

August 6-11 2012 Bergen Norway

# 27th European Crystallographic Meeting



PROGRAMME



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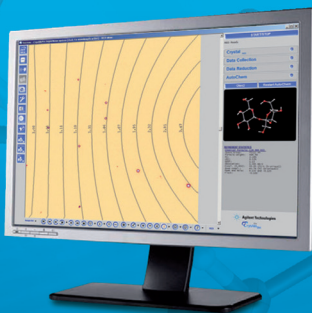
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**Agilent Technologies**

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## Welcome to the ECM 27



The Twenty Seventh European Crystallographic Meeting will be held in Bergen, organized by the Norwegian Crystallographers in August 2012. This will be an excellent opportunity to meet again at the European level, after the XXII IUCr meeting in Madrid, and following the ECM26 held in Darmstadt. We welcome to Bergen all crystallographers and scientist related to Crystallography and Crystal Growth to share with us scientific views on the new achievements of crystallography and Crystal Growth on its many facets. This is also an excellent opportunity to strengthen the links with the IUCr and the Regional Associations AsCa and ACA.

The Program Committee has organized a rich scientific program of Microsymposia and Keynote Lectures to show the growing scientific leadership of the ECA Special Interest Groups and the transversality and networking activity of the General Interest Groups. At the ECM27 there will be commemorations of the important centennial for Crystallography; the **Max Theodor Felix von Laue**, **Walter Friedrich** and **Paul Knipping** seminal experiments achieved by European Crystallographers. The 2011 Nobel Prize in chemistry has been awarded to Professor **Dan Shechtman** for his discovery of quasicrystals and a special symposium on quasicrystals is organized with five invited speaker giving an overview of state of the art researches carried out in the field of quasicrystals. Danny himself will of course also give a plenary talk on his work. The meeting will provide good opportunities to show the strength and leadership of European Crystallography and his connection with society, all being the preamble of 2014 International Year of Crystallography. The UN General Assembly decided to proclaim 2014 the International Year of Crystallography, on June 15 2012. The award ceremonies for the European Crystallographic Association Prizes, sixth Max Perutz, awarded by Prof. Hartmut Fuess, and the fifth Erwin Felix Lewy Bertaut, given to Dr. Pavel V. Afonine, will take place also at the ECM27.

Another important component of the meeting is the ECA Council where the councilors from 33 National Members get together with the three Individual Members representative and the Corporate Associate Members representative to review the work of the Association, elect members of the new Executive Committee and confirm the place for next ECMs.

I have had the opportunity to meet with the Norwegian organizers and visit the beautiful conference venue in Bergen. From these experiences I can tell you that our Norwegian hosts have done everything to make the European Crystallographic Meeting a success and make you feel at home in Bergen, so you can enjoy both the science at the Congress and the charm and beauty of the city and all the Nordic Coast.

So everything is in place for a successful, well attended and well organized, European Crystallographic Meeting, and I am happy to know that you are one of the many who accepted this invitation from the Norwegian Crystallographers to attend the ECM27. I look forward to greet many crystallographers from all parts of the world in Bergen the 6th of August, to start celebrating the Laue Centennial.

**Santiago García-Granda**

President

European Crystallographic Association

**Karl Wilhelm Törnroos**

Chairman of the ECM27

**Carl Henrik Görbitz**

Co-chairman of the ECM27



# Organisation and Committees

## Date

6–11 August 2012

## Conference venue

The Grieg Hall  
Edvard Griegs Plass 1  
5015 Bergen, Norway  
[www.grieghallen.no](http://www.grieghallen.no)

## Scientific organisation

European Crystallographic Association (ECA)  
[www.ecanews.org](http://www.ecanews.org)

## Conference chair

Prof. Dr. Karl Wilhelm Törnroos  
Department of Chemistry  
University of Bergen  
Allégaten 41  
5007 Bergen, Norway  
[karl.tornroos@uib.no](mailto:karl.tornroos@uib.no)

## Conference co-chair

Prof. Dr. Carl Henrik Görbitz  
Department of Chemistry  
University of Oslo  
P.O.Box 1033 Blindern  
0315 Oslo  
[c.h.gorbitz@kjemi.uio.no](mailto:c.h.gorbitz@kjemi.uio.no)

## Programme committee

Conference Secretary  
ECA President  
ECA Past President  
ECA Vice-President  
ECM Past Chair  
IUCr Executive Committee  
ECM28 Chairman

Carl Henrik Görbitz (Oslo/NO)  
Santiago Garcia-Granda (Oviedo/ES)  
John Richard Helliwell (Manchester/GB)  
Andreas Roodt (Bloemfontein/ZA)  
Hartmut Fuess (Darmstadt/DE)  
Elena Boldyreva (Novosibirsk/RU)  
Sandy Blake (Nottingham/UK)

### Focus areas representatives

FA 1 - Ute Krengel (Oslo/NO)

FA 2 - Dmitry Chernyshov (Grenoble/FR)

FA 3 - Xiadong Zou (Stockholm/SE)

FA 4 - Andrew Bond (Odense/DK)

FA 5 - Martin Lutz (Utrecht/NL)

### Representatives of the Special Interest Groups

SIG 1 - Keith Wilson (York/GB)

SIG 2 - Piero Macchi (Bern/CH)

SIG 3 - Artem M. Abakumov (Antwerp/BE)

SIG 4 - Holger Klein (Grenoble/FR)

SIG 5 - Sergey Krivovichev (St.Petersburg/RU)

SIG 6 - Robert Cernik (Manchester/UK)

SIG 7 - Susan Bourne (Cape Town/ZA)

SIG 8 - Robert Cernik (Manchester/UK)

SIG 9 - Martin Lutz (Utrecht/NL)

SIG 11 - Karen Friese (Jülich/DE)

SIG 12 - Julien Haynes (Montpellier/FR)

SIG 13 - Paul Raithby (Bath/UK)

GIG1-YC - Laura Roces (Oviedo/ES)

GIG2-SC - Svend Erik Rasmussen (Aarhus/DK)

### Local organisation

Prof. Dr. Karl Wilhelm Törnroos (Bergen/NO)

Prof. Dr. Carl Henrik Görbitz (Oslo/NO)

Mr. André Bienfait (Bergen/NO)

Prof. Emeritus Dr. Steinar Husebye (Bergen/NO)

Prof. Emerita Dr. Jorunn Sletten (Bergen/NO)

### Conference bureau

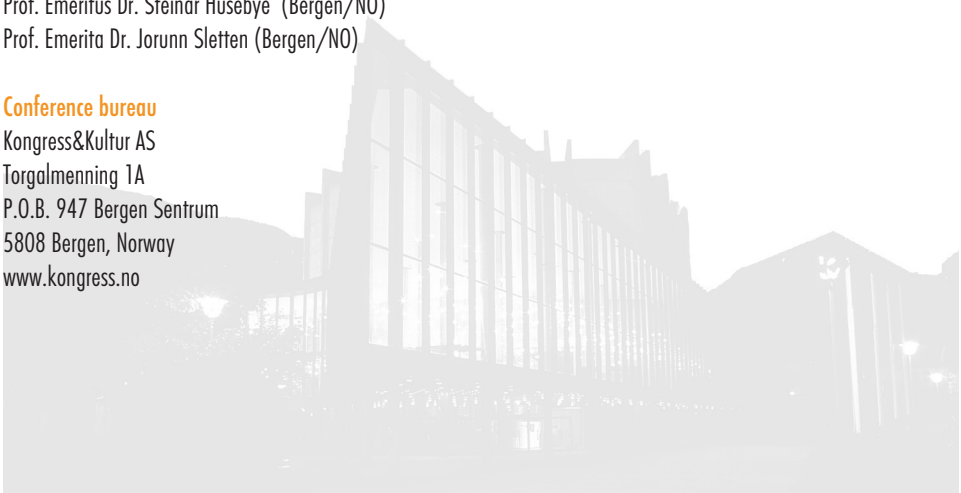
Kongress&Kultur AS

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P.O.B. 947 Bergen Sentrum

5808 Bergen, Norway

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## History of Bergen

The city of Bergen was founded in 1070 AD by Olav Kyrre, king of Norway. He was the son of King Harald Hårdråde who died in the famous battle of Stamford Bridge, Great Britain, in 1066. Olav Kyrre was 10<sup>th</sup> in line of Norwegian kings, and his reign was at a very peaceful time. His nickname Kyrre indeed means peaceful. Population growth, a flourishing trade and increasing papal interest in Norway contributed to the founding of the city.



Bergen, originally called Bjørgvin, started as a small settlement at the east and south shores of Vaagen, a small inlet from the Byfjord (City fjord). Later it spread to the west shore and to areas further south. Bergen is the geographical centre of western Norway. It has an excellent ice-free harbour sheltered from the North Sea by a chain of islands. It is surrounded by mountains and is called 'The city between the seven mountains'.

The thirteenth century was an important period in the history of Bergen. King Haakon Haakonsson made Bergen the capital of Norway and its dependencies Iceland, Greenland and many of the Scottish islands, in 1217. It replaced Trondheim, the first capital, and was itself replaced by Oslo in 1299. King Haakon's son, Magnus the lawmaker, modernized the laws of the country. Civil wars ravaged the city, but it was fortified and castles, monasteries and churches were built. Towards the end of that century Bergen became the city of the northernmost bureau of the Hanseatic League. Bergen was from the beginning an important trade centre and central harbour for western Norway. The Black Death plague in 1349 came to Norway from a foreign ship in the harbour of Bergen. It wiped out one third of Norway's population and was a severe setback also to Bergen.

Norway came under Danish rule towards the end of the fourteenth century. Then Bergen was the centre of trade for all of Norway. The most important trade was that involving dried cod from northern Norway. It was exported to the catholic countries of Europe in connection with the fast. The most important import was grain, clothing and spices. The Hanseatic merchants lived in their own separate quarter of the city, on the east shore of Vaagen, where they built their living quarters and large wharfs, enjoying exclusive trade privileges with the fishermen from the North of Norway. Today, Bergen's old quayside Bryggen where the Hanseatic traders lived, is on UNESCO's list as a World Heritage Site.

The city has been ravaged by many great fires through its history, mainly because of its wooden buildings and narrow streets. The oldest buildings standing today are churches and some of the buildings at the Bergenhus Fortress which are made of stone, among these are the Haakon's Hall from 1261 and the twelfth century St. Mary's church with its twin towers. This church is the oldest building in Bergen.

In 1536, the influence of the Hanseatic League was much reduced and the Saxon merchants were faced with two alternatives; either leave or become Norwegian citizens. Many choose to stay. However, Bergen retained its monopoly of trade with

northern Norway until 1789. For the Middle Ages and up to the 16th century, Bergen was one of the largest cities in the Nordic countries, and the largest city in Norway until the 1830's. After the Hanseatic League was dissolved in 1630, Bergen flourished and continued to be an important shipping and trading centre.

