Optical Absorption Spectroscopy of Minerals: An Overview

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More than 30 years have passed since the systematic study of mineral spectroscopy began in earnest. Now, the spectra of most significant minerals have been surveyed and the spectra of most major rock-forming mineral groups studied in reasonable detail. One of the original goals was to determine quantitative site occupancies for cations in common metamorphic and igneous minerals.

Tabulations of the intensities of absorption bands are poorly developed, but need for it has not grown in the earth-science community. Our understanding of the quantitative aspects of non-linear effects is even less-well developed. These effects include interactions between cations of same oxidation state such as d-d band intensification and pair bands; interactions between cations in different oxidation states such as heteronuclear intervalence charge transfer and intensification of ligand field bands. Even some aspects of homonuclear IVCT are not well understood.

There are significant opportunities for advancements in predictive theory. We would like to be able to consider an arbitrary cation in a site of specified coordination number, geometry and next-nearest neighbors and to be able to accurately predict it's optical spectrum through calculations.

Optical processes involving atomic units on a scale significantly larger than isolated ions yet smaller than several unit cells are poorly understood.

Examples are encountered in the optical spectra of Cu exsolving from plagioclase feldspars, intervalence effects in colored varieties of andalusite, and in the brownish-yellow Fe-oxides or hydrous-oxides in quartz (citrine) and corundum (yellow sapphire).

Opportunities abound to relate mineral spectroscopy to related sciences. Examples include the photochemistry of mineral surfaces, luminescence phenomena, and the development of electro-optic materials.

Instrumentation and the understanding of what is needed to obtain quality data have improved significantly. There is now the need to comprehensively re-assess many early results in view of both this improved understanding and the better structure refinements of minerals now available. A significant portion of our published database on mineral spectroscopy was obtained non-digitally and under conditions which can be improved with current technology. Emerging global electronic communications and computer technology demand that selected spectroscopic data be preserved digitally and made accessible to the global community in digital form.