



## methods of high-pressure single-crystal x-ray diffraction



Satellite workshop of the 27<sup>th</sup> European Crystallographic Meeting (ECM)

**Bergen (Norway), August 4-5, 2012**

Welcome to the workshop "Methods of high-pressure single-crystal diffraction" held from the 4th to the 5th of August in Bergen (Norway) immediately before the 27th European Crystallographic Meeting. This is the second edition of the workshop after the one held in Darmstadt during the 26th European Crystallographic Meeting in 2010.

Single-crystal diffraction provides the most accurate structural data on the compression mechanisms of solids. Its methods for high-pressure studies developed over the last three decades are mature and easy to use in both the laboratory and at synchrotron sources. The aim of this workshop is to demonstrate how to perform single-crystal high-pressure x-ray diffraction measurements in diamond anvil cells using home-laboratory and synchrotron facilities, to complete the data reduction and analysis, and to obtain the highest quality data. The workshop will include both lectures and hands-on exercises. It will be suitable for researchers at all levels.

Experience in single-crystal X-ray diffraction will be assumed, but no previous experience in high-pressure methods is necessary. Participants who have already collected high-pressure data are encouraged to bring their own problematic datasets for discussion and analysis. Different data processing strategies and programs will be presented. The workshop will be interactive through informal discussions on specific interests and the afternoon sessions.

We would like to acknowledge the sponsors of the workshop whose logos are shown below for their generous support which has enabled us to keep costs down and support some student travel.

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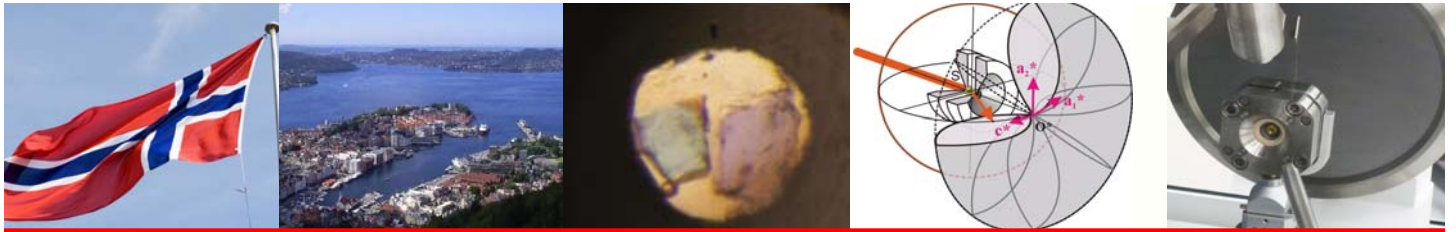
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## Topics and programme

Introduction and overview  
Types of diamond anvil cells and loading  
Data collection procedures  
Equations of state  
Integration of high-pressure single-crystal data  
Integration sessions: software fayre  
High-pressure single-crystal diffraction at synchrotron sources  
Intensity corrections  
Structure refinement: methods & tricks  
Structure validation  
Corrections and refinement: software fayre

**Location:** Science Building of the University of Bergen

**Workshop Fee:** 80 € (senior participants) / 40 € (students)

The number of workshop participants is limited to 50. A small number of student bursaries will be available: applications, including a CV and a recommendation letter from the supervisor, should be sent to grzechnik@xtal.rwth-aachen.de.

