

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 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 Molarrefraktion 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 known¹, 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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¹ 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 spation modes is straightforward even to detect all expected largely, no doubt, to the v cases, such as quartz itself possible to group the absorption cation-anion stretching, anion bending and distortion stretching occurs at the strongest absorption. In a cation-anion bond is the c significant structural change in bond-length changes. He tions at highest frequency s

Moreover, in simple stru hope that certain associatio of known-structure materi groups of phases for such a groups of polymorphs.

These same phases, es value in studying changes i are available which exist in forms, each of which can substance is GeO_2 which ex four-coordinated quartz for

Infra-

In our early work² on show clearly the ability to absorption spectroscopy. T the information and deduct nature of these results is c from their usefulness.

The most significant sp morphs. Spectra for the pol SiO_2 cristobalite, SiO_2 glass isomorphous series BPO_4 ,

² RUSTUM ROY, Isomorphie Symposium on "Defect structu