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DESY Building 25 f, Room 456

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Eigenstate resolving electronic spectroscopy: a straightforward approach to structures and dynamics of excited states

Intrinsic properties of large isolated molecules can be investigated by eigenstate resolving electronic spectroscopy. The rotationally resolved spectra even of medium sized flexible molecules are generally quite congested due to the existence of various conformers, which often spectrally overlap.

The spectral discrimination of conformers by their center frequency due to different zero-point energies or electronic effects is one of the most important benefits of this method compared to other, higher resolving techniques like microwave spectroscopy.

Direct evaluation of the molecular parameters using line position assigned fits are in most cases difficult or impossible. Automated fits without the need for manual quantum number assignments using Genetic or Evolutionary Algorithms have been shown to be very successful in these cases. Information about vibronic coupling between higher vibronic states is contained in the intensities of individual rovibronic transitions and can be used for a more thorough understanding of photophysical processes at high energies.

Applications of the method in order to unravel the mystery why properties of electronically excited states of some flexible molecules are extremely sensitive to the conformation, while others are not, will be given. The limitations and prospects of the method will be discussed.