

## The use of infra-red absorption and molar refractivities to check coordination

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With 3 figures

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### Auszug

Durch experimentelle Untersuchung der Ultrarot-Absorptionsspektren einiger  $\text{SiO}_2$ -Isotope war es möglich, die primäre Koordination, die Atomordnungszahl, das Atomgewicht und die Ionenladung den Absorptions-Wellenlängen der größeren Banden zuzuordnen. Auch die Verwendung der Molrefraktion zur Voraussage und Bestimmung von Änderungen der (primären und sekundären) Koordination wird erläutert.

### Abstract

By an empirical study of the infra-red absorption spectra of some silica isotopes it has been possible to relate primary coordination, atomic number, atomic weight and ionic charge to absorption wave lengths for the major bands. Likewise the utilization of molar refractivity in predicting or determining coordination changes (both primary and secondary) is illustrated.

### Introduction

An attempt has been made at using infra-red absorption spectra and molar refractivities to yield information on coordination of cations in simple structures. The fact that infra-red absorption spectra will distinguish phases, which are quite similar crystallographically, is already well known<sup>1</sup>, and there is no doubt that the differences in such spectra reflect even minor changes of bond length and configuration. Of course, even in slightly complex uniaxial structures it is difficult to make an intelligent guess at assigning particular frequencies to certain vibration modes.

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<sup>1</sup> RUSTUM ROY and E. E. FRANCIS, On the distinction of sillimanite from mullite by infra-red techniques. *Am. Min.* 38 (1953) 725-728.

The use of infra-red

To proceed from the vibration modes is straightforward even to detect all expected bands. Largely, no doubt, to the various cases, such as quartz itself, it is possible to group the absorption bands as cation-anion stretching, cation-anion bending and distortion. Cation-anion stretching occurs at the longest wavelength of the strongest absorption. In a cation-anion bond is the most significant structural change in bond-length changes. Heavily distorted vibrations at highest frequency

Moreover, in simple structures we hope that certain associations of known-structure materials can be grouped of phases for such a series of groups of polymorphs.

These same phases, especially in value in studying changes in structure are available which exist in various forms, each of which can be distinguished by substance is  $\text{GeO}_2$  which exists as four-coordinated quartz for

### Infra-

In our early work<sup>2</sup> on silica we show clearly the ability to distinguish phases by absorption spectroscopy. The nature of the information and deduction from these results is clear from their usefulness.

The most significant series of polymorphs. Spectra for the polymorphs  $\text{SiO}_2$  cristobalite,  $\text{SiO}_2$  glass, and the isomorphous series  $\text{BPO}_4$ , etc.

<sup>2</sup> RUSTUM ROY, Isomorphism in silica. Symposium on "Defect structure in solids"