Exploring conformational dynamics in molecular beams

Understanding the energy pathways that molecules take when passing from one conformation to another could give us an insight into the elusive mechanism of protein folding. It is thus important to understand this dynamics at the very basic level. For this, we are studying simple model systems, like, for instance, aminoacids and weakly bound complexes free of environmental influence in the gas phase.
The conformational dynamics can be triggered by external perturbations, such as excitation by light or collisions. The influence of collisions on conformational distributions is investigated for the benzene-dimer complex. There, it is observed that even very low energy collisions with rare gas atoms can have a profound influence on the structures and a generally applicable model is discussed. In order to investigate aminoacids, these involatile molecules are brought into the gas phase using IR-laser desorption. Their specific conformations are studied via IR-UV double-resonance laser spectroscopy in supersonic molecular beams as well as complementary quantum chemical computations. If a selected conformer is excited by IR photons early in the supersonic expansion, it can isomerize and its population can be collisionally redistributed among other conformers present in the molecular beam. The experimental aspects of the detection and manipulation of different molecular conformations will be exemplified by preliminary results on an IR-laser induced population transfer among phenylalanine conformers.