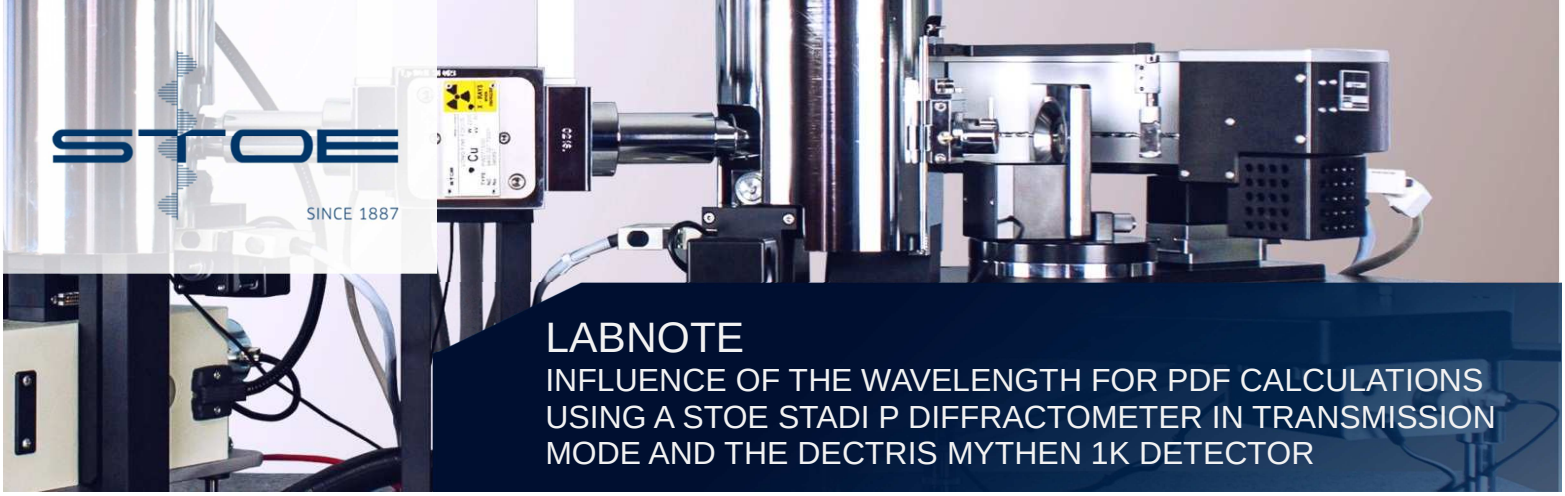

LABNOTE

INFLUENCE OF THE WAVELENGTH FOR PDF CALCULATIONS USING A STOE STADI P DIFFRACTOMETER IN TRANSMISSION MODE AND THE DECTRIS MYTHEN 1K DETECTOR

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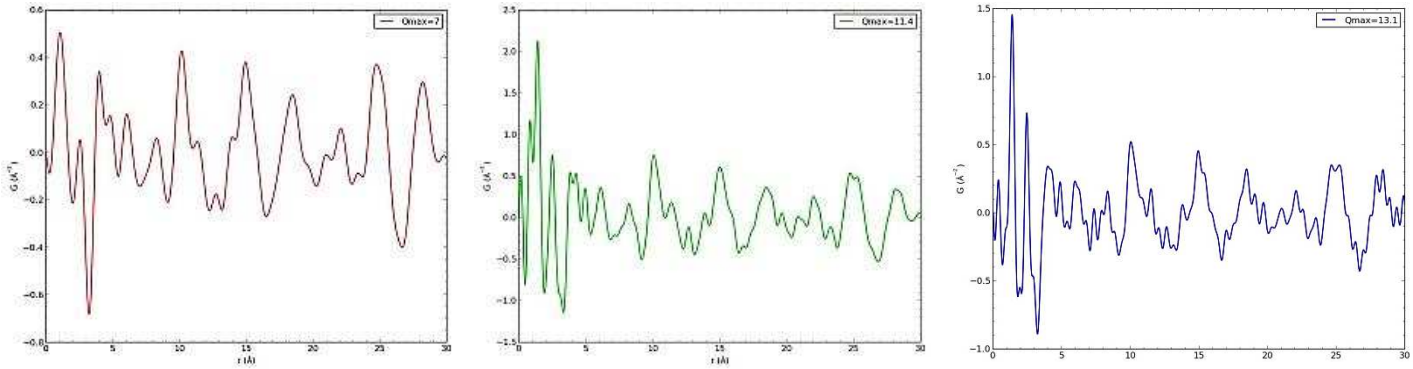
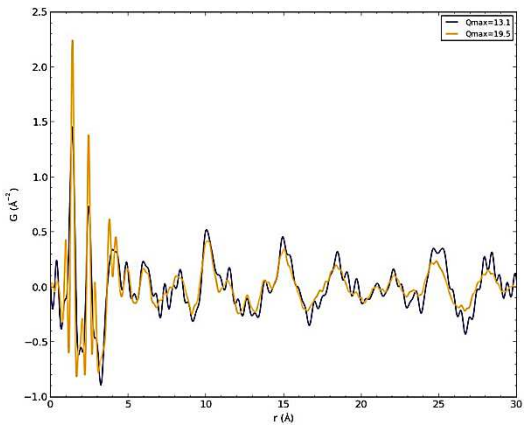
A Stoe Stadi P powder diffractometer with Ge(111) monochromator yielding pure $K_{\alpha 1}$-radiation and the Dectris MYTHEN 1K detector has been chosen for PDF calculation experiments on Naphtalen ($C_{10}H_8$).

For Cu $K_{\alpha 1}$-radiation the Stoe Stadi P has been equipped with a Dectris MYTHEN 1K with 320 µm, for Mo $K_{\alpha 1}$-radiation with a MYTHEN 1K with 450 µm and for Ag $K_{\alpha 1}$-radiation with a MYTHEN 1K with 1mm chip size. Synchrotron data has been taken at beamline X17A at NSLS Brookhaven (λ=0.1839Å). PDF calculations calculated with PDFgetX3 [1] yield a $Q_{(obs\ max)}$ of 7.0 $Å^{-1}$ for Cu-, 11.4 $Å^{-1}$ for Mo-, 13.1 $Å^{-1}$ for Ag-$K_{\alpha 1}$-radiation and 19.5 $Å^{-1}$ for the synchrotron.



G(r) for naphthalen measured with **Cu- (red)**, **Mo- (green)** and **Ag-radiation (blue)**

The direct comparison of the PDF curves of the synchrotron (yellow) and the Ag-$K_{\alpha 1}$- experiment (blue), shows that the resolution of the Ag-data is amazingly similar!



Comparison of the **laboratory setup (blue**) and the **synchrotron experiment (yellow)**

Taking into account that $\lambda_{(synchrotron)}$ has been app. ½ of Ag-$K_{\alpha 1}$, the measuring time (Ag-experiment 18h, synchrotron ½h) is more than reasonable for a laboratory setup.

This makes the Stoe Stadi P with Ag-tube and Dectris MYTHEN 1K an impressive alternative to expensive synchrotron experiments.

[1] Juhas, P., Davis, T., Farrow, C.L. and Billinge, S.J.L., *J. Appl. Cryst.* (2013). **46**, 560-566.