

Raman spectroscopy at the TOFTOF instrument

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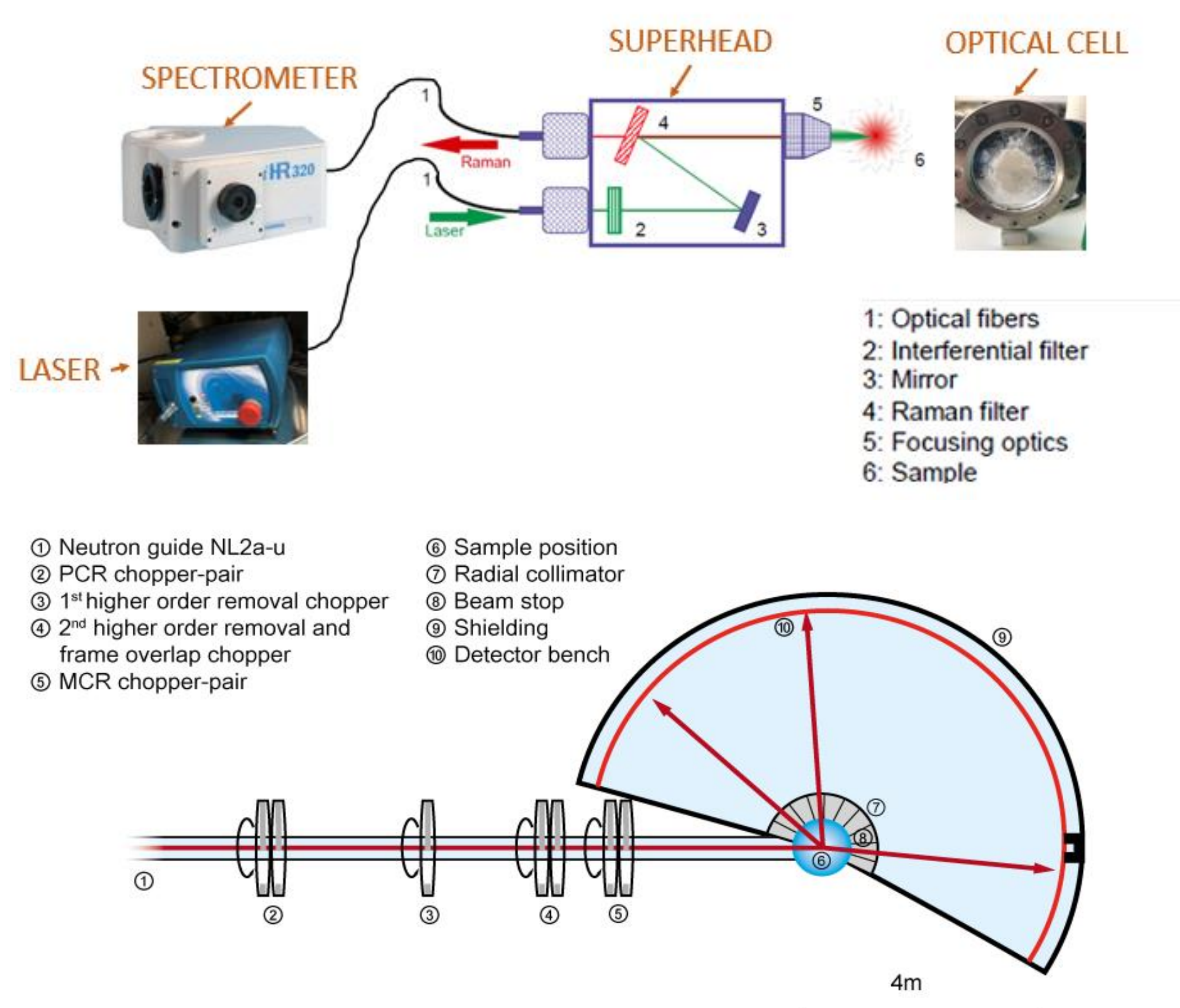
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Introduction

Performing Raman and neutron spectroscopy at the same time under same conditions is useful in order to investigate the sample in unchanged environment. Difference in the environment can lead to differences in the spectra.

To widen the spectral range to covalent bond vibrations a Raman spectrometer was introduced recently to the TOFTOF instrument. Simultaneous neutron and Raman spectroscopy is very powerful to measure sample dynamics of different scale at once. For example, for hydrogen storage samples, like $Mg(NH_2)_2$ or $LiBH_4$, this means that the hydrogen motion is measured in the environment of neighboring atoms and molecules with quasielastic neutron scattering (QENS) and inelastic neutron scattering (INS) and at the same time the sample is probed for chemical reactions with Raman spectroscopy.

