

Poster Presentations

[MS27-P05] Recent results in PDF calculations using a Stoe Stadi P with Ag $K\alpha_1$ -radiation and a Dectris MYTHEN 1K Detector

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Encouraged by observations of the influence of the wavelength and the detector technique using a Stoe Stadi P powder diffractometer in Transmission mode a combination of a Ag-tube, Ge(111)-monochromator yielding pure Ag $K\alpha_1$ -radiation (0.5594 Å) and the new Dectris MYTHEN 1K with 1mm chip size has been chosen to produce data for further PDF calculation experiments on Pigment Yellow 213⁽¹⁾ (C₂₃H₂₁O₉N₅).

An impressive comparison of $G(r)$ calculated with PDFgetX2⁽²⁾ from Data of Pigment Yellow 213 taken in this laboratory setup and from synchrotron data, beamline X17A, NSLS Brookhaven with a wavelength of 0.184 Å, yields a $Q(\text{calc. max})$ of 15 Å⁻¹ for the synchrotron and 13 Å⁻¹ for the laboratory data.

In addition, the same laboratory setup has been used for the investigation of the Jahn-Teller Distortion in different Pyridine Complexes of Copper Halides.

(1) Schmidt, M.U. et al., *Electron diffraction, X-Ray diffraction and pair-distribution-function analyses to determine the crystal structures of Pigment Yellow 213 C23H21N5O9*, Acta Cryst., Sect. B, (2009), **B65**, 189-199.

(2) Qiu, X., Thompson, J.W. and Billinge, S.J.L., *A GUI driven program to obtain the pair distribution function from X-Ray powder diffraction data*, J. Appl. Chem., (2004), **37**, 678.