YOUR PARTNER IN X-RAY DIFFRACTION

STOE since 1887

STOE news

November 2013

Welcome to the 1st issue of the STOE newsletter

We are so pleased to welcome you to the very first issue of the STOE newsletter.

We have a vibrant and loyal user community and we look forward to regularly sharing news about STOE, our products and the exciting scientific developments that we are involved in with you.

We would like to grow our community – so if you know of anyone who would enjoy being added to the distribution list, please let us know at newsletter@stoe.com.

Likewise, if we have you on our distribution list and you do not want to receive this newsletter, please send an email to newsletter@stoe.com for immediate removal.

We hope you find this newsletter useful and enjoyable!

Regards

Your STOE Team

STOE successfully completes shareholder and management succession

Following the retirement of Ms. Bärbel Dollmann (former Managing Director) in 2012, the shareholders of STOE set out to find a suitable long-term successor. The main criteria was:

- Finding a solution that would secure the independence of STOE
- Management of STOE should be „managing owners“, i.e. represented in the shareholder structure

Fulfilling these requirements, Martin Fark joined the leadership team in July 2013. He assumed the role as Co-CEO & CFO and became shareholder.

Martin Fark has a degree in industrial electrical engineering as well as an MBA and is responsible for managing STOE's Commercial Operations and Sales & Marketing.

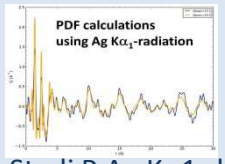
Jens Richter continues to head the scientific areas as Co-CEO & CTO. *"This succession secures that STOE is led with a great sense of ownership that keeps it as customer oriented as you have experienced STOE so far"* Jens Richter commented.

When asked about his first impressions, Martin Fark added *"I am impressed by the strong and loyal, customer base that STOE has build up over its long history. It's our obligation to keep this spirit alive while at the same time set STOE up for future growth."*

Jens Richter and Martin Fark, now heading STOEs scientific and commercial operations

Welcome to the 1st issue of the STOE newsletter...1

STOE successfully completes shareholder and management succession.....1



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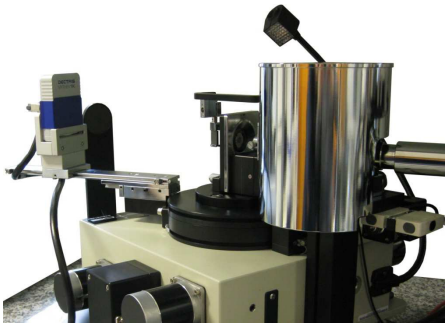
STOE news

Stadi P Ag Kα1-data – a real alternative to expensive synchrotron PDF experiments

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 Naphthalen (C10H8) and Pigment Yellow 213[1] ($C_{23}H_{21}O_9N_5$).



For Cu $K\alpha_1$-radiation the STOE Stadi P has been equipped with a Dectris MYTHEN 1K with 320µm, for Mo $K\alpha_1$-radiation with a MYTHEN 1K with 450µm 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.

Sealed in a 1.0 mm capillary, the samples have been measured on the STOE Stadi P diffractometer in three different ranges:

Range	$2\theta_{start}$ [°]	$2\theta_{end}$ [°]	step [°]	time [s]
1	0,00	53,00	1,00	150
2	40,00	90,00	1,00	300
3	85,00	125,0	1,00	600

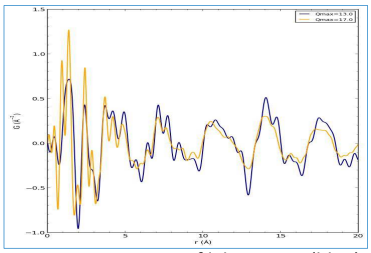
The ranges have been combined and normalized, PDF curves have been calculated using PDFgetX3[2].
The maximum theoretical Q value $Q_{(theo\ max)}$ can be directly calculated from $2\theta_{(max)}$ of the goniometer. For the Stadi P $Q_{(theo\ max)}$ could be 20 $Å^{-1}$ for Ag-$K\alpha_1$-radiation. Certainly, the maximum observed Q value $Q_{(obs\ max)}$ will be lower than the $Q_{(theo\ max)}$.

The comparison of the PDF-curves of Pigment Yellow 213 taken in the laboratory setup with Ag-$K\alpha_1$-radiation and from synchrotron data with a wave-length of 0.184 Å, yields a $Q_{(obs.\ max)}$ of 17 $Å^{-1}$ for the synchrotron (pic_1, blue curve) and 13 $Å^{-1}$ for the laboratory data (pic_1, yellow curve).
For the Naphthalen sample the Q values have been:

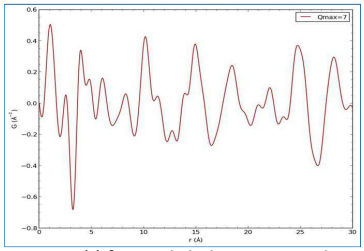
Wavelength [Å]	Q(r) [$Å^{-1}$]	Pic No.
Cu Ka_1 = 1,5406	7,0	2
Mo Ka_1 = 0,7093	11,4	3
Ag Ka_1 = 0,5594	13,1	4
Synchr. = 0,1839	19,5	

The direct comparison (pic_5) of the PDF curves of the synchrotron- (yellow) and the Ag-Ka_1- experiment (blue), shows that the resolution of the Ag-data is amazingly similar!
Taking into account that $I_{(synchrotron)}$ has been approximately ½ of Ag-Ka_1, the measuring time (Ag-experiment 18h, synchrotron ½h) is more than reasonable for this laboratory setup making the Stadi P with Ag-tube and Dectris MYTHEN 1K an impressive alternative to expensive synchrotron experiments.

