CFEL SCIENCE

SEMINAR

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Building 99, Seminar Rooms I+II (EG)

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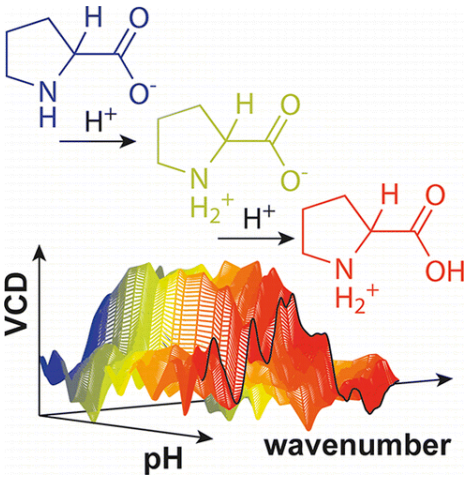
Studying dynamic processes in chiral solutions by quantum cascade laser-based vibrational circular dichroism

Vibrational circular dichroism (VCD) is not only a method of choice for the determination of the absolute configuration but also a very sensitive probe for conformational changes or other dynamic processes in solutions of chiral molecules. Due to the high number of characteristic bands VCD spectra are perfectly suited to be evaluated by multivariate methods and/or global fitting. However, such VCD studies are rare and they are generally hampered by the background absorbance of solvent in the infrared.

As a model dynamic process in solution we chose the pH-titration of l-proline and sequentially recorded VCD spectra using a pump-through flow cell setup. To overcome the high background absorbance of water we used a previously developed VCD-instrument equipped with a quantum cascade laser (QCL) as a high output power light source. On the 3D data (VCD spectra against pH) we performed global fitting of a 2-pK-Henderson−Hasselbalch model. The analysis allowed for extrapolation to pure spectra of fully deprotonated and protonated l-proline. Because full deprotonation and full protonation are only possible at extreme pH, such data is not easily accessible from static experiments. A similar experimental design could as well be useful for studies on other chiral dynamic systems, such as pH- or temperature-dependent conformational equilibria or the time-dependent monitoring of chemical reactions.



Host: Melanie Schnell - CFEL Molecular Physics seminar