The last half of the 19th century was a period of rapid expansion of the city. In 1814 Norway entered a union with Sweden, dominated by the latter. When Norway left the union in 1905 to become an independent kingdom, the Prime Minister Christian Michelsen from Bergen, played a crucial role.

In the nineteenth and twentieth centuries disastrous fires, the last in 1916, led to reconstruction of the central parts of the city. Wider streets and open spaces were built to prevent fires from spreading. Shipping and a growing shipbuilding industry and textile mills contributed to the growth, however manufacturing industry never became of major importance. In 1909, the Bergen railway connecting Bergen with Oslo and the rest of the country was finished. This contributed greatly to the growth of Bergen as a trading and administrative centre.

While Norway kept out of World War I, the German occupation and allied bombings ravaged parts of the city during World War II. The late 1940's and the 1950's were a time of reconstruction. The merchant fleet was also rebuilt and greatly expanded during these years. When oil was found in the Norwegian sector of the North Sea in the 1970's, it was the start of a new era for western Norway. It resulted in a great expansion of many aspects of oil industry in and around Bergen, notably developments of drilling techniques for finding oil at great depths. Important research related to oil is going on in Bergen today, partly in collaboration with the university.

Today, Bergen is a fast growing modern city with one of Europe's largest harbours, known for its oil export facilities. It is the port with largest merchant fleet in Scandinavia. It also houses the main base of the Norwegian Navy. Tourism is also important. Flesland Airport, Bergen is the second busiest airport in Norway and Bergen is known as the 'Gateway to the Fjords'. It is the home harbour for the famous Hurtigruten, whose passenger ships leave Bergen daily for an eleven day round trip along the coast to Kirkenes near the Russian border and back. Bergen is also Norway's most important cruise ship destination. Bergen is the seat of the county of Hordaland and of the bishop of Bjørgvin, and has its own opera and theatre. It is also the city of the University of Bergen founded in 1946. It was originally based on the Bergen Museum where research had been going on since 1825. There are now some 14.000 students at the University. In addition there are several colleges with ca. 10.000 students, including the Norwegian College of Business Administration.

Today new suburbs are growing on the other side of the seven mountains surrounding Bergen. They are connected to the city centre by several road and train tunnels. Also some of the islands west of Bergen are connected to the mainland by large bridges and a fjord north of the city is crossed by a mile long floating bridge. Bergen is considered Norway's most international city. Surnames of German, Dutch and Scottish origin are plentiful, many originating from the Hanseatic era. The population of Bergen is now 265.000 and growing rapidly. In the metropolitan area the population is ca. 390.000.





## Programme overview • Monday, 6th August 2012

09:00 - 18:45 Exhibition mount

12:00 - 18:45 Registration

14:00 - 18:45 Preview Room open, 'Bøygen', no. 16 in venue map

18:45 - 20:00 ECM27 Opening (\*1) - Peer Gynt Hall (R1)

Laue Centennial Lecture **PL1** by Dieter Schwarzenbach: "Laue Centennial. The birth of X-ray diffraction."

20:00 - 21:00 City of Bergen Reception (registered participants only) - Exhibition Hall

\*1 Opening ceremony (ECA President/ECM27 Chair) Lecture by Dieter Schwarzenbach - R1, 18:45 - 20:00  
Followed by City of Bergen Reception in Exhibition Hall 20:00-21:00 (Registered participants only)



## Programme overview • Tuesday, 7th August 2012

08:30 - 09:30	<b>KN1 - R1</b> Jacqueline Cherfils			<b>KN2 - R2</b> Maryjane Tremayne			
Coffee Break 09:30 - 10:00							
10:00 - 12:00	<b>MS 1 - R1</b> Protein crystallization and sample preparation	<b>MS 15 - R2</b> Structural complexity of minerals and inorganic materials	<b>MS 3 - R3</b> Getting the best data from your crystal(s)	<b>MS 41 - R4</b> Dynamics in crystals: experimental techniques and software	<b>MS 39 - R5</b> Electron diffraction and X-ray powder diffraction: getting the best of both worlds	<b>MS 27 - R6</b> Molecular structures in catalysis and magnetism	
Lunch 12:00 - 13:30 (C1, C2[Agilent], C3)							
13:30 - 15:30	<b>MS 4 - R1</b> Phasing challenges. Bootstrapping from a poor start	<b>MS 13 - R2</b> Energy related materials	<b>MS 11 - R3</b> Frontiers in Structural Enzymology	<b>MS 25 - R4</b> Design, structure, and function of multi-component crystals	<b>MS 44 - R5</b> Controlling and Monitoring crystal growth and quality	<b>MS 21 - R6</b> Crystal chemistry of aperiodic crystals and frustrated systems	<b>(C4) - R7</b> Software Fayre 14:00 - 16:15
Poster session 1 with Coffee break 15:30 - 16:30							
16:30 - 17:30	<b>KN3 - R1</b> Olivier Mentré 16:30-17:30			<b>KN4 - R2</b> Paul Midgley 16:30-17:30			
Coffee Break with Sandwich 17:30 - 18:00							
<b>R1 - 18:00 - 19:30</b> Bertaut & Perutz Prize award ceremonies & lectures							

## Programme overview • Wednesday, 8th August 2012

08:30 – 09:30	<b>KN5 – R1</b> Henry Chapman			<b>KN6 – R2</b> Simon Parsons		
	Coffee Break 09:30 – 10:00					
10:00 – 12:00	<b>MS 2 – R1</b> MX at Synchrotron Sources, including X-FELs and time-resolved crystallography	<b>MS 26 – R2</b> Porous materials for gas storage and other applications	<b>MS 5 – R3</b> Advances in refinement and validation. Ligand chemistry	<b>MS 31 – R4</b> "How-to"	<b>MS 37 – R5</b> Electron Crystallography on functional materials	<b>MS 35 – R6</b> Ferroic and multiferroic materials
	Lunch 12:00 – 14:00 (C5, C6)					
14:00 – 16:00	<b>MS 8 – R1</b> Membrane proteins	<b>MS 23 – R2</b> Intermolecular interactions at ambient and extreme conditions	<b>MS 7 – R3</b> Pharmaceutical crystallography - Drug design: success and failures	<b>MS 22 – R4</b> Quasicrystals, their approximants and surfaces: from the atomic to the nanoscale	<b>MS 17 – R5</b> Structural and crystal-physical studies in large volume high-P devices	<b>MS 30 – R6</b> Buy one, get one free: Software for twin handling
	Poster session 1 with Coffee break 16:00 – 17:00					
17:00 – 18:00	<b>KN7 – R1</b> Jens Preben Morth 17:00-18:00			<b>KN8 – R2</b> Simone Techert 17:00-18:00		
Social 18:30	GIG1-Young Crystallographer Mixer 20:30 at Zafran restaurant (registered participants only) Sponsored by Dectris					

## Programme overview • Thursday, 9th August 2012

08:30 - 09:30	<b>KN9 - R1</b> Paola Gilli			<b>KN10 - R2</b> Ross Angel Sponsored by Agilent			
Coffee Break 09:30 - 10:00							
10:00 - 12:00	<b>MS 10 - R1</b> Infection and Disease	<b>MS 14 - R2</b> Materials in operando and in situ crystallography of materials	<b>MS 42 - R3</b> Big "small molecules" and small "macromolecules" - learning techniques from each other	<b>MS 18 - R4</b> New perspectives for charge density analysis: materials properties from inorganics to macromolecules	<b>MS 46 - R5</b> Advances in powder diffraction: structure solution and structure-property relationships	<b>MS 24 - R6</b> Bioinformatics informs MX	<b>(C7) - R7</b> Quasicrystal symposium'
Lunch 12:00 - 14:00 (C8[Bruker&Incoatec], C9)							
14:00 - 16:00	<b>MS 9 - R1</b> EM and MX for viruses, assemblies and biological nano-machines	<b>MS 43 - R2</b> Hot topics and structures in molecular chemistry	<b>MS 47 - R3</b> 3rd Generation Synchrotrons - Radiation Damage/ Impact on Crystals	<b>MS 50 - R4</b> X-ray or neutron optics and instrumentations	<b>MS 20 - R5</b> Probing crystal structures at the nanoscale by quantitative electron crystallography	<b>MS 34 - R6</b> Aperiodic, short-range ordered and non-crystalline materials at ambient and non-ambient conditions	<b>(C10) - R7</b> Software Fayre 14:00 - 16:15
Poster session 2 with Coffee break 16:00 - 17:00							
17:00 - 18:00	<b>KN11 - R2</b> Michael Rossmann 17:00-18:00			<b>KN12 - R2</b> Knut Urban 17:00-18:00			
Social	Conference dinner(*2) Fløien folkerestaurant (Registered participants only)						



## Programme overview • Friday, 10th August 2012

08:30 – 09:30	<b>KN13 – R1</b> Randy Read			<b>KN14 – R2</b> Mark Spackman		
Coffee Break 09:30 – 10:00						
10:00 – 12:00	<b>MS 6 – R1</b> Bioinformatics informs MX	<b>MS 12 – R2</b> Molecular recognition	<b>MS 49 – R3</b> Crystallographic teaching	<b>MS 40 – R4</b> Structure prediction for crystalline and amorphous molecular solids	<b>MS 38 – R5</b> Structure solution of minerals and inorganics by electron crystallography	<b>MS 36 – R6</b> Towards megabar pressures: complex and geo-materials
Lunch 12:00 – 13:30 (C11, C12)						
13:30 – 15:30	<b>MS 45 – R1</b> MX- Difficult problems and how to tackle them	<b>MS 16 – R2</b> Crystal chemistry and phase transitions in materials at non-ambient conditions	<b>MS 29 – R3</b> Likely to be useful: Statistical software packages	<b>MS 33 – R4</b> Neutrons and high-resolution X-ray diffraction for bio-crystallography	<b>MS 19 – R5</b> The importance of low temperature in charge density studies: history and future	<b>MS 32 – R6</b> Optimizing the use of Databases
Poster session 2 with Coffee break 15:30 – 16:30						
16:30 – 17:30	<b>KN15 – R1</b> Björn Winkler 16:30 – 17:30			<b>KN16 – R2</b> Neil Champness 16:30 – 17:30		
Pause 17:30 – 17:45						
Closing ceremony – R1 17:45 – 18:30 Poster prize awards						

- \*1 Opening ceremony (ECA President/ECM27 Chair) Lecture by Dieter Schwarzenbach – R1, 18:45 – 20:00  
Followed by City of Bergen Reception in Exhibition Hall 20:00-21:00 (Registered participants only)
- \*2 Conference dinner at ‘Fløien folkerestaurant’. Registered participants only.  
Participants must arrive at 19:30 using the Fløibanen funicular. Return ticket included.
  
