ENGINEERING RESEARCH INSTITUTE
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TENTH QUARTERLY REPORT

ON

INFRARED STUDIES OF CRYSTALS

16 November 1953 to 15 February 1954

By

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TABLE OF CONTENTS

TENTH QUARTERLY REPORT

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I. INTRODUCTION

Purpose of the Research

This has been outlined previously (cf. Report of June, 1953) and does not need to be repeated here. The main emphasis has continued on the determination of the positions of the hydrogen atoms in mica and brucite. Work has also been started on gypsum ($Ca\ SO_4\ 2H_2O$) i.e., a crystal containing water of crystallisation.

Personnel

The following have been engaged on the work reported here:

Professor G.B.B.M. Sutherland, Director (Part time)
Mrs. C. Y. Pan Liang (Half time)
Mr. A. Dockrill (Part time)
Mr. G. Allen (Part time)
Mr. M. Hass (Part time, voluntary)

II. ACCOUNT OF WORK DONE

A. Mica Problem

The principal effort has been directed to the elucidation of the biotite spectrum near 3μ in terms of the coupled vibrations of eight OH groups in the unit cell. The earlier treatment (mentioned in the last report) was over-simplified. The new treatment may be summarised briefly by saying that the eight OH stretching vibrations couple to give eight modes of vibration of the unit cell. There are two centres of symmetry in the unit cell, one of which belongs to four of the oxygen atoms and the other to the other four. There is a C_2 axes parallel to the b axes of the crystal. It is assumed that there is negligible interaction between OH groups separated by a layer of K ions. This means that the four active frequencies will reduce to two pairs of frequencies identical in numerical value. The first pair are associated with the band at 2.83μ, since there should be no component along the c axis. The second pair are associated with the 2.73μ band, since the major change of electric moment is now along the c axis. (cf. Ninth Quarterly Report). The quantitative agreement with the observed spectra is now very good, apart from a small anomaly connected with the 2.73μ band. This last point is being checked experimentally and will also be reinvestigated theoretically.

From the data it is now possible to determine the orientation of the OH groups in the unit cell with considerable accuracy, and this is being done. The full details (experimental and theoretical) will form the subject of a separate technical report.

B. Brucite

Since our previous results indicated that the unit cell in Brucite was larger than that found by X-ray work, one of our crystals (which were greatly superior to those on which the early X-ray work had been done) was sent to Dr. Megaw in Cambridge, England. She has made a fresh investigation but arrived at the same structure as before, i.e., two $Mg(OH)_2$ ionic groups per unit cell. We are therefore making another attempt to see whether the complexities of the OH absorption in Brucite can possibly be accounted for in terms of the original X-ray unit cell. A detailed treatment by group theory is now in progress.

C. Gypsum

The absorption spectrum of thin plates of gypsum has been obtained between 2μ and 20μ, using polarised radiation and various angles of inclination. Some of the bands are too intense for absorption work so the reflection spectrum is being obtained in these regions. It is possible to deduce the absorption spectrum from the reflection spectrum.

The gross features of these spectra can largely be accounted for in terms of assignments made by previous workers on the Raman spectrum of gypsum. However, all the bands show some fine structure and interesting dichroic effects. A good deal more experimental work has to be done using different aspects of the crystal before any detailed interpretation can be attempted.

III. FUTURE PROGRAM

Work will continue on the theoretical interpretation of the spectra of mica and brucite. The experimental work will be concentrated on completing the data on gypsum, especially the reflection spectrum.