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Abstract

Chiral characterization of materials using Raman spectroscopy

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Abstract:
Recently, developments in optical filters have enabled the facile use of Raman spectroscopy to detect low-frequency vibrational (LFV) modes. We presented a new method for differentiating racemic from enantiopure crystals by using, for the first time, Raman spectroscopy to characterize the LFV modes of crystalline organic materials composed of chiral molecules. The LF-Raman spectra of racemic and enantiopure crystals exhibit a significant variation, which we attribute to different hydrogen-bond networks in the chiral crystal structures. Across a representative set of amino acids, we observed that when comparing racemic versus enantiopure crystals, the available LFV modes and their relative scattering intensity are strong functions of side chain polarity. Thus, LF-Raman can be used as a complementary method to the currently used methods for characterizing crystal's chirality. The pharmaceutical industry is in need of new techniques to identify the chirality of solids due to regulatory and safety concerns regarding the biological activity of enantiomers. Since we found the LF-Raman spectra of racemic and enantiopure crystals are significantly different, we set out to demonstrate the capabilities of our method for chiral purity investigation. For that we used a model system based on chiral crystals of enantiopure, racemic crystals and their mixtures in various ratios. Using this method, we were able to identify small amounts, as low as 1% w/w, of an enantiomer in racemic crystals. Comparing the achieved sensitivity for enantiomeric excess measurement in chiral crystals to that of circular dichroism and X-ray diffraction measurements showed that LF-Raman attains high sensitivity in solids that is similar to chiral optical methods used for solutions. Overall, our proposed approach of using Raman spectroscopy for determining enantiomeric excess in crystals is simple, fast, and offers a high degree of chiral sensitivity.

Biography:
Dr. Hagit Aviv is a lab manager and a research associate in the Molecular Photonics Laboratory in the Department of Chemistry at Bar-Ilan University. Her research focuses on Raman Spectroscopy of nanostructure and atomic force microscopy of thin films. She also designs and characterizes nano devices. Her work has been published in several esteemed journals in her field and she leads sevelar collaborative projects in the private sector.

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