- C1: ECA Council Meeting 1, 12:00-13:30 in R4. SIG’s meet in individual groups in R1 and R2.
- C2: Agilent Technologies Seminar 12:00 – 13:30 in R6.
- C3: GIG2-SC meeting 12:00 – 13:30 in R3.
- C4: Software Fayre 14:00 – 16:15 in R7.
- C5: ECA Programme Committee Meeting (closed) 12:00 – 14:00. SIG’s and IM’s meet in individual groups in R1 and R2.  
‘Glassrommet’, no. 10 in venue map (10 pax) available if needed.
- C6: IUCr Commission on Journals Meeting (closed) 12:00 – 14:00 in seminar room ‘Bukken’, no. 11 in venue map.
- C7: Quasi Crystal Symposium in Celebration of the 2011 Nobel Prize 10:00 – 12:00 in R7.  
Sponsored by The Nobel Committees for Physics and Chemistry, The Royal Swedish Academy of Sciences
- C8: Bruker & Incoatec Seminar 12:30 – 13:30 in R6.
- C9: ECA Council Meeting 2, 12:00 – 14:00 in R4.
- C10: Software Fayre 14:00 – 16:15 in R7.
- C11: ECA Council Meeting 3, 12:00 – 13:30 in R4.
- C12: GIG2-SC meeting 12:00 – 14:00 in R3.

Seminar room codes: R1: Peer Gynt  
R2: Scene  
R3: Trolldag  
R4: Klokkelklang  
R5: Gjendine  
R6: Nina  
R7: PG2



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25-29 August 2013



ECM  
28

DATE FOR YOUR DIARY

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## Scientific programme • Introduction

The scientific programme of ECM27 covers the following focus areas and fields of crystallography which are promoted by the programme committee as well as the Special Interest Groups (SIGs 1–13) and the General Interest Group (GIG 1).

### Focus Areas

- FA 1 Biological and macromolecular crystallography
- FA 2 Materials and minerals
- FA 3 Physical including fundamental crystallography
- FA 4 Chemical crystallography
- FA 5 Experimental and computational techniques

### Microsymposia (MS)

#### Focus Area 1 Biological and macromolecular crystallography

- MS 1 Protein crystallization and sample preparation
- MS 2 MX at Synchrotron Sources, including X-FELs and time-resolved crystallography
- MS 3 Getting the best data from your crystal(s)
- MS 4 Phasing challenges. Bootstrapping from a poor start
- MS 5 Advances in refinement and validation. Ligand chemistry
- MS 6 Bioinformatics informs MX
- MS 7 Pharmaceutical crystallography - Drug design: success and failures
- MS 8 Membrane proteins
- MS 9 EM and MX for viruses, assemblies and biological nano-machines
- MS 10 Infection and Disease
- MS 11 Frontiers in Structural Enzymology
- MS 12 Molecular recognition

#### Focus Area 2 Materials and Minerals

- MS 13 Energy related materials
- MS 14 Materials in operando and in situ crystallography of materials
- MS 15 Structural complexity of minerals and inorganic materials
- MS 16 Crystal chemistry and phase transitions in materials at non-ambient conditions
- MS 17 Structural and crystal-physical studies in large volume high-P devices

#### Focus Area 3 Physical including fundamental crystallography

- MS 18 New perspectives for charge density analysis: materials properties from inorganics to macromolecules
- MS 19 The importance of low temperature in charge density studies: history and future
- MS 20 Probing crystal structures at the nanoscale by quantitative electron crystallography
- MS 21 Crystal chemistry of aperiodic crystals and frustrated systems
- MS 22 Quasicrystals, their approximants and surfaces: from the atomic to the nanoscale

## Focus Area 4 Chemical crystallography

- MS 23 Intermolecular interactions at ambient and extreme conditions  
 MS 24 Polymorphism and chirality in molecular crystals  
 MS 25 Design, structure, and function of multi-component crystals  
 MS 26 Porous materials for gas storage and other applications  
 MS 27 Molecular structures in catalysis and magnetism

## Focus Area 5 Experimental and computational techniques

- MS 28 Imaging using diffraction, spectroscopy or coherent signals  
 MS 29 Likely to be useful: Statistical software packages  
 MS 30 Buy one, get one free: Software for twin handling  
 MS 50 X-ray or neutron optics and instrumentations

## General crystallography

- MS 31 "How-to"  
 MS 32 Optimizing the use of Databases  
 MS 48 Historical Aspects of Crystallography  
 MS 49 Crystallographic teaching

## Shared between two or three FA's

- MS 33 Neutrons and high-resolution X-ray diffraction for bio-crystallography  
 MS 34 Aperiodic, short-range ordered and non-crystalline materials at ambient and non-ambient conditions  
 MS 35 Ferroic and multiferroic materials  
 MS 36 Towards megabar pressures: complex and geo-materials  
 MS 37 Electron Crystallography on functional materials  
 MS 38 Structure solution of minerals and inorganics by electron crystallography  
 MS 39 Electron diffraction and X-ray powder diffraction: getting the best of both worlds  
 MS 40 Structure prediction for crystalline and amorphous molecular solids  
 MS 41 Dynamics in crystals: experimental techniques and software  
 MS 42 Big "small molecules" and small "macromolecules" - learning techniques from each other  
 MS 43 Hot topics and structures in molecular chemistry  
 MS 44 Controlling and Monitoring crystal growth and quality  
 MS 45 MX- Difficult problems and how to tackle them  
 MS 46 Advances in powder diffraction: structure solution and structure-property relationships  
 MS 47 3rd Generation Synchrotrons - Radiation Damage/Impact on Crystals

MS	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47
FA1	×									×			×		×
FA2		×	×	×	×	×								×	
FA3		×				×	×	×							
FA4	×							×	×	×	×				
FA5	×		×	×			×		×			×	×	×	
GIG								×			×	×		×	×

## Special Interest Groups

SIG 1	Macromolecular crystallography
SIG 2	Charge, spin & momentum density
SIG 3	Aperiodic crystals
SIG 4	Electron crystallography
SIG 5	Mineral and inorganic crystallography
SIG 6	Instrumentation & experimental techniques
SIG 7	Molecular interaction and recognition
SIG 8	Powder diffraction
SIG 9	Crystallographic computing
SIG 11	Crystallography under extreme conditions
SIG 12	Crystallography of functional materials
SIG 13	Molecular structure & chemical properties
GIG 1	Young Crystallographers

48 microsymbiosia (1-27, 29-47, 49-50) are organised with six sessions running parallel: in the mornings (10:00 – 12:00) and in the afternoons (13:30 – 15:30 Tuesday and Friday, 14:00-16:00 Wednesday and Thursday). In each microsymbiosium there are five lectures, 30+30 (invited lectures) and 20+20+20 (selected lectures) minutes long, respectively. You are kindly requested to carefully check the time table of each MS session. MS 28 has only posters, MS 48 (with two lectures) is arranged during lunch time Friday 10th, 12:00 – 13:30 in seminar room Trolldtog in conjunction with the founding meetings for a new general interest group for senior crystallographers, GIG2.

## Posters

A poster session is scheduled daily between 15:30 – 16:30 (on Tuesday and Friday) and 16:00 – 17:00 (on Wednesday and Thursday).

**Poster session 1 on Tuesday, 7th August and on Wednesday, 8th August:** odd numbers, e.g. MS1-P1

**Poster session 2 on Thursday, 9th August and on Friday, 10th August:** even numbers, e.g. MS1-P2

Poster boards have the same number as the abstract in the Programme Book. On the presentation days, authors are kindly requested to set up their poster on the corresponding board with the supplied material before 10:00

Posters should be removed no later than 18:00 on the second day.

Authors of posters are also kindly requested to stay at their poster for discussion during the official poster session.

**All abstracts are identified by a code in a form PLn, KNn or MSn-Oi/Pi.**

**PL:** plenary lecture

**KN:** keynote lecture

**O:** oral presentation

**P:** poster presentation

**n, i:** sequence numbers



### THE NOBEL COMMITTEES FOR PHYSICS AND CHEMISTRY

THE ROYAL SWEDISH ACADEMY OF SCIENCES

The 2011 Nobel Prize in chemistry has been awarded to Professor Dan Shechtman for his discovery of quasicrystals. Indeed his observation of a diffraction pattern with icosahedral symmetry in 1982 has been a revolution in crystallography, with a paradigm shift that changed our understanding of long range order in solid state materials. The seminal paper by D. Shechtman, I. Blech, D. Gratias and J.W. Cahn ("Metallic phase with long range orientational order and no translation symmetry", 1984, Phys. Rev. Lett. **53**, 1951-1954) has opened a very active field in mathematics, crystallography, physics and chemistry.

In celebration of this Nobel Prize, a special symposium on quasicrystals is organised at the ECM27. Five invited speakers will give an overview of the state-of-the-art for research carried out in the field of quasicrystals. The symposium is aimed at none-specialist and will offer a unique opportunity to everyone to discover this fascinating field. We are proud to acknowledge the financial support by The Nobel Committees for Physics and Chemistry, The Royal Swedish Academy of Sciences for this symposium and the plenary lecture given by Dan Shechtman, Wednesday 8th, 18:40-19:40.

The above will be complemented by more specific Microsymposia dedicated to aperiodic crystals; MS 15, 21, 22 and 34.

Organiser: Marc de Boissieu (Saint Martin d'Heres/FR)

Time& Place: Thursday 9<sup>th</sup>, 10:00-12:00 Seminar room 'PG2'

Title of the five presentations:

1. **W. Steurer** (Zürich/CH) "Decagonal quasicrystals"
2. **C. Pay Gomez** (Uppsala/SE) "Structure of the icosahedral CdYb quasicrystal"
3. **H. Euchner** (Stuttgart/DE) "Tetrahedron dynamics in the  $i$ -ZnMgSc quasicrystal and its  $1/1$  periodic approximant Zn<sub>6</sub>Sc"
4. **J. Ledieu** (Nancy/FR) "Quasicrystal and approximant surfaces: structural determination and pseudomorphy"
5. **R. Lifshitz** (Tel Aviv/IL) "Soft quasicrystals"

## Scientific programme • Crystallographic Software Fayre

At the ECM27 Congress 2012 in Bergen there will be a Software Fayre, where authors of academic and/or open-source software can present their new developments. The Software Fayre will be held on Tuesday, 7th and Thursday 9th. During the Tutorial Sessions, authors will demonstrate the features of their software on one or more practical examples.

