CFEL SCIENCE

SEMINAR

3rd June 2021 - 10:00 h Zoom virtual meeting

https://desy.zoom.us/j/91202137161 (Meeting-ID: 912 0213 7161, Password: 845021)

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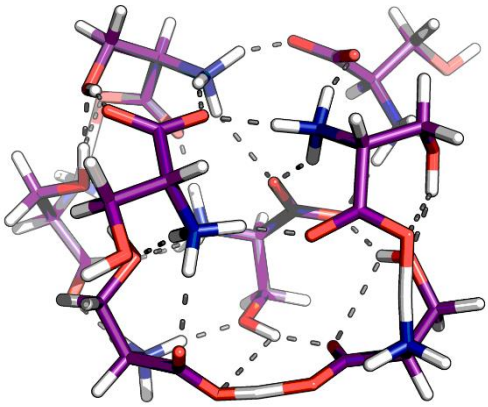
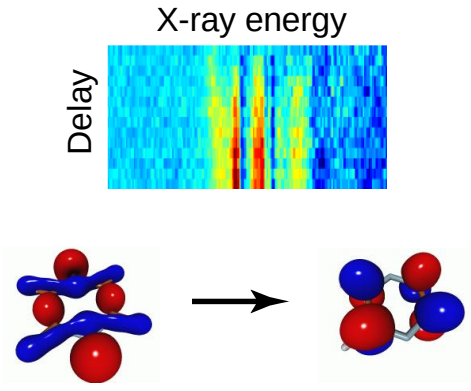
Infrared and soft X-ray probes of structure and dynamics

The amino acid serine is long known to form a protonated “magic-number” cluster containing eight monomer units that shows an unusually high abundance in mass spectra and has a remarkable homochiral preference. We present the structure of Ser_8H^+ determined by a combination of infrared spectroscopy and *ab initio* molecular dynamics simulations. The three-dimensional structure that we determine is ~25 kcal·mol^{-1} more stable than the previous most stable published structure and explains both the homochiral preference and the experimentally observed facile replacement of two serine units.

In the second part, dynamics in UV-excited pyrazine are tracked with soft X-rays in a table-top setup. The participation of the optically dark ^1A_u ($n\pi^*$) state is assigned by a combination of experimental X-ray core-to-valence spectroscopy, electronic structure calculations, and nonadiabatic dynamics simulations. The ^1A_u ($n\pi^*$) state is populated in 200±50 femtoseconds after electronic excitation and plays a key role in the relaxation of pyrazine to the ground state.





Host: Melanie Schnell / CFEL Molecular and Ultrafast Science Seminar