Setup Description



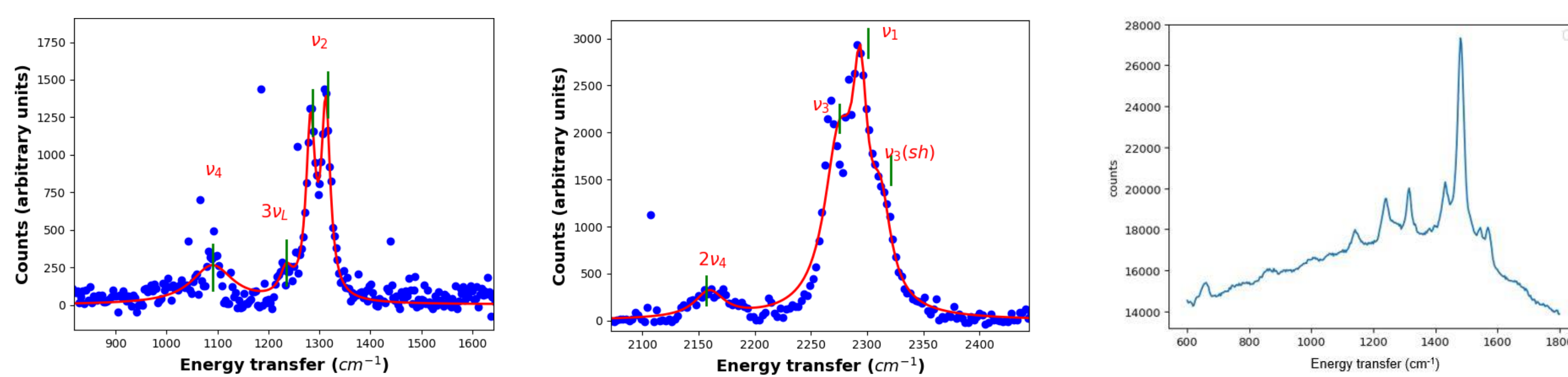
The Raman setup consists of:

- Laser (785 nm) and Control Unit (IPS IO785SHOO9OB-IS-TH-L)
- Spectrometer (Horiba iHR 320 and Sincerity CCD Detection System J810050),
- Camera and Shutter Unit (Horiba SDrive-500)
- Superhead
- Mirror and Lens System
- Sample

The TOFTOF setup consists of:

- Neutron guide
- Choppers
- Ionization chamber
- Sample and sample holder
- Radial collimator
- Flight chamber
- Detectors
- Beam stop

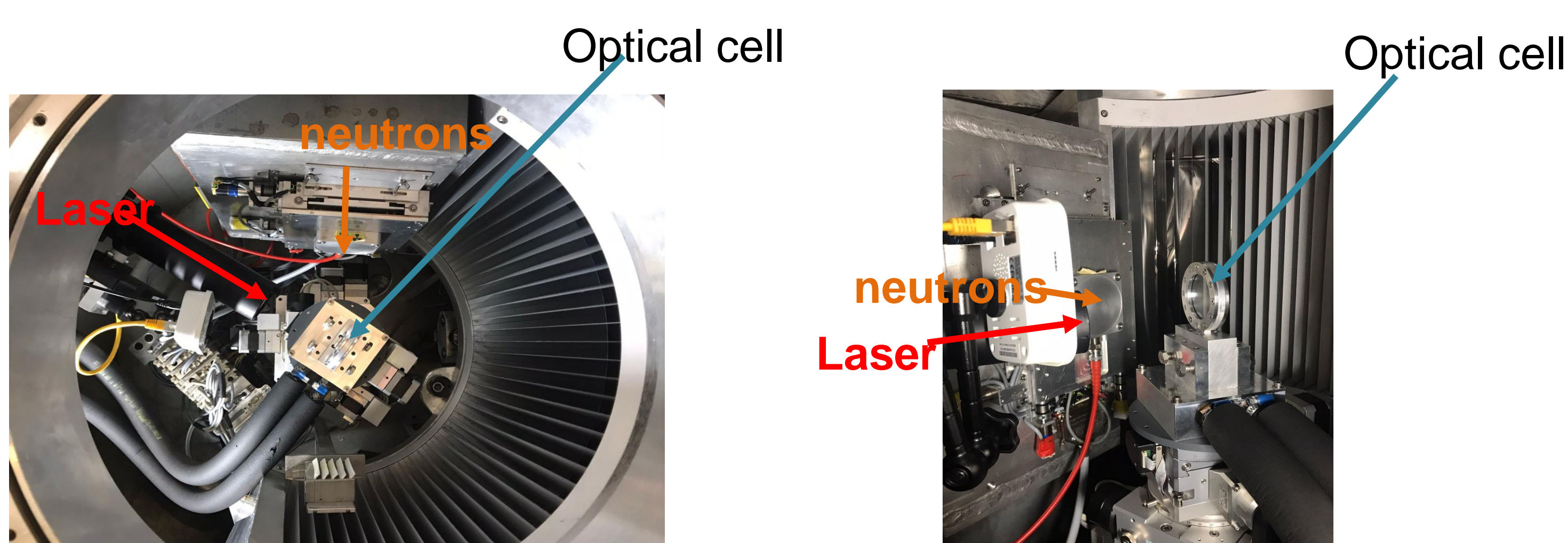
First Results



Test of the raman spectrometer with $LiBH_4$:

- Successful measurement of the molecular vibrations
- Bending and stretching modes fits to literature

Next steps



- Installation of Raman setup into TOFTOF
- Alignment of the Raman beam to the neutron beam
- Characterization of the temperature profile of the sample cell
- Combined in-situ Raman and neutron spectroscopy

Scientific Applications and References

In-situ Measurement of

- Aqueous liquids
- Measurement of non-polar groups and carbon bonds
- Chemical reactions
- Stability of proteins and polymers
- Lattice vibrations (internal and external)
- Phase transitions

1) <https://www.horiba.com/deu/automotive/products/detail/action/show/Product/raman-fiber-probes-1674/>

2) <https://www.horiba.com/pl/scientific/products/optical-spectroscopy/detectors/scientific-cameras-for-spectroscopy-cdd-ingaas-emccd/ccds/details/ihr320-imaging-spectrometer-198/>

3) https://en.wikipedia.org/wiki/Optical_spectrometer