Experimental report

13/04/2021

Proposal: TEST-3137 **Council:** 4/2020

Title: Investigating the interaction ofnoble gases with C60 cage.INS of 3He@C60 and 4He@C60

Research area:

This proposal is a new proposal

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Stephane ROLS

Local contacts: Stephane ROLS

Samples: C60
3He@C60
4He@C60

Instrument	Requested days	Allocated days	From	To
PANTHER	2	2	16/09/2020	21/09/2020
			10/03/2021	11/03/2021

Abstract:

Experimental Report: Test-3137

Mohamed Aouane

31/03/2021

Title: Investigating the interaction of noble gases with C_{60} cage. INS of $^3He@C_{60}$
Instrument: PANTHER
Experimental Team: S. Rols - M. Aouane
Date of Experiment: 08/03/2021 to 09/03/2021

1 Introduction

Endofullerenes are supramolecular complexes, each of which consists of a small atom/molecule enclosed by a fullerene (in this case a C_{60}) cage. Endofullerenes offer an ideal particle in a box setting to observe translational quantization, which leads to energy levels sensitive to the interaction potential between the trapped atom/molecule and the cage where it's trapped, giving a perfect probe into non-bonded interactions. The goal of this experiment was to observe transitions of arising purely from the atomic translational quantization modes due to the confinement in a nearly spherical cage of the ^3He and from the energy level structure a derivation of the confining potential for the complex should be feasible

2 Samples

For this experiment, the following samples were used at a temperature around 2K:

- $^3He@C_{60}$: Around 1047mg with a filling factor around 45%
- C_{60}: Mass matching blank fullerene
- E_i used: 19, 40, 60 and 130 meV

The filling factor refers to the percent of ^3He filled cages versus the total cages in the sample, made with the molecular surgery method. Both samples were in powder form and wrapped in an Al foil.

3 Experiment

The INS experiment were conducted at 2K and for the different incident energies in order to exploit the large C_{60} band gap and observe as many translational modes coming from the ^{3}He atom before the C_{60} vibrational modes start appearing around 33 meV. This is done in order to see if the system behaves like a particle in a box, a harmonic oscillator or a model that lies in between *e.g.* an anharmonic oscillator. In order to correct the effects of the C_{60} and the Al foil used as a sample holder as much as possible, the following measurements were done at each energy mentioned previously:

- ^{3}He@C_{60} runs
- Blank C_{60} runs
- Empty Al foil runs
- Vanadium run

The Al foil contribution was subtracted from the sample runs and data was normalized to vanadium.

