Pre-resonant enhancement of Amide Raman bands in small oligo-peptides and proteins detected by synchrotron-based UV Resonant Raman scattering

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Ultra-violet Resonant Raman (UVRR) is widely used to investigate organic systems whenever the complexity of the molecules analyzed do not allow to get an easy and unique interpretation of the spontaneous Raman vibrational spectra. One of the most important applications of UV Resonant Raman in the deep-UV range (below 300 nm) is the investigation of peptides systems. It requires the use of an UV laser source able to generate the excitation wavelengths needed to selectively approach the energy of resonances occurring in the specific system. Although these class of measurements are generally performed by using fixed energy lasers, the possibility of having, instead, a tunable radiation source in the deep-UV range allow to "map" the whole resonance landscape range. First, it allows a better selection of the resonant conditions, even by applying small changes in the excitation energies. Secondary, by an attempt choice of such excitation energy it is possible to match experimental conditions where the sample self—absorption is negligible but their pre-resonance effects are sufficiently marked to enhance specific Raman bands.

In this contribution, we will introduce the synchrotron-based resonant Raman scattering instrument working in the UV spectral range, newly developed on IUVS at Elettra synchrotron radiation facility in Trieste. As example of a possible application we have investigated the enhancement of the Amide band intensity in model peptide systems above 230 nm of excitation wavelength. We have used specific small peptides model systems such e.g. NAGMA and NALMA discovering that the Amide-II band strongly enhances its intensity between 270 and 230 nm on incident radiation. These findings have been explained by means of quantum mechanics simulations.

Keywords: UV Resonant Raman; peptides; proteins.

References

[1] S. A. Oladepo, K. Xiong, Z. Hong, S. A. Asher, J. Handen, I. K. Lednev, *Chem. Rev*. **112**, 2604–2628 (2012).