Python plug-ins for advanced data processing with TopSpin NMR software

Studentský projekt

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TopSpin is a piece of software for controlling Bruker nuclear magnetic resonance (NMR) spectrometers and handling NMR data. In recent versions of TopSpin, a Python programming interface was added, thus enabling the data handling with all the power of Scientific Python on the spot. In this call we invite a motivated bachelor student, with programming skills, to implement a few advanced data processing algorithms in Python using the new TopSpin Python API so as to provide the users of our NMR laboratory at Matematicko-fyzikální fakulta in Troja, as well as NMR practitioners elsewhere, with an extended TopSpin functionality.

The current project will include three tasks:

1) *Improved spectral baseline correction*. It is designed to be a two-step procedure consisting of classification of baseline points and their interpolation, both steps implying interactive parameter optimization.
2) *Symmetrization of quadrupolar MAS spectra*. Magical-angle-spinning (MAS) sidebands in quadrupolar NMR spectra (see Figure) are often lacking in the symmetry inherent to first-order quadrupolar interactions. One proper way to fix it is to localize the pairs of opposite sidebands and replace them with their average intensities.
3) *Building rotor-synchronized spectra from arbitrarily sampled NMR signals*. This means picking rotary echoes from a signal acquired in a conventional MAS NMR experiment, which relies on periodic pattern recognition algorithm and the accuracy of signal period measurements.

The resulting programs will start a TopSpin Python plug-ins library with the possibility of further publication, depending on code quality. Some of the relevant algorithms have been already implemented as stand-alone Python scripts by the *vedoucí* but not necessarily in their best way. The student is thus welcome to bring forth his/her ideas how to improve that, as well as to propose new numerical recipes for the existing and emerging problems.

<u>Further reading:</u> Python Programming in TopSpin – a user manual by Bruker BioSpin (2021)