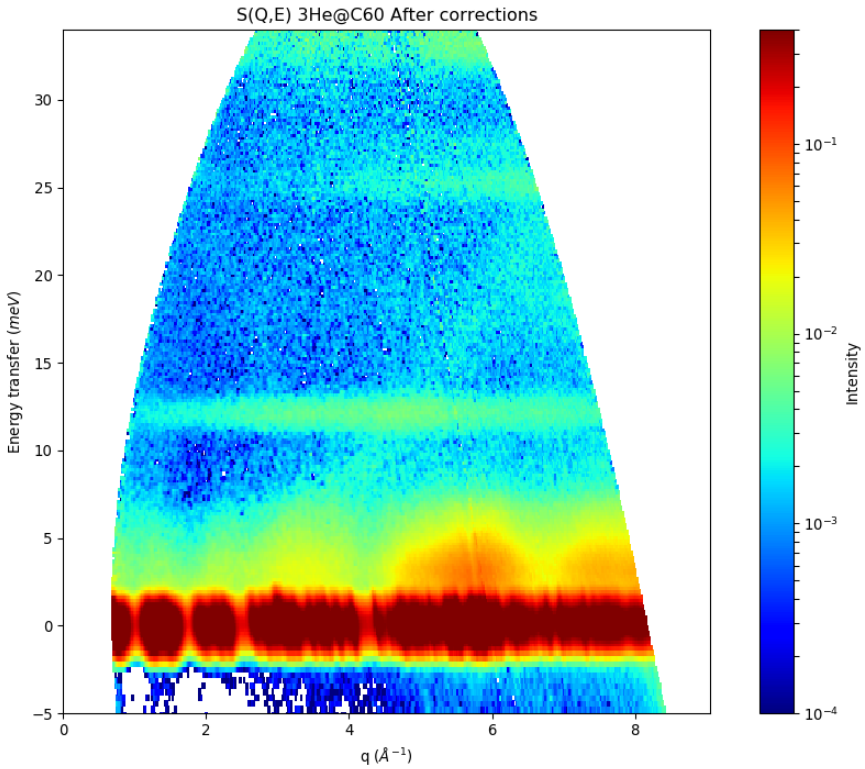

Figure 1: The S(Q,E) obtained for ^{3}He@C_{60} at 40meV

In this report only the 40 meV results will be shown since it's the ones where transitions coming from the ^{3}He atom are observed clearly without much loss in resolution.
In Fig[1], after corrections, a first transition is observed around 12 meV, corresponding to the first transition from the ground state to the first excited state for ^{3}He@C_{60} alongside a doublet around 25/27 meV corresponding to a transition from the ground state to the second excited states which is split in this case, showing that there is some anharmonicity in the potential allowing a symmetry breaking. In order to see the transitions more clearly (Notably the doublet) Fig[2] shows the plot obtained when grouping all detectors for both the ^{3}He@C_{60} sample and the blank fullerene cage.

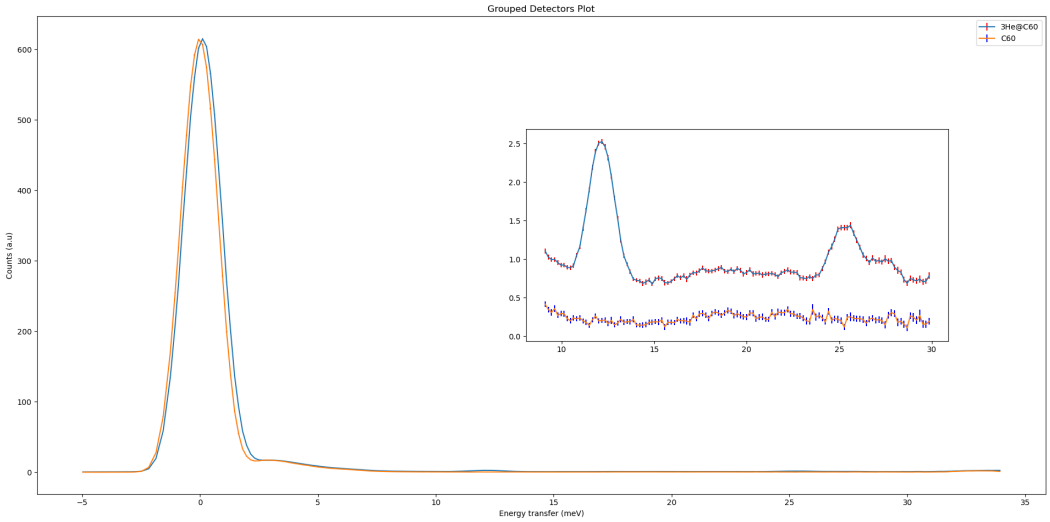

Figure 2: The grouped detectors plot

In Fig[2], the elastic peaks of both samples measured were re-scaled to be at approximately the same height. The inset of the graph shows the transitions mentioned in Fig[1], the first transition 12 meV and around 25/27 meV the doublet corresponding to the split energy level represented in Fig[1] with a Gaussian that has a first peak at 25 meV and a shoulder that appears at 27 meV.
These preliminary results on PANTHER show that the idea of an anharmonic oscillator model is a good start.