

Poster Presentations

[MS41-P05] To deuterate or not to deuterate? That is the question

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Accepted wisdom when performing powder diffraction experiments with neutrons is to deuterate the sample, wherever possible, as collecting data from the hydrogenous analogue is complicated by the large incoherent scattering background contribution from hydrogen. However, current generation high-flux, medium-resolution continuous wavelength (CW) instruments can overcome this background problem. [1-5] Here, I present the case for not deuterating materials as, with proper optimisation procedures for the instrument set-up, data collection strategy and correction techniques, it is possible to investigate a wide range of systems. Details will be given to the ongoing project to study the incoherent scattering cross section of H as a function of incident neutron wavelength and the effects on the measured data. The lack of an in-depth study to accurately quantify its variation with wavelength in diffraction is surprising, as it is the largest contributing factor to the absorption coefficient that is used in both single-crystal and powder neutron diffraction experiments to calculate the optimal absorption correction and sample size for hydrogen containing compounds. The practical effect is that the attenuation of the neutron beam (both incident and scattered) by the sample changes as a function of neutron wavelength and path length through the sample, with striking implications for quantitative analysis of time-of-flight (t-o-f) neutron data. The aim is to collect the necessary information to implement an empirical correction routine for CW and t-o-f data as a function of wavelength in the thermal neutron range. This correction will allow a significant number of users to perform routine data collections on hydrogenous materials

without the need for deuteration (and the often observed changes in properties upon deuteration) impacting directly research in technologically important fields such as proton conductors, fuel cells and pharmaceuticals.

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