**Registration is through the webpage** <http://ecm27.ecanews.org>

**Speakers:**

- David Allan (Diamond Light Source, United Kingdom)
- Ross J. Angel (Padova, Italy)
- Tiziana Boffa-Ballaran (Bayreuth, Germany)
- Karen Friese (Jülich, Germany)
- Andrzej Grzechnik (Aachen, Germany)
- Michael Hanfland (European Synchrotron Radiation Facility, France)
- Clivia Hejny (Innsbruck, Austria)
- Ronald Miletich (Vienna, Austria)
- Michael Probert (Durham, United Kingdom)

**Convenors:** Karen Friese & Tonci Balic-Zunic

**Programme:** Ross J. Angel & Tiziana Boffa-Ballaran

**Organising Committee:** Karl Törnroos (local), Andrzej Grzechnik, Clivia Hejny & Ronald Miletich



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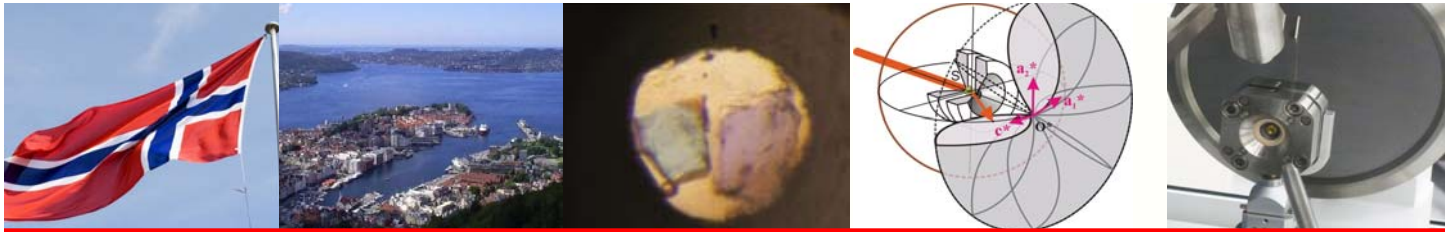
## Programme

### Day 1

08:00-08:30	Registration
08:30-08:40	K. Friese, <i>Welcome</i>
08:40-09:00	R.J. Angel, <i>Overview</i>
09:00-10:00	R. Miletich, <i>Types of DACs and how to load them</i>
10:00-10:30	Coffee Break
10:30-11:45	C. Hejny, <i>Data collection procedures</i>
11:45-12:30	T. Boffa-Ballaran, <i>Equations of state</i>
12:30-13:45	Lunch
13:45-14:30	R.J. Angel, A. Grzechnik, <i>Indexing and integration overview</i>

## Afternoon Parallel Sessions

14:30-18:00	R. Miletich, <i>DAC demonstration</i>	
14:30-15:30	A. Grzechnik, K. Friese, <i>Integration with Stoe software</i>	M. Probert, <i>Integration with Bruker software</i>
15:30-16:30	C. Hejny, <i>Integration with Crystalis</i>	All speakers: <i>Open session on Integration</i>
16:30-17:00	Coffee Break	
17:00-18:00	R.J. Angel, <i>Integration for point detectors</i>	A. Grzechnik, K. Friese, <i>Integration with XDS</i>
18:00	Close	
19:00	Workshop dinner	



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## Programme

### Day 2

08:30-09:00	D.R. Allan, <i>How to perform HP single-crystal diffraction at Diamond</i>
09:00-09:30	M. Hanfland, <i>How to perform HP single-crystal diffraction at ESRF</i>
09:30-09:45	<i>Discussion</i>
09:45-10:30	R.J. Angel, <i>Absorption and other intensity corrections</i>
10:30-11:00	Coffee Break
11:00-11:30	<i>General discussion, requests for afternoon sessions</i>
11:30-12:30	K. Friese, <i>Refinements to high-pressure data</i>
12:30-13:30	Lunch

## Afternoon Parallel Sessions

13:30-14:30	R.J. Angel, <i>Absorption corrections with Absorb</i>	<i>Open sessions and problem solving</i>
14:30-15:30	K. Friese, A. Grzechnik, <i>H.P. refinement, mostly Jana2006</i>	<i>Open sessions and problem solving</i>
15:30-16:00	Coffee Break	
16:00-17:00	T. Boffa-Ballaran, <i>Fitting equations of state (EoSfit)</i>	R.J. Angel, <i>Post-refinement parametric data handling</i>
17:00-17:30	<i>General discussion.</i>	