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Fluorescence of trivalent neodymium in various materials excited by a 785 nm laser

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Abstract

The nature of the fluorescence in the frequency-shift range of 1000–2500 cm^{-1} observed in the Raman spectra of many minerals when excited by a 785 nm laser has been investigated. Among the trivalent rare earths only Nd^{3+} has the combination of a good ionic-radius match to substitute for Ca^{2+} and an arrangement of energy levels to produce fluorescence in the frequency-shift range of interest. Raman/fluorescence spectra of six calcium-based minerals, namely fluorite, calcite, powellite, scheelite, apatite, and grossular/tsavorite, have been obtained at both room temperature and liquid-nitrogen temperature and transition assignments made for the majority of fluorescence lines in fluorite, powellite, scheelite, and grossular/tsavorite. The room-temperature results agree closely with results on individual minerals obtained by previous workers for fluorite and scheelite. The liquid-nitrogen-temperature results as well as the transition assignments for powellite and grossular/tsavorite are new. The Nd concentration has been measured by laser-ablation induction-coupled-plasma mass spectrometry (LA-ICP-MS) and correlated with Nd^{3+} fluorescence intensity where possible. For fluorite, the fluorescence intensity increases at least linearly with concentration at levels up to a few parts per million and then saturates at higher levels due to concentration quenching. Analysis of room-temperature Raman/fluorescence spectra of a much larger group of minerals available on the RRUFF web site shows that strong or very strong Nd^{3+} fluorescence is much more likely in calcium-based minerals than in non-calcium-based ones and is completely absent for minerals containing iron in the chemical formula. Nd^{3+} fluorescence is best understood in fluorite and less well understood in the other five minerals. Further study of calcite, apatite, and grossular/tsavorite is necessary to improve the understanding of the charge-compensation mechanisms and increase the number of identified transitions in calcite and apatite. The results of this work indicate that Nd^{3+} fluorescence in calcium-based minerals, when excited by a 785 nm laser, has potential uses in three areas: mineral identification, structure characterization and determination of trace-element concentration.

Keywords: Raman spectrum fluorescence, neodymium fluorescence, rare-earth impurities in minerals, laser-ablation induction-coupled-plasma mass spectrometry, LA-ICP-MS