Experimental report

06/02/2020

Proposal: 7-02-184 **Council:** 10/2018

Title: Studying the motion of TEA cationsin the dielectric material TEA(TCNQ)2 using quasi-elastic neutron scattering

Research area: Materials

This proposal is a new proposal

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Samples: Triethylammonium bis-7,7,8,8-tetracyanoquinodimethane

Instrument	Requested days	Allocated days	From	To
IN13	11	6	25/07/2019	31/07/2019

Abstract:

We wish to perform a detailed study of the elastic incoherent structure factor for the organic magneto-electric material triethylammonium bis-7,7,8,8-tetracyanoquinodimethane (TEA(TCNQ)2). This material shows some very interesting behaviour within the capacitance and dielectric loss, where anomalies occur at two temperatures; 220 and 120 K. The lower temperature is related to the freezing out of magnetic fluctuations as the sample enters an ordered magnetic state. The high temperature transition is related to the freezing of the TEA cation, where above 220 K, the TEA cation is randomly fluctuating. Below 220 K the TEA cations freeze into a static state, accompanied by a large dielectric anomaly, but there is relatively little information regarding this. We want to perform QENS measurements to pin down the behaviour of the TEA cation to answer questions on how the cations jump and re-orientate themselves.

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Dr Adam Berlie

$TEA(TCNQ)_2$ shows some interesting behaviour; it does not undergo a true Peierls or SP distortion as the 1D TCNQ stacks decrease in distance as the temperature is lowered. At 220 K, the TEA cations also freeze, where above this one the TEA molecules flip between orientations. We have previously shown that this systems shows two dielectric anomalies; one at this order disorder transition and another at 120 K, where the systems enters a magnetic singlet ground state. We have performed QENS measurements to fully understand what the TEA cation does and these have been extremely fruitful (see Fig 1). We have used IN13 and conducted fixed window scans on the elastic line to study the motion of the TEA cations. We have found that there are two processes that enter the measurement time scale; one around 100 K, which we believe to be methyl group rotation, and another at 200 K, which we believe is related to the molecule flipping over a radius of 1.7 Å. QENS measurements have provided an estimate of the activation energy for this process of ~ 1000 K, where we are currently analysing QENS data from both IRIS and IN13 to get out more information on the timescales of the two different processes.

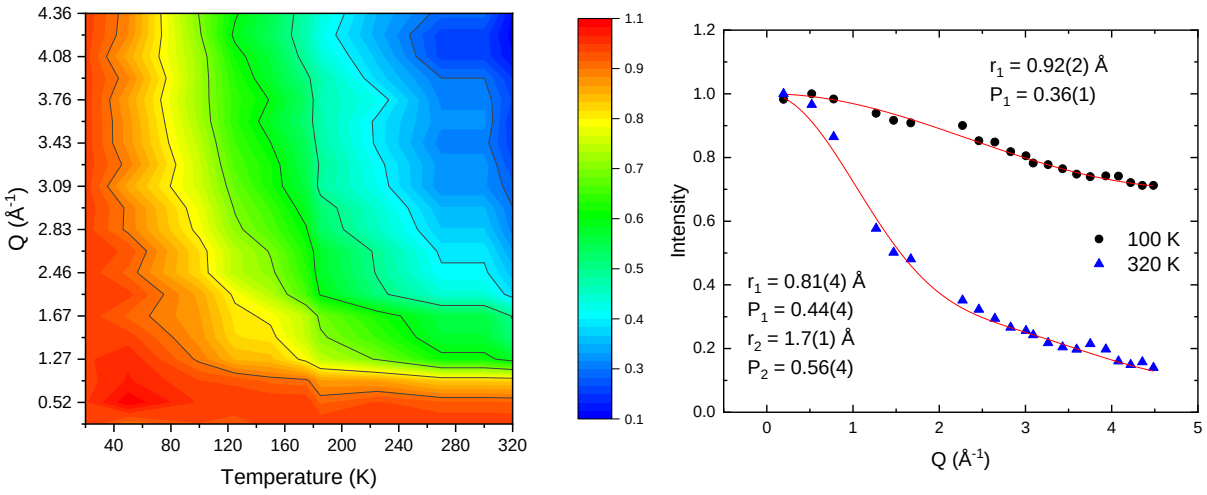

Figure 1: Elastic fixed window scan from IN13 where the left graph shows a contour plot of the data over a wide temperature range and the right graph shows two selected temperatures with representative fits to the EISF.