Chair and Organiser: **Martin Lutz** (Utrecht/NL)

### Programme:

Tuesday 7th, 14:00-16:15 Tutorial Session Seminar room 'PG2'

14:00-14:45

**S. Hovmöller** (Stockholm/SE) "Single crystal diffraction from powders, using rotation electron diffraction (RED)"

14:45-15:30

**P. Oleynikov** (Stockholm/SE) "New developments in the Automated 3D Electron Diffraction Tomography software"

15:30-16:15

**B. Dittrich** (Göttingen/DE) "Introduction to MolecoolQt"

Thursday 9th, 14:00-16:15 Tutorial Session Seminar room 'PG2'

14:00-14:45

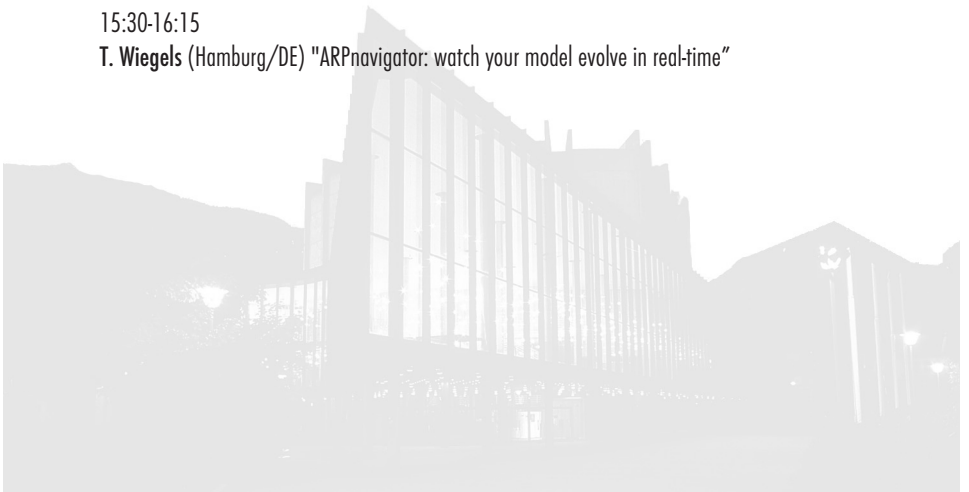
**M. Lutz** (Utrecht/NL) "Intensity integration with Eval15"

14:45-15:30

**I. Usón** (Barcelona/ES) "ARCIMBOLDO"

15:30-16:15

**T. Wiegels** (Hamburg/DE) "ARNavigator: watch your model evolve in real-time"



## Special Meetings

### Monday August 6 2012

13:00-16:00 ECA Executive Committee Meeting

### Seminar room

Auditorium 2, U-Level  
Realfagbygget (Science building)  
Allégaten 41

### Tuesday August 7 2012

12:00-13:30 ECA Council Meeting 1

12:00-13:30 GIG2-Senior Crystallographers

Klokkeklang

Troldtog

### Wednesday August 8 2012

12:00-14:00 ECA Programme Committee Meeting

12:00-14:00 IUCr Commission on Journals

20:30-23:00 GIG1-Young Crystallographers Mixer (Registered participants only)

Sponsored by DECTRIS

Klokkeklang

Bukken

Zafran restaurant

Nygårdsgaten 53

### Thursday August 9 2012

12:00-14:00 ECA Council Meeting 2

Klokkeklang

### Friday August 10 2012

12:00-13:30 ECA Council Meeting 3

12:00-13:30 GIG2-Senior Crystallographers

#### MS-48 Historical Aspects of crystallography

12:00-12:20

**S. Garcia-Granda** (Oviedo/ES)

“X-rays and crystallography. A story through the stamps”

12:20-12:40

**A.A. Chuev** (Moscow/RU)

“History of the establishment and development of X-ray analysis methods in Russia - The USSR. The first 20 years”

## Scientific programme • Satellite conference and workshops

### Methods of High-Pressure Single Crystal X-ray Diffraction

Dates: 4–5 August 2012  
Venue: The Science building, University of Bergen  
Allégaten 41  
5007Bergen, Norway

Organisers: Karen Friese (Jülich/DE) & Tonci Balic Zunic (Copenhagen/DK)

For further information, please refer to the ECM27 website: <http://ecm27.ecanews.org/satellite-meetings.html>

### IUCr Workshop on Diffraction Data Deposition (DDD)

This full-day Workshop is organised by the DDD Working Group (WG), appointed by the IUCr Executive Committee to define the need for and practicalities of routine deposition of primary experimental data in X-ray diffraction and related experiments. It will take the form of a one-day workshop to review progress during the Working Group's first year of activity.

Objective: To help frame a policy to be drafted by the IUCr DDD WG on raw diffraction data deposition for final approval by the IUCr Executive Committee.

Date: 6 August 2012  
Venue: The Science building, University of Bergen  
Allégaten 41  
5007 Bergen, Norway

Organisers: John Helliwell (Manchester/UK) & Brian McMahon (Chester/UK)

For further information, please refer to this website: <http://www.iucr.org/resources/data/dddwg>





## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • morning

08:30 – 09:30	Peer Gynt	Scene
	<b>KN1 Jacqueline Cherfils</b> <i>CNRS, France</i> Regulation of Arf GTPases in Cellular Traffic Chair: Tom Terwilliger	<b>KN2 Maryjane Tremayne</b> <i>School of Chemistry, University of Birmingham, United Kingdom</i> Structure solution from powder diffraction; new developments, applications and avenues Chair: Radomir Kuzel
09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	Peer Gynt	Scene
	<b>MS 1: Protein crystallization and sample preparation</b> Chairs: Axel Scheidig, Susanna Törnroth-Horsefield	<b>MS 15: Structural complexity of minerals and inorganic materials</b> Chairs: Oleg Siidra, Olivier Perez
	10:00 <b>MS1-01 Elias Vlieg</b> <i>Radboud University Nijmegen, Netherlands</i> Record Resolution Protein Crystals Using an Efficient Convection-free Growth Geometry	10:00 <b>MS15-01 Thorsten M. Gesing</b> <i>Inorganic Chemistry, University Bremen, Germany</i> Mullite-type dibismuth-nonaoxometallates-(III): The effects of strontium doping
	10:30 <b>MS1-02 Bernadette Byrne</b> <i>Imperial College London, United Kingdom</i> Producing stable membrane protein for structural studies	10:30 <b>MS15-02 Marie Colmont</b> <i>France</i> From simple O(Bi,M)4 entities to the large family of bismuth based oxyphosphate compounds: use of High Resolution Electron Microscopy Imaging to the deduction of new structure types
	11:00 <b>MS1-03 Christian Betzel</b> <i>University of Hamburg, Germany</i> Latest Methods to grow and prepare micro- and nano-Crystals for future Free-Electron-Laser and Synchrotron Radiation Sources	11:00 <b>MS15-03 Henrik Friis</b> <i>Canada</i> From calcite to the first natural hexaniobate or 350 years of mineral science
	11:20 <b>MS1-04 Naomi E. Chayen</b> <i>Imperial College London, United Kingdom</i> Smart materials for protein crystallization	11:20 <b>MS15-04 Yuri Grin</b> <i>MPI für Chemische Physik fester Stoffe, Germany</i> Crystallography of shadows: local disorder in intermetallic compounds
	11:40 <b>MS1-05 Anja Burkhardt</b> <i>DESY - Hasylab, Germany</i> High Pressure Freezing of Macromolecular Crystals	11:40 <b>MS15-05 Julien Haines</b> <i>CNRS, France</i> Negative linear compressibility and complex high-P structure in Zn[Au(CN) <sub>2</sub> ] <sub>2</sub>
12:00 – 13:30	<b>Lunch (C1, C2[Agilent], C3)</b>	

C1: ECA Council Meeting 1, 12:00-13:30 in R4. SIG's meet in individual groups in R1 and R2.

C2: Agilent Technologies Seminar 12:00 – 13:30 in R6.

C3: GIG2-SC meeting 12:00 – 13:30 in R3.

## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • morning

09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	<b>Troldtog</b>	<b>Klokkeklang</b>
	<b>MS 3: Getting the best data from your crystal(s)</b> <b>Chairs: Gordon Leonard, Jan Dohnalek</b>	<b>MS 41: Dynamics in crystals: experimental techniques and software</b> <b>Chairs: Francesca Fabbiani, Navraj Pannu</b>
	10:00 <b>MS3-01 James M Holton</b> <i>UCSF/LBNL, United States</i> The battle of signal vs noise, and how to tip the balance in your favor	10:00 <b>MS41-01 Antonija Kuzmanic</b> <i>Max F. Perutz Laboratories, Austria</i> Implications of conformational heterogeneity in protein crystals: from interatomic distance measurements to entropy estimation
	10:30 <b>MS3-02 Matthew W. Bowler</b> <i>EMBL, France</i> Extracting the maximum data from your samples - advanced sample evaluation at the ESRF	10:30 <b>MS41-02 Carole A. Morrison</b> <i>School of Chemistry, University of Edinburgh, United Kingdom</i> Bananas, pears and other fruitful discussions: modelling atomic motions in molecules
	11:00 <b>MS3-03 Kazuhiro Yamada</b> <i>Institute of Molecular Biology and Biophysics, ETH, Switzerland</i> ISWI a crystal resolution improvements through packing engineering	11:00 <b>MS41-03 Loes M.J. Kroon-Batenburg</b> <i>Utrecht University, Netherlands</i> EVAL15 as a tool for studying crystal properties in detail: dynamic and static disorder
	11:20 <b>MS3-04 Marcus Mueller</b> <i>Dectris Ltd., Switzerland</i> Getting best data using photon counting pixel detectors	11:20 <b>MS41-04 Anders O. Madsen</b> <i>Department of Chemistry, University of Copenhagen, Denmark</i> Entropies from Diffraction Experiments: Towards Polymorph Prediction
	11:40 <b>MS3-05 James Foadi</b> <i>MPL - Imperial College, United Kingdom</i> Clustering procedures for the optimal selection of datasets from multiple crystals in macromolecular crystallography	11:40 <b>MS41-05 Boris Zakharov</b> <i>Russia</i> X-ray diffraction and spectroscopic study of selected complexes of amino acids with carboxylic acids at high pressures and low temperatures
12:00 – 13:30	<b>Lunch (C1, C2[Agilent], C3)</b>	

C1: ECA Council Meeting 1, 12:00-13:30 in R4. SIG's meet in individual groups in R1 and R2.

C2: Agilent Technologies Seminar 12:00 - 13:30 in R6.

C3: GIG2-SC meeting 12:00 - 13:30 in R3.

## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Gjendine	Salong Nina
	<b>MS 39:</b> Electron diffraction and X-ray powder diffraction: getting the best of both worlds <b>Chairs:</b> Holger Klein, Christian Baerlocher	<b>MS 27:</b> Molecular structures in catalysis and magnetism <b>Dietmar Stalke, Deon Visser</b>
	<b>10:00</b> <b>MS39-01</b> <b>Mauro Gemmi</b> <i>Istituto Italiano di Tecnologia, Italy</i> The interplay between x-ray powder and electron diffraction: the case of experimental petrology	<b>10:00</b> <b>MS27-01</b> <b>Nicoline Cloete</b> <i>University of the Free State, South Africa</i> Ethylene tetramerisation: link between catalyst precursor structure and catalysis
	<b>10:30</b> <b>MS39-02</b> <b>Lynne B. McCusker</b> <i>Laboratory of Crystallography, ETH Zurich, Switzerland</i> Electron microscopy as seen through the eyes of a powder diffractionist	<b>10:30</b> <b>MS27-02</b> <b>Peter B. Brenner</b> <i>University of Würzburg, Germany</i> The trans-Influence of the Boryl Ligand in Square-Planar Platinum(II) Complexes
	<b>11:00</b> <b>MS39-03</b> <b>A. Ken Inge</b> <i>Stockholm University, Sweden</i> SU-66: Combining X-ray powder diffraction, electron diffraction and IR spectroscopy	<b>11:00</b> <b>MS27-04</b> <b>Wieslaw Lasocha</b> <i>J.Haber Institute of Catalysis, Jagiellonian University, Poland</i> Synthesis and crystal structure of few new decavanadates
	<b>11:20</b> <b>MS39-04</b> <b>Tereza Brunatova</b> <i>Czech Republic</i> Study of Titanate Nanotubes by X-ray and Electron Diffraction and Electron Microscopy	<b>11:20</b> <b>MS27-05</b> <b>Theunis Jacobus Muller</b> <i>Universteit of the Free State, South Africa</i> Crystallographic and kinetic investigation of nitrosyl, cyanide and acetonitrile complexes of Rh(I)/(III)
	<b>11:40</b> <b>MS39-05</b> <b>Ute Kolb</b> <i>Johannes Gutenberg-Universität Mainz, Germany</i> Electron diffraction structure analysis of organic nano sized crystals	
12:00 – 13:30	Lunch (C1, C2[Agilent], C3)	

C1: ECA Council Meeting 1, 12:00-13:30 in R4. SIG's meet in individual groups in R1 and R2.

C2: Agilent Technologies Seminar 12:00 – 13:30 in R6.

C3: GIG2-SC meeting 12:00 – 13:30 in R3.

## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Peer Gynt	Scene
	<p>MS 4: Phasing challenges. Bootstrapping from a poor start  <b>Chairs:</b> Keith Wilson, Clemens Vonrhein</p>	<p>MS 13: Energy related materials  <b>Chairs:</b> Serena Margadonna, Yaroslav Filinchuk</p>
	<p>13:30 <b>MS4-01</b> <b>Thomas C Terwilliger</b>  <i>Los Alamos National Laboratory, United States</i>                      Molecular replacement and model-building using distant homology models as templates</p>	<p>13:30 <b>MS13-01</b> <b>Lorenzo Malavasi</b>  <i>University of Pavia, Italy</i>                      Local structure investigation of clean energy materials through pair distribution function</p>
	<p>14:00 <b>MS4-02</b> <b>Gerard Bricogne</b>  <i>Global Phasing Ltd., United Kingdom</i>                      Classical-style MAD phasing with wavelength interleaving and kappa goniometry on PROXIMA-1</p>	<p>14:00 <b>MS13-02</b> <b>Martin Dornheim</b>  <i>Helmholtz-Zentrum Geesthacht, Germany</i>                      Characterization of hydrogen storage materials both at the laboratory level and at the scale for prototype tanks</p>
	<p>14:30 <b>MS4-03</b> <b>Kevin D Cowtan</b>  <i>University of York, United Kingdom</i>                      The Nautilus software for automated nucleic acid model building</p>	<p>14:30 <b>MS13-03</b> <b>Marco Milanesio</b>  <i>Universita del Piemonte Orientale, Italy</i>                      Investigating Repeated Gas adsorption in zeolites for solar cooling applications</p>
	<p>14:50 <b>MS4-04</b> <b>Navraj S Pannu</b>  <i>Netherlands</i>                      A novel function for the combination of SAD phasing, density modification and refinement</p>	<p>14:50 <b>MS13-04</b> <b>Rune E. Johnsen</b>  <i>Denmark</i>                      In situ XRPD studies of Li intercalation in graphite in working Li-ion batteries</p>
	<p>15:10 <b>MS4-05</b> <b>Sun-Shin Cha</b>  <i>Korea Ocean Research and Development Institute, Republic of Korea</i>                      Zinc-binding to protein surface and its application to phase determination</p>	<p>15:10 <b>MS13-05</b> <b>Hilde Grove</b>  <i>IFE, Norway</i>                      Changing Properties of Hydrogen Storage Materials by Halide Substitution</p>
15:30 – 16:30	<b>Poster session 1 with Coffee break</b>	
16:30 – 17:30	Peer Gynt	Scene
	<p><b>KN3</b> <b>Olivier Mentré</b>  <i>UCCS, France</i>                      Phase Homology and Structural Prediction in Extended Series of Inorganic Bi-based Compounds  <b>Chair:</b> Karl Wilhelm Törnroos</p>	<p><b>KN4</b> <b>Paul A. Midgley</b>  <i>University of Cambridge, United Kingdom</i>                      Towards Routine Structure Solution using Precession Electron Diffraction  <b>Chair:</b> Sven Hovmöller</p>
17:30 – 18:00	<b>Coffee Break with Sandwich</b>	
18:00 – 19:30	<b>Peer Gynt</b>	
	<p>Bertaut &amp; Perutz Prize award ceremonies &amp; lectures  <b>Chairs:</b> Andreas Roodt, Santiago Garcia-Granda</p>	

## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Troidtog	Klokkeklang
	<b>MS 11: Frontiers in Structural Enzymology</b> <b>Chairs: Jaqueline Cherfils, Menico Rizzi</b>	<b>MS 25: Design, structure, and function of multi-component crystals</b> <b>Chairs: Petra Bombicz, Laszlo Fabian</b>
	<b>13:30 MS11-01 Ilme Schlichting</b> <i>Max Planck Institute for Medical Research, Germany</i> Serial femtosecond crystallography provides new approaches to structural enzymology	<b>13:30 MS25-01 Ulrich J. Griesser</b> <i>University of Innsbruck/Inst. of Pharmacy, Austria</i> Value and Perspectives of Multicomponent Crystals in Pharmaceutical Development
	<b>14:00 MS11-02 Juan A. Hermoso</b> <i>Spanish National Research Council (CSIC), Spain</i> Advances in bacterial cell-wall remodeling enzymes. Implications in virulence and antibiotics resistance	<b>14:00 MS25-02 Gerard F.R. Coquerel</b> <i>University of Rouen, France</i> 'Hybrid salt-cocrystals and exotic stoichiometries in host-guest compounds: troubles in nomenclature!...'
	<b>14:30 MS11-03 Francesca Cutruzzola</b> <i>Sapienza University of Rome, Italy</i> Human DOPA decarboxylase: structural snapshots of PLP binding	<b>14:30 MS25-03 Filip Topić</b> <i>University of Jyväskylä, Finland</i> Predictable Supramolecular Motifs in Cocrystals of (Thio)urea with Ph4P <sup>+</sup> Halides
	<b>14:50 MS11-04 Daniel Burschowsky</b> <i>University of Oslo, Department of Chemistry, Norway</i> Reaction Mechanism of Chorismate Mutase, a Model Enzyme for Pericyclic Reactions, Finally Resolved	<b>14:50 MS25-04 Andreas Lemmerer</b> <i>University of the Witwatersrand, South Africa</i> Covalent Assistance to Supramolecular Synthesis: The Use of Hydrogen Bonding Modifying Groups to Control the Assembly of Co-Crystal
	<b>15:10 MS11-05 Chun-Jung Chen</b> <i>National Synchrotron Radiation Research Center, Taiwan</i> Structural insights into enzyme catalysis of sulfate reduction in <i>Desulfovibrio gigas</i>	<b>15:10 MS25-05 Alessandra Crispini</b> <i>Department of Chemistry, University of Calabria, Italy</i> Crystallization and co-crystallization of Zn(II) heteroleptic complexes: modulation of properties.
15:30 – 16:30	<b>Poster session 1 with Coffee break</b>	
17:30 – 18:00	<b>Coffee Break with Sandwich</b>	

## Scientific programme Tuesday, 7<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Gjendine	Salong Nina
	<p>MS 44: Controlling and Monitoring crystal growth and quality  <b>Chairs: Dino Aquilano, Alexander Van Driessche</b></p>	<p>MS 21: Crystal chemistry of aperiodic crystals and frustrated systems  <b>Chairs: Sven Lidin, Gwilherm Nenert</b></p>
	<p>13:30 <b>MS44-01</b> <b>Pablo Cubillas</b>  <i>The University of Manchester, United Kingdom</i>            Uncovering the molecular assembly of metal organic frameworks through scanning force microscopy</p>	<p>13:30 <b>MS21-01</b> <b>Artem Abakumov</b>  <i>University of Antwerp, Belgium</i>            Modulations and short range order in perovskites with lone pair A-cations</p>
	<p>14:00 <b>MS44-02</b> <b>Mike Sleutel</b>  <i>Vrije Universiteit Brussel, Belgium</i>            In situ observations of impurity effects during protein crystallization</p>	<p>14:00 <b>MS21-02</b> <b>Andreas Schönleber</b>  <i>University of Bayreuth, Germany</i>            Modulated structure and magnetic order in MOCl (M = Ti, V, Cr, Fe) at low temperatures</p>
	<p>14:30 <b>MS44-03</b> <b>Nobutaka Numoto</b>  <i>Kyoto University, Japan</i>            Crystallization behaviors of protein molecules in high magnetic forces fields</p>	<p>14:30 <b>MS21-03</b> <b>Thomas Richard Welberry</b>  <i>Australian National University, Australia</i>            Diffuse scattering resulting from macromolecular frustration</p>
	<p>14:50 <b>MS44-04</b> <b>Wolfgang Hornfeck</b>  <i>German Aerospace Center, Germany</i>            Time-resolved Crystallization of Charged Colloidal Silica Spheres</p>	<p>14:50 <b>MS21-04</b> <b>Olivier Perez</b>  <i>CRISMAT / ENSICAEN, France</i>            Complex ordering in Metal Organic Framework</p>
	<p>15:10 <b>MS44-05</b> <b>Edward J. Daniel</b>  <i>University of Oulu, Finland</i>            xtalPiMS: A tool for managing your crystallization experiments</p>	<p>15:10 <b>MS21-05</b> <b>Julia Dshemuchadse</b>  <i>ETH Zurich, Switzerland</i>            Structural Characteristics of Complex Intermetallics</p>
15:30 – 16:30	<b>Poster session 1 with Coffee break</b>	
17:30 – 18:00	<b>Coffee Break with Sandwich</b>	

## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • morning

08:30 – 09:30	Peer Gynt	Scene
	<b>KN5 Henry Chapman</b> <i>DESY, Germany</i> Femtosecond Protein Nanocrystallography with an X-ray Free-Electron Laser Chair: David Brown	<b>KN6 Simon Parsons</b> <i>University of Edinburgh, United Kingdom</i> Absolute Structure Determination Chair: Martin Lutz
09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	Peer Gynt	Scene
	<b>MS 2: MX at Synchrotron Sources, including X-FELs and time-resolved crystallography</b> Chairs: Henry Chapman, Ilme Schlichting	<b>MS 26: Porous materials for gas storage and other applications</b> Chairs: Luigi Nassimbeni, Alessia Bacchi
	10:00 <b>MS2-01 Richard Neutze</b> <i>University of Gothenburg, Sweden</i> Visualising rapid structural changes in photosynthetic reaction centres with XFEL radiation	10:00 <b>MS26-01 Kari Rissanen</b> <i>University of Jyväskylä, Finland</i> Porous Molecular Crystals based on Halogen and Hydrogen Bonds
	10:30 <b>MS2-02 Junko Yano</b> <i>Lawrence Berkeley National Laboratory, United States</i> Taking Snapshots of Photosynthetic Water Oxidation: Towards Time-Resolved X-ray Spectroscopy and Crystallography	10:30 <b>MS26-02 Michael Mastalerz</b> <i>Ulm University, Germany</i> Porous Crystalline Materials from Discrete Organic Molecules
	11:00 <b>MS2-03 Marius Schmidt</b> <i>UW-Milwaukee, United States</i> 5-Dimensional Crystallography	11:00 <b>MS26-03 Gaelle Ramon</b> <i>University of Cape Town, South Africa</i> Thermo and solvatochromic coordination frameworks with 4-(pyridin-4-yl)benzoic acid
	11:20 <b>MS2-04 Yves Watier</b> <i>ESRF, France</i> Humidity controlled Protein Powder Diffraction, application on an urchin-like polycrystal of the Mayaro virus nsp3 macrodomain	11:20 <b>MS26-04 Yaroslav Filinchuk</b> <i>Universite Catholique de Louvain, Belgium</i> Get more for your porous system: heats of adsorption from powder diffraction data
	11:40 <b>MS2-05 Uwe Mueller</b> <i>Helmholtz-Zentrum Berlin, Germany</i> Improvement of the diffraction quality of macromolecular crystals at European synchrotrons using the HCl dehydration control device	11:40 <b>MS26-05 Stephen A Moggach</b> <i>The University of Edinburgh, United Kingdom</i> GPa pressure modification of a scandium microporous MOF
12:00 – 14:00	<b>Lunch (C5, C6)</b>	

C5: ECA Programme Committee Meeting (closed) 12:00 – 14:00. SIG's and IM's meet in individual groups in R1 and R2. 'Glassrommet', no. 10 in venue map (10 pax) available if needed.

C6: IUCr Commission on Journals Meeting (closed) 12:00 – 14:00 in seminar room 'Bukken', no. 11 in venue map.



## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • morning

09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	<b>Troidtog</b>	<b>Klokkeklang</b>
	<p><b>MS 5: Advances in refinement and validation. Ligand chemistry</b>  <b>Chairs: Garib Murshudov, Isabel Uson</b></p>	<p><b>MS 31: "How-to"</b>  <b>Chairs: Susanne L. Coles, Laura Rocas</b></p>
	<p>10:00 <b>MS5-01</b> <b>Oliver S. Smart</b>  <i>Global Phasing Ltd., United Kingdom</i>            Better ligand representation in BUSTER protein-complex structure determination</p>	<p>10:00 <b>MS31-01</b> <b>Santiago Garcia-Granda</b>  <i>University Oviedo, Spain</i>            How to apply to the EC Framework Programs: Opportunities for young scientists</p>
	<p>10:30 <b>MS5-02</b> <b>Tom B Burnley</b>  <i>Utrecht University, Netherlands</i>            Ensemble refinement of protein crystal structures in PHENIX</p>	<p>10:30 <b>MS31-02</b> <b>Harold R. Powell</b>  <i>MRC Laboratory of Molecular Biology, United Kingdom</i>            Il Buono, il brutto, il cattivo - strategies for better lectures</p>
	<p>11:00 <b>MS5-03</b> <b>Saulius Grazulis</b>  <i>VU Institute of Biotechnology, Lithuania</i>            Use of the Crystallography Open Database as a source of prior knowledge for molecular modelling</p>	<p>11:00 <b>MS31-03</b> <b>John R Helliwell</b>  <i>University of Manchester, United Kingdom</i>            How to present results in scientific articles</p>
	<p>11:20 <b>MS5-04</b> <b>Ciaran G Carolan</b>  <i>European Molecular Biology Laboratory, Germany</i>            Automated Identification of Ligands in Macromolecular Electron Density Maps</p>	<p>11:20 <b>MS31-04</b> <b>Alessia Bacchi</b>  <i>Dipartimento di Chimica, University of Parma, Italy</i>            How to survive in Academia</p>
	<p>11:40 <b>MS5-05</b> <b>Thomas Lütteke</b>  <i>Justus-Liebig-University Giessen, Germany</i>            New Features and Improvements in Carbohydrate 3D Structure Validation</p>	<p>11:40 <b>MS31-05</b> <b>Elena Boldyreva</b>  <i>Novosibirsk State University, Russia</i>            How to ensure the future of crystallography - a teaching perspective</p>
12:00 – 14:00	<b>Lunch (C5, C6)</b>	

C5: ECA Programme Committee Meeting (closed) 12:00 – 14:00. SIG's and IM's meet in individual groups in R1 and R2. 'Glassrommet', no. 10 in venue map (10 pax) available if needed.

C6: IUCr Commission on Journals Meeting (closed) 12:00 – 14:00 in seminar room 'Bukken', no. 11 in venue map.

## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Gjendine	Salong Nina
	<b>MS 37: Electron Crystallography on functional materials</b> <b>Chairs: Xiaodong Zou, Joke Hadermann</b>	<b>MS 35: Ferroic and multiferroic materials</b> <b>Chairs: Christine Martin, Manuel Hinterstein</b>
	<b>10:00 MS37-01 Louisa Meshi</b> <i>Ben Gurion University of the Negev, Israel</i> Structure determination of intermetallics using Precession Electron Diffraction	<b>10:00 MS35-01 Jérôme Rouquette</b> <i>ICGM UMR CNRS 5253 Equipe C2M, France</i> Structural Origin of the Ferroelectric Fatigue in Lead Zirconate Titanate (PZT)
	<b>10:30 MS37-02 Junliang Sun</b> <i>Stockholm University, Sweden</i> Electron Crystallography on porous materials	<b>10:30 MS35-02 Roger D Johnson</b> <i>University of Oxford, United Kingdom</i> Giant Improper Ferroelectricity in the Ferroaxial Magnet CaMn7O12
	<b>11:00 MS37-03 Enrico Mugnaioli</b> <i>Johannes</i> <i>Gutenberg-Universität Mainz, Germany</i> Structure investigation of nanocrystalline small-molecule organics and MOF by ADT and simulated annealing	<b>11:00 MS35-03 David I Woodward</b> <i>University of Warwick, United Kingdom</i> Depoling studies of lead-free $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ - $\text{K}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ piezoelectric ceramics
	<b>11:20 MS37-04 David I Woodward</b> <i>University of Warwick, United Kingdom</i> 'Digital' Electron Diffraction	<b>11:20 MS35-04 Semën Gorfman</b> <i>University of Siegen, Germany</i> Observation of low - symmetry phase in $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ by optical birefringence microscopy
	<b>11:40 MS37-05 Osman Adiguzel</b> <i>Firat University, Department of Physics, Turkey</i> Diffraction Studies on Displacive Transitions in Copper Based Shape Memory Alloys	<b>11:40 MS35-05 Claire V. Colin</b> <i>Institut Néel, CNRS and Université Joseph Fourier, France</i> Symmetry adapted analysis of the magnetic and structural phase diagram of $\text{Bi}_{1-x}\text{Y}_x\text{CrO}_3$
12:00 – 14:00	Lunch (C5, C6)	

C5: ECA Programme Committee Meeting (closed) 12:00 – 14:00. SIG's and IM's meet in individual groups in R1 and R2. 'Glassrommet', no. 10 in venue map (10 pax) available if needed.

C6: IUCr Commission on Journals Meeting (closed) 12:00 – 14:00 in seminar room 'Bukken', no. 11 in venue map.

## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Peer Gynt	Scene
	MS 8: Membrane proteins Chairs: J. Preben Morth, Gergely Katona	MS 23: Intermolecular interactions at ambient and extreme conditions Chairs: Elena Boldyreva, Paola Gilli
	14:00 <b>MS8-01</b> <b>Petra Fromme</b> <i>Arizona State University, Department of Chemistry, United States</i> Femtosecond nanocrystallography of membrane proteins opens a new Era	14:00 <b>MS23-01</b> <b>Olga V. Grineva</b> <i>Chemistry Department of M.V. Lomonosov MSU, Russia</i> Intermolecular halogen...halogen contacts in crystals with heteroatomic halogens
	14:30 <b>MS8-02</b> <b>Poul Nissen</b> <i>Aarhus University, Denmark</i> Membrane transporters and bilayers studied by X-ray crystallography	14:30 <b>MS23-02</b> <b>Anna Olejniczak</b> <i>Poland</i> Ten polymorphs of NH • • • N bonded DABCO hydroiodide - and even more!
	15:00 <b>MS8-03</b> <b>Simone Weyand</b> <i>Imperial College London, United Kingdom</i> The structure of the human Histamine H1 receptor in complex with Doxepin	15:00 <b>MS23-03</b> <b>Vera Vasylyeva</b> <i>Germany</i> Fluorine substituents disturb the aggregation of molecules
	15:20 <b>MS8-04</b> <b>Juho A T Kellosalo</b> <i>University of Helsinki, Institute of Biotechnology, Finland</i> The structure of a sodium pumping pyrophosphatase: clues to catalytic mechanism	15:20 <b>MS23-04</b> <b>Andrew G P Maloney</b> <i>University of Edinburgh, United Kingdom</i> Application of the PIXEL Method to Transition Metal Complexes
	15:40 <b>MS8-05</b> <b>Linda C Johansson</b> <i>University of Gothenburg, Sweden</i> Serial Femtosecond Crystallography Using Crystals Grown in Lipidic-Sponge Phases	15:40 <b>MS23-05</b> <b>Janusz S Lipkowski</b> <i>Polish Academy of Sciences, Poland</i> The Structure of Hydrophobic Hydration
16:00 – 17:00	<b>Poster session 1 with Coffee break</b>	
17:00 – 18:00	Peer Gynt	Scene
	<b>KN7</b> <b>Jens Preben Morth</b> <i>NCMM, Norway</i> Listeria Monocytogenes Lmo0818 – Exploring a putative Ca <sup>2+</sup> -ATPase, to understand Calcium ion specificity Chair: Ute Krengel	<b>KN8</b> <b>Simone E. Techert</b> <i>Max Planck Institute for Biophysical Chemistry, Germany</i> Time Resolved Crystallographic Processes in Molecular Systems Chair: Mark Spackman
18:00 – 18:40	<b>Coffee Break with Sandwich</b>	
18:40 – 19:40	<b>Peer Gynt</b>	
	<b>PL2</b> <b>Dan Shechtman</b> <i>Technion, Haifa, Israel</i> Quasi-periodic materials discovery – the role of TEM Chair: Sven Lidin	
20:30	<b>GIG1-Young Crystallographer Mixer at Zafran restaurant (Registered participants only)</b> Sponsored by Dectris	

## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Troidtog	Klokkeklang
	<p><b>MS 7: Pharmaceutical crystallography - Drug design: success and failures</b>  <b>Chairs: Rick Engh, Michael Hennig</b></p>	<p><b>MS 22: Quasicrystals, their approximants and surfaces: from the atomic to the nanoscale</b>  <b>Chairs: Cesar Pay Gomez, Thomas Weber</b></p>
	<p><b>14:00</b> <b>MS7-01</b> <b>David Brown</b>  <i>University of Kent, United Kingdom</i>                      Perspectives on Structure Based Drug design – A Changing landscape</p>	<p><b>14:00</b> <b>MS22-01</b> <b>Ryuji Tamura</b>  <i>Tokyo University of Science, Japan</i>                      Structural and Magnetic Ordering in Cd-based Crystalline Approximants</p>
	<p><b>14:30</b> <b>MS7-02</b> <b>Thomas Bertrand</b>  <i>SANOFI, France</i>                      A Structure-Based Approach To Selective PI3Kbeta Inhibition</p>	<p><b>14:30</b> <b>MS22-02</b> <b>Pawel Kuczera</b>  <i>AGH - University of Science and Technology, Poland</i>                      The physical space approach to the structure refinement of decagonal quasicrystals. Are three dimensions enough?</p>
	<p><b>15:00</b> <b>MS7-03</b> <b>Andreas Heine</b>  <i>Philipps-University Marburg, Germany</i>                      Starting Small and Getting Bigger: From Molecular Probes to Fragments and Leads</p>	<p><b>15:00</b> <b>MS22-03</b> <b>Marc de Boissieu</b>  <i>France</i>                      Diffuse scattering and phason modes in the Zn-Sc binary icosahedral quasicrystal</p>
	<p><b>15:20</b> <b>MS7-04</b> <b>Puja Pathuri</b>  <i>Astex Pharmaceuticals Inc., United Kingdom</i>                      Discovery of novel allosteric inhibitors of HCV NS3/4a enzyme via structure-based drug design</p>	<p><b>15:20</b> <b>MS22-04</b> <b>Taylan Ors</b>  <i>ETH Zurich, Switzerland</i>                      Structure analysis of decagonal ZnMgDy quasicrystal</p>
	<p><b>15:40</b> <b>MS7-05</b> <b>Steffi Munack</b>  <i>University of Oslo, Norway</i>                      Enzyme inhibitors as tuberculosis drugs – a structure guided approach</p>	<p><b>15:40</b> <b>MS22-05</b> <b>Arina Alexandrovna Pankova</b>  <i>Samara State University, Russia</i>                      Multi-shell nanoclusters with the <math>\gamma</math>-brass polyhedral core in intermetallics</p>
<b>16:00 – 17:00</b>	<b>Poster session 1 with Coffee break</b>	
<b>18:00 – 18:40</b>	<b>Coffee Break with Sandwich</b>	

## Scientific programme Wednesday, 8<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Gjendine	Salong Nina
	<p><b>MS 17:</b> Structural and crystal-physical studies in large volume high-P devices  <b>Chairs:</b> Konstantin Kamenev, Andrzej Grzechnik</p>	<p><b>MS 30:</b> Buy one, get one free: Software for twin handling  <b>Chairs:</b> Regine Herbst-Irmer, Michal Dusek</p>
	<p>14:00 <b>MS17-01</b> <b>Wilson Crichton</b>  <i>ESRF, France</i>                      New opportunities with the large-volume device at ID06, ESRF</p>	<p>14:00 <b>MS30-01</b> <b>Ina Dix</b>  <i>Novartis Institutes of Biomedical Research, Switzerland</i>                      Discover the Cosmos of Reciprocal Space – Twins as a Routine Case?</p>
	<p>14:30 <b>MS17-02</b> <b>Norimasa Nishiyama</b>  <i>Deutsches Elektronen Synchrotron DESY, Germany</i>                      The Large Volume Press Beamline at the extension of PETRA III</p>	<p>14:30 <b>MS30-02</b> <b>Berthold Stöger</b>  <i>Vienna University of Technology, Austria</i>                      Twin refinement with Jana2006: from polytypism to modulated phases</p>
	<p>15:00 <b>MS17-03</b> <b>Craig L Bull</b> (invited)  <i>University of Edinburgh, United Kingdom</i>                      Single-Crystal Neutron Diffraction 10 GPa and Beyond</p>	<p>15:00 <b>MS30-03</b> <b>Mathias Meyer</b>  <i>Agilent Technologies, Poland</i>                      Twin samples with CrysAlisPro: Experiments, unit cell finding, data reduction and post corrections</p>
	<p>15:20 <b>MS17-04</b> <b>Y. Le Godec</b> (invited)  <i>IMPMC, UPMC, France</i>                      New Scientific Opportunities with next Generation Portable Large Volume HighP/T/Stress/Tomography Cells</p>	<p>15:20 <b>MS30-04</b> <b>Martin Lutz</b>  <i>Utrecht University, Netherlands</i>                      Oligo-diffractometry using EVAL15</p>
	<p>15:40 <b>MS17-05</b> <b>Martin Bremholm</b>  <i>Department of Chemistry, Aarhus University, Denmark</i>                      Discovery of novel post-perovskites by high pressure methods</p>	<p>15:40 <b>MS30-05</b> <b>Simon Parsons</b>  <i>University of Edinburgh, United Kingdom</i>                      Facilities for Handling Twins in CRYSTALS</p>
16:00 – 17:00	<b>Poster session 1 with Coffee break</b>	
18:00 – 18:40	<b>Coffee Break with Sandwich</b>	

## Scientific programme Thursday, 9<sup>th</sup> August 2012 • morning

08:30 – 09:30	Peer Gynt	Scene
	<b>KN9 Paola Gilli</b> <i>University of Ferrara, Italy</i> Towards the unification of intermolecular forces: The hydrogen bond as a charge-transfer interaction Chair: Jacco van de Streek	<b>KN10 Ross J Angel</b> <i>University of Padova, Italy</i> Minerals and materials at high pressures: the challenges of complexity Chair: Simon Parsons Sponsored by Agilent
09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	Peer Gynt	Scene
	<b>MS 10: Infection and Disease</b> Chairs: Sine Larsen, Pirkko Heikinheimo	<b>MS 14: Materials in operando and in situ crystallography of materials</b> Chairs: Werner Paulus, Poul Nordby
	<b>10:00 MS10-01 Jack C. Leo</b> <i>Max Planck Institute for Developmental Biology, Germany</i> Type Ve secretion: a novel autotransport mechanism	<b>10:00 MS14-01 Guy Ouvrard</b> <i>University of Nantes, France</i> Operando characterization of lithium battery electrode materials
	<b>10:30 MS10-02 Tommi Kajander</b> <i>University of Helsinki, Finland</i> Factor H ligand complexes - Structural studies on complement regulation and disease	<b>10:30 MS14-02 Andrew M Beale</b> <i>Utrecht University, Netherlands</i> An eye on the inside: imaging of catalytic particles under reaction conditions
	<b>11:00 MS10-03 Annabelle Varrot</b> <i>CERMAV, France</i> Fucose binding lectins from opportunistic pathogens and blood group antigens	<b>11:00 MS14-03 David S. Wragg</b> <i>University of Oslo, Norway</i> Watching the MTO process with time and space resolved X-ray diffraction
	<b>11:20 MS10-04 Konrad Büsow</b> <i>Germany</i> Crystal structure of human lysosome-associated membrane protein 3 (LAMP-3)	<b>11:20 MS14-04 Pierre Fertey</b> <i>Synchrotron Soleil, France</i> In-situ diffraction determination of the structural response of GaAsO4 submitted to an applied electric field
	<b>11:40 MS10-05 Marte I Flydal</b> <i>University of Bergen, Norway</i> Phenylalanine Hydroxylase from Legionella pneumophila: a Thermostable Dimer	<b>11:40 MS14-05 Philipp Urban</b> <i>Leipzig University, Germany</i> Diffusion processes in $(\text{GeTe})_n(\text{Sb}_2\text{Te}_3)$ ( $4 \leq n \leq 12$ ) crystals investigated by synchrotron radiation
12:00 – 14:00	<b>Lunch (C8[Bruker&amp;Incoatec], C9)</b>	

C8: Bruker & Incoatec Seminar 12:30 – 13:30 in R6.

C9: ECA Council Meeting 2, 12:00 – 14:00 in R4.

