NYO 1447-74
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FINAL REPORT

Spectra of Rare Earth Ions and Hydrogen Molecules

Prepared by

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The Johns Hopkins University
Baltimore, Maryland

Period: November 1, 1952 - October 31, 1971

AT(30-1)-1447
AT(11-1)-3272

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ABSTRACT

The research reported here was carried out under Contracts AT(30-1)-1447 and AT(11-1)-3272 from its inception on November 1, 1952 to October 31, 1971. These nineteen years of AEC sponsorship of spectroscopic research at The Johns Hopkins University saw a spectacular increase in scientific interest in research related to optical phenomena in solids and gaseous plasmas. Although it was not the purpose of this work to deal directly with the development of these devices, the three main areas of research (experimental spectrum analysis of the isotopic hydrogen molecules, experimental level analysis of rare earth ions in crystals, and development of the theory of atomic structure of complex atoms) have proved to be of fundamental importance for technological developmental work carried on in other laboratories. Books by the principal investigators have been published in each of these fields.

Details are discussed in separate sections below under the following headings:

1. Spectra of Molecular Hydrogen and Its Isotopes
2. Rare Earth Crystal Spectra
3. Theoretical Spectroscopy
4. Rare Earth and Uranium Free Ion Spectra
5. Publications

This research was carried out under the direction of G. H. Dieke until his death in August, 1965. Between this date and November 1, 1967, it was shared by L. Madansky and H. M. Crosswhite; from November, 1967 on, B. R. Judd and H. M. Crosswhite were the contract directors.

1. Spectra of Molecular Hydrogen and Its Isotopes.

The isotopic molecular spectra of H_2 are of great theoretical interest, since they represent the simplest molecular system for which detailed spectroscopic data are available. At the beginning of this work, the basic electronic structure was known for H_2 , D_2 , and DH , and a beginning had been made on T_2 and TH . However, as new experimental techniques developed it became evident that a remeasurement of all spectra would be needed to bring the work up to a uniformly high quality. This rather massive program was still incomplete at the time of Professor Dieke's death in 1965, and the effort since then has been to bring his work into a form suitable for publication. His entire H_2 line list (not including vacuum ultraviolet data) with all known classifications and energy levels has been published by Wiley-Interscience ("The Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke," edited by H. M. Crosswhite (1972)). Extensive D_2 and T_2 classifications had also been completed by Dieke and these tables have been evaluated and are now nearly ready for publication. This work is being continued with the assistance of an NSF grant. The experiments on the mixed molecules DH , TH and TD are much more difficult, and as the experimental work on these mixed molecules was left in a more primitive state, it does not appear that more can be done with these without a much higher level of assistance than now appears feasible.

2. Rare Earth Crystal Spectra.

The importance of Dieke's studies of the energy level structures of rare earth ions in crystals can best be realized by comparing the present state of experimental knowledge with that in 1952. Before that time it was not possible to obtain rare earths of the quality required for spectroscopic research, with the result that much of the published data was confused by frequent impurities. The availability of high-purity materials and the use of high magnetic fields and spectrographs with higher resolution than had previously been used resulted in comprehensive understanding of the experimental facts, especially as regards the highly symmetric $LaCl_3$ and related crystals. Parallel developments of the theory

of $4f^N$ atomic structures in crystals (see the next section) has permitted clear quantum number assignments to be made for nearly all the observed levels in these crystals. A summary of a large part of Dieke's work has been published by Wiley-Interscience ("Spectra and Energy Levels of Rare Earth Ions in Crystals," by G. H. Dieke, edited by H. M. Crosswhite and Hannah Crosswhite (1968)). Further clarifications have been made as the experiments have been refined and as the details of the theoretical interpretation have been further explored. Much of this more sophisticated work has been made possible by advances in computer technology. Details can be found in the list of publications given in Section 5.

3. Theoretical Spectroscopy.

The first decade of AEC sponsorship was principally concerned with perfecting and exploiting experimental techniques, the empirical analysis however being greatly assisted by the developments in theoretical spectroscopy by other groups. Dieke's death in 1965 brought this phase to an end, and the subsequent emphasis has been on a fuller development of theory, leading to a sharper interpretation of the experimental results.

The electronic structure of ions with configurations containing open-shell f electrons is very complex. In free-ion spectroscopy one examines transitions between two separate configurations, at least one of which must contain inequivalent open-shell electrons. As long as the theoretical apparatus was in a relatively primitive state, interpretation of such spectra beyond the very lowest levels was difficult, and progress was slow.

In the early 1950's (largely through electron paramagnetic resonance experiments) it became clear that the ground states of rare earth ions in crystals were of configurations containing only $4f$ electrons. This result inspired a great deal of interest in theoretical analysis of $4f^N$ structures, especially concerning the application of Racah algebra and the refinement of symmetry considerations for these systems. The experimental work of Hellwege in the late 1940's had shown that the optical spectra observed in these crystals was the result of transitions between levels of the

$4f^N$ configuration only. These transitions are normally forbidden as electric dipole radiation by the parity selection rule, but may however appear in crystals in which the site occupied by the rare earth ion does not have a center of symmetry. The importance of this fact to the theoretical treatment is that in this case only equivalent electrons are involved and a radical simplification in the symmetry properties is possible. Some hint of this had been given by Racah, but even he apparently did not realize the full implications of the group-theoretical arguments.

The application of group-theoretical methods to atomic systems has had a much broader reach than to these specific crystal problems, the larger scope in fact being an examination of the fundamental mathematical structure of atomic and nuclear theory. Atomic-beam and free-ion spectroscopic problems have also been clarified, as the methods developed are useful in the treatment of the dimpler d- and p-shell atoms and ions.

Details can be found in the publications listed in Section 5 from 1967 on, principally by B. R. Judd and Lloyd Armstrong.

4. Rare Earth and Uranium Free Ion Spectra.

A large part of the interpretation of the rare earth crystal spectra can be interpreted in terms of parameters used to describe the unperturbed trivalent ion. This is the so-called "free ion" model. But it is apparent from the systematic variation of these parameters from host to host that this method masks effects more properly attributable to the environment.

In 1957, preliminary studies of rare earth metal spark spectra were begun with the objective of obtaining the unperturbed free-ion energy levels, so that direct comparison to the crystal spectra could be made.

Sponsorship of this work was taken over by the Air Force Office of Scientific Research in 1959, which continued until 1968. AEC interest continued in this effort however in that several problems involving theoretical analysis of some of these spectra were investigated.

Beginning in 1966, similar experimental and theoretical studies of doubly and triply ionized metal spark spectra of uranium were begun. Most of the experimental work has been finished but the analysis has not been completed.

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ABSTRACT

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