 Jun 77 - 31 May 80

by

10 Elliot R. Bernstein
Principal Investigator

11 Aug 1980

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report summarizes the important results of the grant research. It includes a statement of the problem studied, a list of personnel supported during the life of the grant, and a list of publications which resulted from the supported research.		

Statement of Problem Studied

Optical and magnetic resonance investigations of inorganic molecular solids were performed. We have studied magnetic resonance, Raman scattering, and optical spectra of various transition metal hexafluorides. The aim of these studies was to begin a program to determine the dynamical energy properties of transition metal molecular crystal systems.

Scientific Personnel Supported During This Period

Lawrence Dennis, Postdoctoral Fellow

Daniel Michalopoulos, Graduate Student

John D. Webb, Graduate Student

Elliot R. Bernstein, Principal Investigator (summer salary)

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Summary of Important Results

The important results for this research fall into two categories. The first is a study of the Jahn Teller Effect in iridium hexafluoride (IrF_6). This work is significant because it lays the foundation for a detailed analysis of the vibronic coupling in molecules and solids. The careful analysis of three of the degenerate electronic states of IrF_6 by absorption and Raman scattering studies of low temperature crystals has enabled us to determine linear and quadratic vibronic coupling parameters and how vibronic coupling interferes with interactions in the solid. We have performed a theoretical analysis of the energy levels of IrF_6 .

The second area of important contributions is in the analysis of electron paramagnetic resonance data for an octahedral Γ_8 state. We have demonstrated for the first time that such a state, even in a cubic environment, evidences anisotropic behavior and highly complicated magnetic resonance spectra.

Publications

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