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Computational assignment of vibrational frequency bands facilitates the identification of Raman spectra

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Spectroscopic parallax is the measure of the distance between two stars or celestial objects and relies on the stellar spectral type and luminosity class defined by the Morgan-Keenan classification system. UV, IR (infrared), Raman or optical spectrographic instruments are 'integrated' in many telescopes and are used to obtain information on brightness, temperature (surface), density and velocities. Stars are classified based on their type and on their brightness, which allow us to obtain distances to them, however, with previous classification systems, the star's size, i.e. dwarf, giant or supergiant and composition (heavy metal versus carbon stars) were also used. The Morgan-Keenan classification offers information on the star color, i.e. very blue and the type, however, the infrared wavelengths are approximately >9000 Å. We therefore tend to speak of near-infrared spectra. Spectra can be ulterior division into continuous, band and linear. Band spectra are usually descriptive of molecular compounds and are the ones that we investigated. We are going to concentrate on the interpretation of Raman band spectra of a small biological peptide, i.e. human glutathione (GSH), but we the same approach can be applied to gain stellar information. Our method consisted in using vibrational dynamics (VD), the study of atomic oscillations within a molecule. We previously obtained experimental vibrations for the peptide through Raman or IR spectroscopies available in the literature. These techniques have been widely used in the past, but the assignment of vibrational frequency bands is still challenging. In recent years, researchers have used ab initio and other computer simulation methods that facilitate band recognition. The goal of this work was to apply computational vibrational dynamics studies to the structure of human glutathione, and to then compare these values with its IR and Raman frequencies. By analyzing both simulation results and by comparing them with empirical data, we gained important information about the vibration modes of glutathione. This study showed that some bands that may not be visible in Raman or IR spectra can be 'detected' with this technique. Furthermore, our findings illustrate that most peaks obtained experimentally match those achieved in the computational simulation. Vibrational dynamics was therefore not just effective in understanding the structure of glutathione, but it can also be used to refine the quality of experimental Raman-IR data.

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