

A CRITICAL ANALYSIS OF VIBRATIONAL SPECTROSCOPY IN LABORATORY TEST

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Abstract: Vibrational spectroscopy includes several different techniques, the most important of which are mid-infrared (IR), near-IR, and Raman spectroscopy. Raman and mid-IR spectroscopy are complementary techniques and usually both are required to completely measure the vibrational modes of a molecule. Vibrational spectrometry covers a series of well-established analytical methodologies suitable to be employed for both qualitative and quantitative purposes. In the first part of this review, we will focus on theoretical aspects related to vibrational techniques; in the second part, the most important papers, published during the period 2010-2019 related to clinical analysis performed with vibrational spectroscopy techniques will be critically discussed.

Keywords: Vibrational Spectroscopy, Critical Analysis, Laboratory

INTRODUCTION

Vibrational spectroscopy includes several different techniques, but the most important techniques are mid-infrared (IR), near-IR (NIR), and Raman spectroscopy. Both mid-IR (MIR) and Raman spectroscopy provide characteristic fundamental vibrations that are employed for the elucidation of molecular structure and are the topic of this review. Near IR spectroscopy measures the broad overtone and combination bands of some of the fundamental vibrations (only the higher frequency modes) and is an excellent technique for rapid and accurate quantization. Vibrational spectroscopy is used to study a very wide range of sample types and can be carried out from a simple identification test to an in depth, full spectrum, qualitative and quantitative analysis. Samples may be examined either in bulk or in microscopic amounts over a wide range of temperatures and physical states (e.g., gases, liquids, latexes, powders, films, fibers, or as a surface or embedded layer).

Vibrational spectroscopy has a very broad range of applications and provides solutions to a host of important and challenging analytical problems. Raman and mid-IR spectroscopy are complementary techniques and usually both are required to completely measure the vibrational modes of a molecule. Although some vibrations may be active in both Raman and IR, these two forms of spectroscopy arise from different processes and different selection rules. In general, Raman spectroscopy is best for symmetric vibrations of non-polar groups, whereas IR spectroscopy is best at the asymmetric vibrations of polar groups.

Every molecule has a unique fingerprint of vibrational frequencies, which makes Raman and Fourier transform infrared (FTIR) spectroscopy highly specific techniques for molecular identification. Both techniques can be employed noninvasively, making them ideal for biomedical applications. Raman and FTIR spectroscopy are sometimes referred to as "sister" techniques and provide complementary information about molecules, but they differ in several fundamental ways.

Raman spectroscopy arises from the inelastic scattering of ultraviolet, visible, or near infrared light when a photon interacts with a molecule. Raman scattering is an inherently weak process and, as such, samples are typically illuminated by laser light. Light scattered by the sample is diffracted into individual wavelengths by a spectrograph and collected by a detector such as a charge coupled device or complementary metal-oxide semi-conductor sensor. One disadvantage of Raman spectroscopy in the biomedical arena, however, is its inherently weak signal, which can be overwhelmed by sample fluorescence. Therefore, there is an increasing demand for clinical analysis, which obliges hospital laboratories and public health systems to make a large number of determinations and justifies the use of powerful mechanized commercial systems. These kinds of methods involve the use of high amounts of expensive and specific reagents, which are out of the economical possibilities of many countries.

Vibrational spectroscopy offers complete information on the chemical composition of samples regarding both major and minor compounds, which present many characteristic bands in the studied range. Additionally, the presence of trace compounds can be modeled in some cases through the multivariate treatment of the whole IR or Raman spectra of well characterized samples based on the influence of molecules at low concentration levels on the size and shape of the bands of major compounds. Vibrational spectroscopy is an attractive modality for the analysis of biological samples, providing a complete noninvasive acquisition of the biochemical fingerprint of the sample. It has been demonstrated that these data provide the means to assay multiple functional responses of a biological system at a spatial resolution as low as a micrometer within the sample. The objective of this article is to review new developments in applications of vibrational spectroscopy (Raman and FTIR) in clinical diagnostics, covering the period between 2010 and 2019. Prior to a review on this subject, it is useful to give a short introduction on the concept of the vibrational spectroscopy, followed by discussion of the quantitative and qualitative biomedical investigations of the technique.

VIBRATIONAL SPECTROSCOPY-THEORETICAL ASPECTS

Molecular vibrations can be excited via two physical mechanisms: the absorption of light quanta and the inelastic scattering of photons, as can be seen in Figure 1. Direct absorption of photons is achieved by irradiation of molecules with polychromatic light that includes photons of energy matching the energy difference between two vibrational energy levels, the initial (ground state) and the final (first excited state) vibrational state. In IR spectroscopy, the vibrational transitions are induced by absorption of light quanta.

PRINCIPAL

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