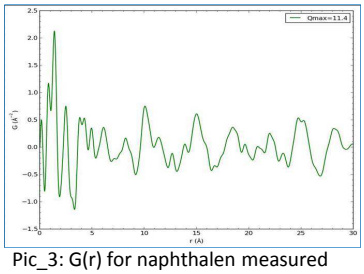
[1] Schmidt, M.U. et al., *Acta Cryst*. (2009).**B65**, 189-199.
[2] Juhas, P., Davis, T., Farrow, C.L. and Billinge, S.J.L., *J. Appl. Cryst*. (2013). **46**, 560-566.



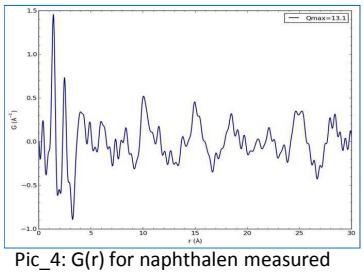
Pic_1: Comparison of laboratory- (blue) and synchrotron experiment (yellow)



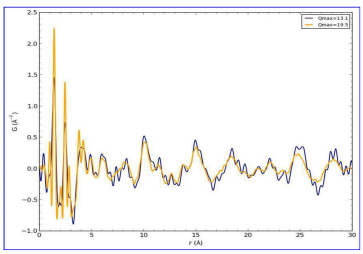
Pic_2: G(r) for naphthalen measured with Cu Ka_1



Pic_3: G(r) for naphthalen measured with Mo Ka_1



Pic_4: G(r) for naphthalen measured with Ag Ka_1



Pic_5: Comparison of the laboratory setup (blue) and the synchrotron experiment (yellow)

STOE news

STOE Powder XRD Users Meeting
What a success!

We were pleased to host the first STOE Powder XRD Users Meeting on September 5th and 6th at our facility in Darmstadt.

21 people from 5 countries participated in the meeting. These participants came from a range of Universities, Research Centers as well as the Pharmaceutical Industry and had a variety of backgrounds and experience in a wide range of techniques.

The meeting has proven to be a valuable event in which to exchange experiences and ideas with and among the participants.

A clear highlight was the presentation of the results of PDF calculations given by Dragica Podgorski from the group of Professor Schmidt, at Goethe University, in Frankfurt.

In addition to providing a forum for the exchange of excellent scientific content, it was our pleasure to host a backyard barbecue, with lot's of meat, local beer and fun! We will never forget the midnight factory tours.

We are still impressed by spirit of these events and we look forward to hosting our next user meeting.

Save the date:
STOE Single Chrystal
XRD Users Meeting
18. & 19. September 2014
in Darmstadt









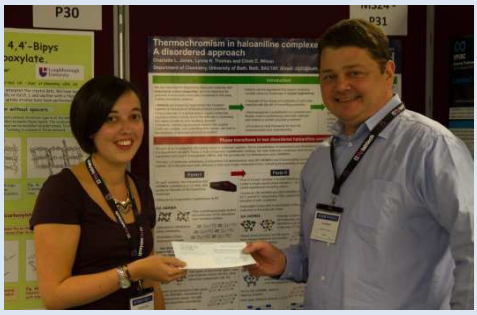


STOE news

Charlotte Jones receives STOE poster prize at ECM

Ms. Charlotte L. Jones, Dept. of Chemistry at University Bath, received the STOE poster prize in recognition for the best poster on functional materials presented by a student at ECM 28 in Warwick this year.

STOE is proud to be the sponsor of the award for her outstanding research.



Jens Richter congratulates Charlotte L. Jones at ECM 2013 in Warwick

STOE supports the International Year of Crystallography

Crystals – familiar to all in gemstones, glittering snowflakes or grains of salt – are everywhere in nature. The study of their inner structure and properties gives us our deepest insights into the arrangement of atoms in the solid state - insights that advance the sciences of chemistry, solid-state physics and, perhaps surprisingly, biology and medicine. A century has passed since crystals first yielded their secrets to X-rays. In that time, crystallography has become the very core of structural science, showing us the structure of DNA, allowing us to understand and fabricate computer memories, showing us how proteins are created in cells, and helping us to design powerful new materials and drugs.

That is why in July 2012 the General Assembly of the United Nations adopted the resolution that 2014 should be the International Year of Crystallography, 100 years since the award of the Nobel Prize for the discovery of X-ray diffraction by crystals.

STOE is proud to support the IUCr through a range of activities which will be presented at the opening Ceremony in Paris on January 20-21, 2014.

Meet STOE - Upcoming Events

December 2013
5.-7.: Tage der Seltenen Erden, Stuttgart, Germany

January 2014
20.-21.: Opening Ceremony International Year of Crystallography, Paris, France

March 2014
6.-8.: Hemdsärmelkolloquium, Köln, Germany

10.-11.: Chemiedozententagung, Paderborn, Germany

16.-20.: ACS National Meeting, Dallas, USA

17.-20.: DGK Annual, Berlin, Germany

April 2014
7.-10.: BCA Spring Meeting, Loughborough, UK

21.-25.: MRS Spring Meeting, San Francisco, California

May 2014
24.-28. ACA Annual Meeting, Albuquerque, USA

June 2014
15.-18.: EPDIC14, Aarhus, Denmark

July 2014
28.-1.8. Denver X-Ray Conference, Big Sky, USA

August 2014
5.-12.: IUCr Congress, Montréal, Canada

September 2014
18.-19.: STOE Single Crystal User Meeting, Darmstadt, Germany

Imprint

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