



## 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**

We would like to invite you 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 a software fayre.

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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](mailto: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)
- Tonci Balic-Zunic (Copenhagen, Denmark)
- 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)

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

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

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