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Polarisation analysis of QENS on per-deuterated proteins.

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Deuterated samples are used in neutron scattering to investigate the dynamics of hydrogen atoms by contrast matching, due to the low incoherent and high coherent cross-sections of deuterium. The use of fully deuterated proteins has been restricted so far to the study of light hydration water or the collective dynamics of proteins in D_2 O.

In order to study kinetic isotope effects of the internal dynamics of proteins, we produced two D_2 O hydrated powders : a protonated Green-Fluorescent Protein and its deuterated counterpart with 99% H \rightarrow D labelling. We recently performed QENS experiments combined with polarisation analysis on LET, ISIS, on the usual space range probed with proteins (r \in [2.5Å^, 20Å]) and at the pico-second time scale corresponding to structural relaxation. Polarisation analysis enables to separate the coherent and the incoherent parts of scattering. Unexpectedly, it shatters the usual assumption that neutrons probe mainly collective dynamics in fully-deuterated proteins.

We came across the conclusion that in this space region, where the structural pattern is weakly dependent on the size or the secondary structure of the proteins, the magnitude of the coherent contribution of scattering is fairly lower than the incoherent one. It is verified at both very low (T=2K) and high (T=310K) temperatures and compared to non-polarized experiments on IN5, ILL.

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