

IRTG TUTORIAL SERIES
How to convert, display and analyse (optical) spectra
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Optical Spectroscopy of Functional Nanosystems
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Optical spectra of (in)organic functional materials provide a wealth of information. Examples are spectral shifts due to a change in 'solvent', an increase in linewidth when going from a highly ordered, crystalline environment to a disordered, amorphous environment; the vibronic progression present in most spectra of organic molecules provides information about the energies of vibrations coupling to electronic transitions and the relative intensities yield the coupling strength. In supramolecular systems the changes in optical spectra upon self-assembly are indicative of the mutual arrangement of molecules (H-, J-aggregates) as well as about disorder present in aggregates. To retrieve this information, however, spectra must be appropriately converted and presented.

Here, I will briefly repeat quantum mechanical expressions that describe optical transitions in molecules. To connect quantum-mechanical properties of molecules to measurable quantities we will discuss, which quantities are actually measured in an experiment, and which transformations are required to make this connection correctly. Since spectra are often (essentially always) recorded as function of wavelength, but we are mostly interested in energy differences, the Jacobian transformation will be introduced as well. All transformations together can strongly change the shape and position of spectra, which is important to realise if spectra are to be analysed quantitatively.

Finally, I will discuss some examples to highlight which information can be retrieved from (changes in) optical spectra of functional organic molecules.

Please **bring your laptop** to the tutorials!!
The tutorials take place

Thursday, 20 th July:	9.15 to 10.45 am	S74 (NWII)
Friday, 21 st July:	9.15 to 10.45 am	S74 (NWII)

or remotely via zoom:

<https://uni-bayreuth.zoom.us/j/63364766941?pwd=VjJ1dkIyVjRxZlZLcTdUZU1jdTJzUT09>
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