VIBRATIONAL SPECTROSCOPY OF GAS-PHASE PEPTIDES: A MODEL FOR UNDERSTANDING THE SECONDARY STRUCTURE OF PROTEINS

ISABELLE COMPAGNON, JOS OOMENS, *FOM Institute for Plasma Physics "Rijnhuizen", Nieuwegein, The Netherlands*; GERT VON HELDEN, GERARD MEIJER, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*.

Experiments on biomolecules in the gas phase, where the interaction with the environment is eliminated or controlled, provide fundamental insight into their structure and function. Understanding the formation of the secondary structure in peptides is a key point in the protein-folding problem. The aim of this project is to identify the intrinsic factors responsible for conformational stability, as well as the influence of a controlled environment. Particularly, the combination of IR and UV hole burning spectroscopy with molecular beam techniques has recently yielded detailed information on the structure of low energy conformations of a variety of biomolecules, among which several small peptides.

In this contribution, the mid- and far-IR radiation produced by the Free Electron Laser for Infrared eXperiments (FELIX) is applied to address the local organization of peptides, i.e. the "secondary structure". We introduced a UV chromophore (benzyloxycarbonyl, referred to as Z) protecting function in the peptide[1], which allows us to extend the application of IR/UV hole burning spectroscopy to any peptide, instead of only those containing an aromatic amino-acid (Trp, Phe, Tyr). We investigate the mid-IR signature of two capped model peptides in the wavelength range beyond the well-known Amide bands (1500-1800 cm^{-1}), which are commonly used as a diagnostic of the intramolecular H-bonding network. The 1000-1500 cm^{-1} range offers a wealth of information leading to a precise assignment of the peptide's backbone conformation[2]. The far IR region ($<$1000 cm^{-1}) contains a number of bands that are poorly predicted by DFT calculations, which may be due to the presence of strongly anharmonic vibrations. Hence, the IR signature of the Amide bands and the mid-IR fingerprint of the backbone bands are quite complementary and offer a very detailed description of the secondary structure of peptides.

1. I. Compagnon, J. Oomens, J.M. Bakker, G. Meijer, G. von Helden *Phys. Chem. Chem. Phys.* **7**, 13-15 (2005)
2. I. Compagnon, J. Oomens, G. Meijer, G. von Helden, to be published.