Experimental report

21/04/2022

Proposal: **EASY-881** **Council:** 10/2020

Title: Density of states and EINS of protonated and deuterated GFP in view of an analysis including quantum effects

Research area: Biology

This proposal is a new proposal

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Experimental team:

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Samples: pGFP

Instrument	Requested days	Allocated days	From	To
IN1	8	8	03/10/2021	04/10/2021

Abstract:

There is a growing number of indications that quantum mechanics might play a role for the functioning of certain biomolecules, as for instance through tunnelling effects or quantum entanglement. As quantum effects depend on the mass of the scatterer, their signature should be detectable when comparing a protonated protein with its per-deuterated counterpart. We use both versions of GFP powders (already disposable).

We propose to record the density of states at low temperature over a broad energy domain to permit data analysis within a newly developed approach taking into account quantum effects. Former analysis on IN5 displayed bad resolution results over 150 meV, which unabled us to investigate all internal motions and normalise our data.

We will measure the general densities of states on IN1 Lagrange up to 300 meV, at a temperature of 2.5 K using a displex for cooling. Thus we will have complementary results to our Panther experiment, in term of energy and Q range (this proposal is already accepted for next beamtime). We ask for 4 hours of measurement per sample (2 of them), and 4 hours for the corrections (empty cell and vanadium), in total 1 day of beamtime for Lagrange.

Preliminary Report on LAGRANGE, EASY-881

Nidriche Agathe, Peters Judith

EASY-881 experiment is an easy access experiment on LAGRANGE that lasted about a day in total. The purpose was to acquire Inelastic Neutron Scattering at high energy transfers ω up to 400 meV, in order to spot vibrationnal discrepancies between two proteins, one fully deuterated and the other one not, to search for mass effects that could lead to evidence of quantum effects occuring at this scale.

This experiment was performed on protonated and deuterated powders of Green Fluorescent Proteins , both hydrated at 40% in D_2O. Vanadium, empty cell, Cadmium and both samples intensities were acquired for a few hours from 22 to 400 meV, at 2K with the use of a displex.

Despite the non ideal shape of flat empty cell to carry the sample (Lagrange is fitted for cylindrical sample holders), the data acquired displays, as expected, quite important differences between both protonated and deuterated sample.

Analysis is planned to be performed to the light of Gainaru et Al 2014 article [1], estimating the impact of quantum tunneling over classical over-barrier crossing thanks to the large isotope effect observable in water vibrationnal density of states. Effects are expected to be smaller with proteins which are much more complex systems.

Also as expected, the intensity spectrum of dGFP is less intense due to an incoherent contribution that is reduced because of deuteration. Careful analysis of the data must be performed to understand what stems from water and what stems from the protein in the dGFP sample intensities.

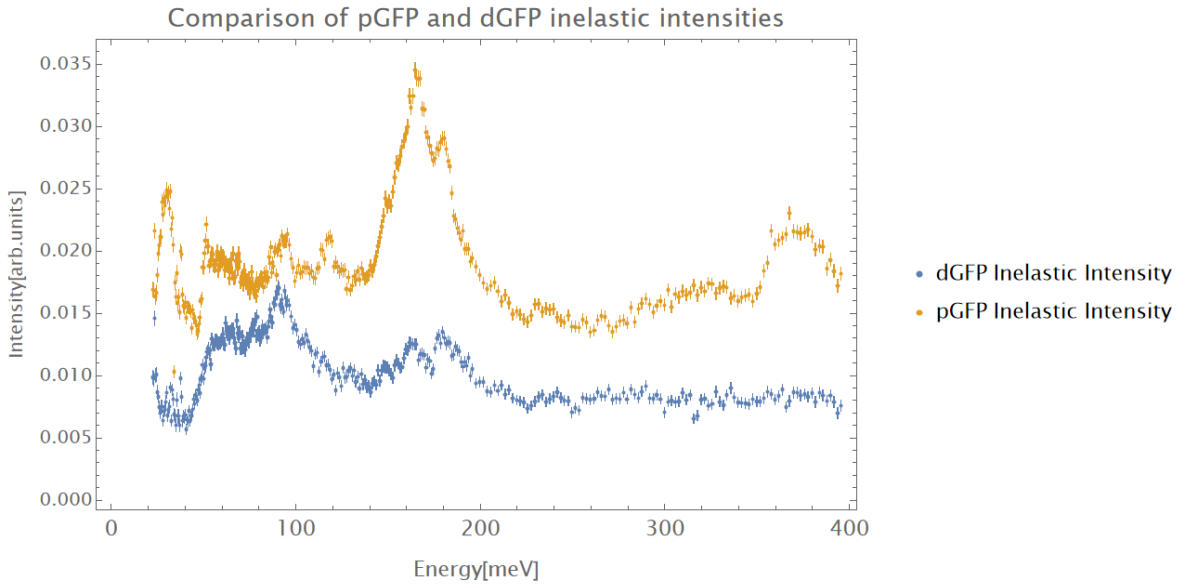

Figure 1 : Comparison of inelastic intensities of pGFP and Dgfp..

[1] Gainaru, C., Agapov, A. L., Fuentes-Landete, V., Amann-Winkel, K., Nelson, H., Köster, K. W., Kolesnikov, A. I., Novikov, V. N., Richert, R., Böhmer, R., Loerting, T., & Sokolov, A. P. (2014). Anomalously large isotope effect in the glass transition of water. In Proceedings of the National Academy of Sciences (Vol. 111, Issue 49, pp. 17402–17407). Proceedings of the National Academy of Sciences. https://doi.org/10.1073/pnas.1411620111