Karlsruhe Institute of Technology

Tritium Laboratory Karlsruhe

B.Th/ M.Th

Development of spectral fitting software

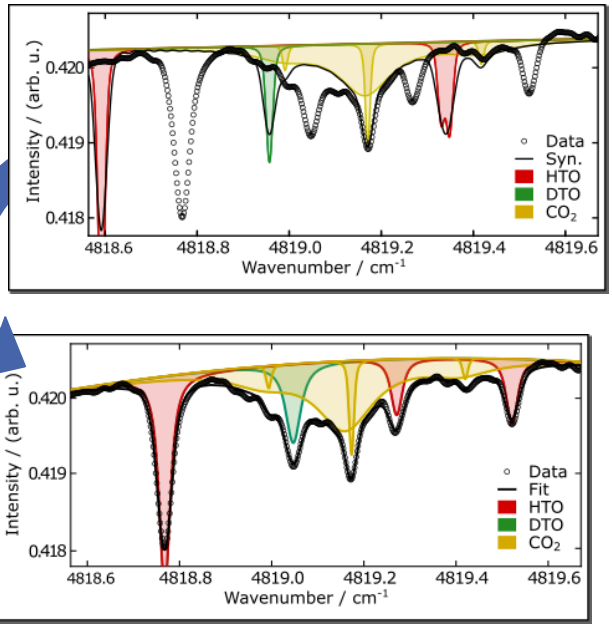
Motivation

Exchanging the hydrogen with tritium (^{3}H) in molecules (e.g. water, ammonia and methane) drastically influences the rotational and vibrational energy structure in the molecule. Therefore, high-resolution infrared spectra of so-called *tritiated* molecules allow for fundamental tests to quantify these isotope shift and symmetry breaking effects.

However, as precise theoretical predictions are not available a versatile spectral fitting tool needs to be developed. This software will be key to future fundamental research programs at TLK!

Your task

- Learn from existing python-software
- Develop your own software to fit Fourier transform infrared spectroscopy (FTIR) spectra
- Learn about Molecular Spectroscopy
- Implement quantum-mechanical models for the rotational and vibrational states for efficient fitting (opt.)
- Implement machine learning methods (opt.)
- Test software with real spectra, validate your results
- Analyse data of tritiated methane spectra (opt.)



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