

Experimental report

06/03/2024

Proposal: 6-05-1044

Council: 4/2021

Title: Neutron scattering experiment on non-linear optical materials

Research area: Other...

This proposal is a continuation of 6-05-1019

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Samples: [(PhSn)4S6], Ph=Phenyl (C6H5)
[(MeSn)4S6], Me=Methyl (CH3)

Instrument	Requested days	Allocated days	From	To
D4	2	2	13/04/2023	15/04/2023

Abstract:

Recently a new class of molecular materials has been found which exhibits strong non-linear optical effects: Irradiating the sample with a low power IR Laser produces a broad and continuous light spectrum covering the visible regime. This emitted white light is highly directional and has a brilliance comparable to a Laser. The origin of this effect is, as of yet, unknown. This White-Light Emission (WLE) only occurs in amorphous samples while in a crystalline state these materials exhibit the well known Second Harmonics Generation (SHG) effect. These observations suggest that the WLE effect is linked to the amorphous structure. We propose neutron diffraction experiments to gain information on the structural cause of the WLE effect.

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This was a continuation from experiment 6-05-1019. The following samples were measured including the first experiment: (1) $[(\text{NpSn})_4\text{S}_6]$, (2) $[(\text{CpSn})_4\text{S}_6]$, (3) $[(\text{PhSn})_4\text{S}_6]$, (4) C_2Cl_4 and (5) $\text{C}_3\text{Cl}_6\text{O}$.

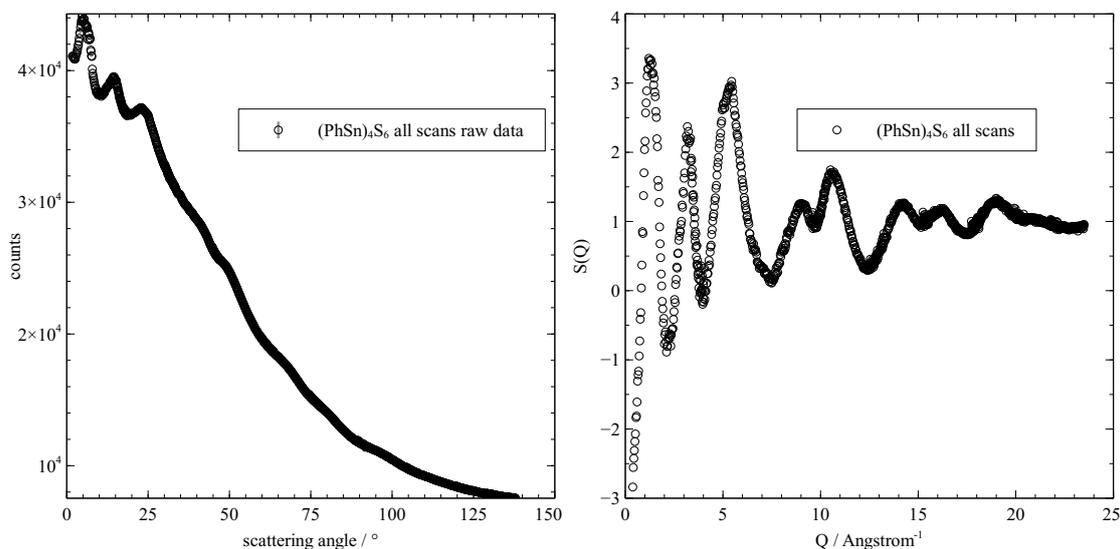


Figure 1: Data for sample (3). Left is raw data showing tremendous incoherent scattering contributions from hydrogen. Right shows the structure factor $S(Q)$ that was extracted from this data.

The first experiment took place in 2020 and due to difficulties with suppliers of deuterated chemicals as well as the more complicated synthesis routes using deuterated educts we were not able to bring all desired samples. Samples (1) and (2) were measured that time but it quickly became clear, that deuteration was not 100% successful so that an unknown H/D ratio made correction of incoherent scattering contributions difficult. Similar difficulties concerning sample preparation were still present during the preparation of experiment 6-05-1044 in 2021 and when it became clear that our cooperation partners performing the synthesis would not be able to deliver this time as well we contacted the beamline staff to first delay and later cancel the experiment. We were pleasantly surprised, but surprised nonetheless, when in 2023 we received information that the beamtime for this experiment would be scheduled. Given the good results from the previous

experiment we decided to use non-deuterated samples (2) and (3) this time to avoid the synthesis problems and were allowed to bring chlorated solvents (4) and (5) as backup samples for another project which did not require much measurement time. Figure 1 shows the data gathered for sample (3). Despite not deuterating the sample the data correction expertise of the beamline staff allowed us to extract a sensible structure factor. Figure 2 shows a comparison between the data gathered for sample (2) in 2020 (partly-deuterated) and 2023 (non-deuterated). For this sample we therefore now have H/D substitution contrast data which will hopefully be useful though the non-deuterated data will be useful regardless.

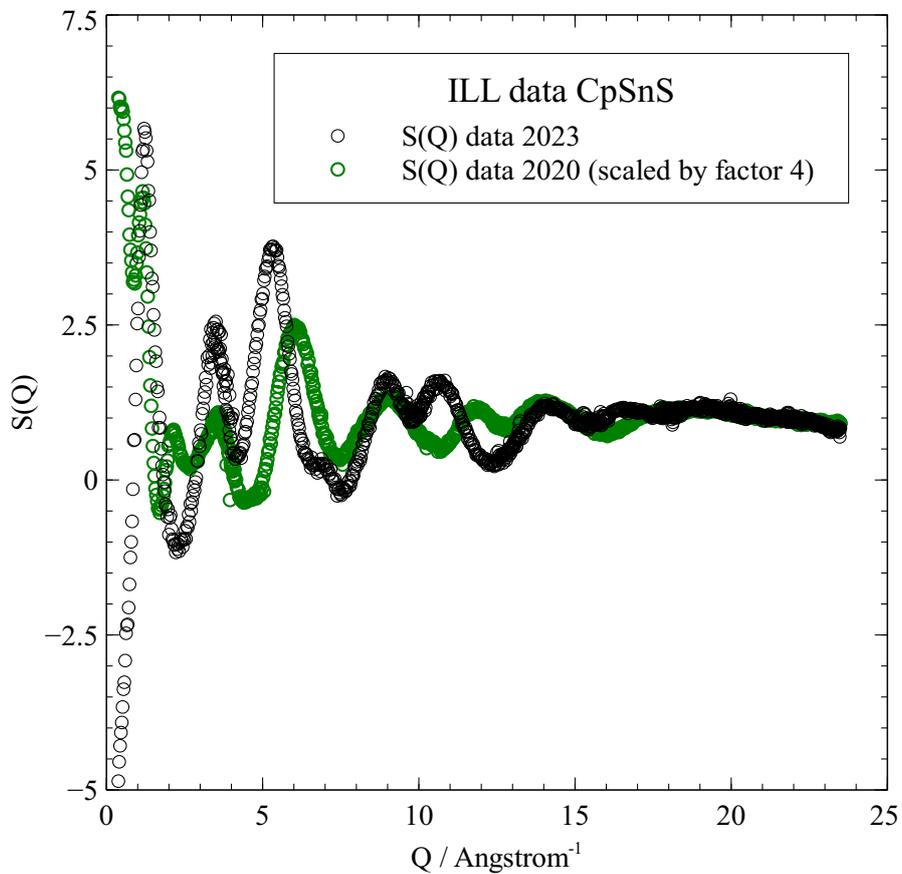


Figure 2: Structure factors $S(Q)$ for sample (2) extracted from partly deuterated material in 2020 compared to the non-deuterated material from this experiment.