## Scientific programme Thursday, 9<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Troldtog	Klokkeklang
	<p><b>MS 42:</b> Big "small molecules" and small "macromolecules" - learning techniques from each other</p> <p><b>Chairs:</b> Thomas Schneider, Vratislav Langer</p>	<p><b>MS 18:</b> New perspectives for charge density analysis: materials properties from inorganics to macromolecules</p> <p><b>Chairs:</b> Hazel Sparkes, Benoit Guillot</p>
	<p>10:00 <b>MS42-01</b> <b>David Flot</b> <i>ESRF, France</i> Small molecule Crystallography on Macromolecular Biology Beam Line at the ESRF</p>	<p>10:00 <b>MS18-01</b> <b>Nour Eddine Ghermani</b> <i>Université Paris Sud 11 Faculté de Pharmacie, France</i> Electron properties of pharmaceutical molecules</p>
	<p>10:30 <b>MS42-02</b> <b>Michal Dusek</b> <i>Institute of Physics ASCR, Czech Republic</i> When small molecule data are lacking resolution</p>	<p>10:30 <b>MS18-02</b> <b>Maciej Kubicki</b> <i>Adam Mickiewicz University, Poland</i> Charge density analysis of macromolecules: case studies of small protein and DNA fragment</p>
	<p>11:00 <b>MS42-03</b> <b>Carl Henrik Görbitz</b> <i>Norway</i> Finally: The crystal structure of L-tryptophan</p>	<p>11:00 <b>MS18-03</b> <b>Maura Malinska</b> <i>University of Warsaw, Faculty of Chemistry, Poland</i> Experimental Charge Density Analysis of the Nature of C-Br • • • N≡C Interactions in Biologically Active Compound</p>
	<p>11:20 <b>MS42-04</b> <b>Weixiao Yuan</b> <i>Wahlgren University of Gothenburg, Sweden</i> Crystallization of bacterioferritin from Blastochloris viridis</p>	<p>11:20 <b>MS18-04</b> <b>Jozef Kozisek</b> <i>STU Bratislava, Slovakia</i> Electronic structure of Tetrakis(<math>\mu_2</math>-Acetato)-diaqua-di-chromium (II) complex, <math>[C_8H_{16}Cr_2O_{10}]</math></p>
	<p>11:40 <b>MS42-05</b> <b>Amber L. Thompson</b> <i>University of Oxford, United Kingdom</i> When Small Molecules Get Large – A Journey into the Unknown</p>	<p>11:40 <b>MS18-05</b> <b>Dorothee C Liebschner</b> <i>National Cancer Institute, United States</i> Topological analysis of hydrogen-bonds and weak interactions in protein helices</p>
12:00 – 14:00	Lunch (C8[Bruker&Incoatec], C9)	

C8: Bruker & Incoatec Seminar 12:30 – 13:30 in R6.

C9: ECA Council Meeting 2, 12:00 – 14:00 in R4.

## Scientific programme Thursday, 9<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Gjendine	Salong Nina
	<b>MS 46:</b> Advances in powder diffraction: structure solution and structure-property relationships <b>Chairs:</b> Lukas Palatinus, Michele Catti	<b>MS 24:</b> Bioinformatics informs MX <b>Chairs:</b> Ulli Englert, Luigi Nassimbeni
	<b>10:00</b> <b>MS46-01</b> <b>Dan Xie</b> <i>Chevron ETC, United States</i> The 2D-XPD charge flipping method for structure solution from powder diffraction data	<b>10:00</b> <b>MS24-01</b> <b>Laszlo Fabian</b> <i>University of East Anglia, United Kingdom</i> Structural relationships between chiral and racemic cocrystals
	<b>10:30</b> <b>MS46-02</b> <b>Stephen Hull</b> <i>The ISIS Facility, Rutherford Appleton Laboratory, United Kingdom</i> Neutron Scattering Studies of Ionically Conducting Oxides	<b>10:30</b> <b>MS24-02</b> <b>Alessia Bacchi</b> <i>Dipartimento di Chimica, University of Parma, Italy</i> Trekking on hills and valleys in the polymorph landscape of TPB
	<b>11:00</b> <b>MS46-03</b> <b>Jordi Rius</b> <i>CSIC-Institut de Ciència de Materials de Barcelona, Spain</i> Advances in TALP, a direct-space LS strategy for solving molecular crystals from powders	<b>11:00</b> <b>MS24-03</b> <b>Nikoletta B Bathori</b> <i>Cape Peninsula University of Technology, South Africa</i> Chiral Discrimination in the Solid State by using the Dutch Resolution Method
	<b>11:20</b> <b>MS46-04</b> <b>Dmitry Chernyshov</b> <i>SNBL at ESRF, France</i> Modulation Enhanced Diffraction - from Theory to Experiment	<b>11:20</b> <b>MS24-04</b> <b>Joe Ridout</b> <i>Durham University, United Kingdom</i> High Pressure / Low Temperature Polymorphism in Simple Aromatic Systems
	<b>11:40</b> <b>MS46-05</b> <b>Céleste A. Reiss</b> <i>PANalytical, Netherlands</i> An alternative method for quantitative XRPD analysis; partial least square regression	<b>11:40</b> <b>MS24-05</b> <b>Roberto Centore</b> <i>Italy</i> An entire class of compounds forming polar crystals and showing single-crystal-to-single-crystal transitions between polar phases
12:00 – 14:00	Lunch (C8[Bruker&Incoatec], C9)	

C8: Bruker & Incoatec Seminar 12:30 – 13:30 in R6.

C9: ECA Council Meeting 2, 12:00 – 14:00 in R4.



## Scientific programme Thursday, 9<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Peer Gynt	Scene
	MS 9: EM and MX for viruses, assemblies and biological nano-machines Chairs: Michael Rossmann, Anke Terwisscha van Scheltinga	MS 43: Hot topics and structures in molecular chemistry Chairs: Tony Linden, Amber Thomson
	14:00 <a href="#">MS9-01</a> <b>Sarah J. Butcher</b> <i>University of Helsinki, Finland</i> Packaging of the membrane-containing thermophilic virus STIV2	14:00 <a href="#">MS43-01</a> <b>Francesca P. A. Fabbiani</b> <i>Georg-August-Universität Göttingen, Germany</i> Host-guest interactions in cyclodextrin inclusion complexes at extreme conditions
	14:30 <a href="#">MS9-02</a> <b>Janet Vonck</b> <i>Max Planck Institute of Biophysics, Germany</i> Fatty acid synthase: insights in the substrate shuttling mechanism by cryo-EM	14:30 <a href="#">MS43-02</a> <b>G. Dan Pantos</b> <i>University of Bath, United Kingdom</i> Solution and Solid-State Supramolecular Chemistry of Naphthalenediimides
	15:00 <a href="#">MS9-03</a> <b>Federico Forneris</b> <i>University of Utrecht, Netherlands</i> Modularity and conformational changes as key features of the complement system	15:00 <a href="#">MS43-03</a> <b>Dietmar Stalke</b> <i>Georg-August University Goettingen, Germany</i> Low Valent Silicon
	15:20 <a href="#">MS9-04</a> <b>Ivo Tews</b> <i>University of Southampton, United Kingdom</i> Malarial vitamin B6 biosynthesis	15:20 <a href="#">MS43-04</a> <b>Marina A. Petrukina</b> <i>University at Albany, SUNY, United States</i> Self-assembly of highly charged fullerene fragment: Structural mystery resolved
	15:40 <a href="#">MS9-05</a> <b>Matthias Wilmanns</b> <i>EMBL, Germany</i> The architecture of the muscle filament myomesin by a hybrid structural biology	15:40 <a href="#">MS43-05</a> <b>Loredana Erra</b> <i>European Synchrotron Radiation Facility, France</i> Exploring the solid state conformation and assembly of cyclic peptoids derivatives
16:00 – 17:00	<b>Poster session 2 with Coffee break</b>	
17:00 – 18:00	Peer Gynt	Scene
	<a href="#">KN11</a> <b>Michael G. Rossmann</b> <i>Purdue University, United States</i> Combining crystallography and electron microscopy for virus structure determinations Chair: Petra Fromme	<a href="#">KN12</a> <b>Knut W. Urban</b> <i>Forschungszentrum Juelich, Germany</i> Picometer Electron Microscopy Chair: Peter Oleynikov
	<b>Conference dinner(*2)</b> Fløienfolke restaurant	

- \*2 Conference dinner at 'Fløien folkerestaurant'. Registered participants only.  
Participants must arrive at 19:30 using the Fløibanen funicular. Return ticket included.

## Scientific programme Thursday, 9<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Troidtog	Klokkeklang
	<b>MS 47: 3rd Generation Synchrotrons - Radiation Damage/Impact on Crystals</b> <b>Chairs: Matthias Wilmanns, Sean McSweeney</b>	<b>MS 50: X-ray or neutron optics and instrumentations</b> <b>Chairs: Hermann Franz, Esko Oksanen</b>
	<b>14:00 MS47-01 Kristina Djinovic-Carugo</b> <i>Dept. Struct. and Comput. Biol., Univ. Vienna, Austria</i> Current understanding of X-ray induced radiation damage on macromolecular crystals	<b>14:00 MS50-01 Horst Schulte-Schrepping</b> <i>Deutsches Elektronen-Synchrotron, Germany</i> Beamlines and Optics at PETRA III
	<b>14:30 MS47-02 Gleb Bourenkov</b> <i>EMBL-Hamburg, Germany</i> Systematic characterization of radiation sensitivity and its applications for MX data collection	<b>14:30 MS50-02 Clemens Schulze-Briese</b> <i>DECTRIS Ltd., Switzerland</i> MX at third generation synchrotrons: better data from real crystals
	<b>15:00 MS47-03 Lukas Lomb</b> <i>Max-Planck-Institute for medical Research, Germany</i> Serial femtosecond crystallography: structure determination and radiation damage analysis	<b>15:00 MS50-03 Joerg Wiesmann</b> <i>Incoatec GmbH, Germany</i> Multilayer Optics for X-ray Analytical Equipment - The past, the present and the future
	<b>15:20 MS47-04 Hans-Petter Hersleth</b> <i>Department of Molecular Biosciences, Univ. of Oslo, Norway</i> Radiation damage in haem and flavoproteins studied by in-situ single-crystal spectroscopy	<b>15:20 MS50-04 Gail N. Iles</b> <i>Helmholtz-Zentrum-Berlin, Germany</i> The New Neutron Laue Diffractometer at HZB
	<b>15:40 MS47-05 Desiree Heintz</b> <i>DESY - Hasylab, Germany</i> The Role of Hydrogen Abstraction in X-ray Radiation Damage	<b>15:40 MS50-05 Daniel M. Többers</b> <i>Helmholtz-Zentrum Berlin, Germany</i> E9 upgraded: the fine-resolution neutron powder diffractometer at BER II
16:00 – 17:00	<b>Poster session 2 with Coffee break</b>	

## Scientific programme Thursday, 9<sup>th</sup> August 2012 • afternoon

14:00 – 16:00	Gjendine	Salong Nina
	<p><b>MS 20:</b> Probing crystal structures at the nanoscale by quantitative electron crystallography</p> <p><b>Chairs:</b> Ute Kolb, Loisa Meshi</p>	<p><b>MS 34:</b> Aperiodic, short-range ordered and non-crystalline materials at ambient and non-ambient conditions</p> <p><b>Chairs:</b> Olga Degtyareva, David Keen</p>
	<p>14:00 <b>MS20-01</b> <b>Peter Oleynikov</b> <i>Stockholm University, Sweden</i></p> <p>Crystal structure determination using automated electron diffraction tomography</p>	<p>14:00 <b>MS34-01</b> <b>Ingo Loa</b> <i>The University of Edinburgh, United Kingdom</i></p> <p>Barium-IVc: A truly complex elemental crystal structure</p>
	<p>14:30 <b>MS20-02</b> <b>Lukas Palatinus</b> <i>Institute of Physics of the AS CR, Czech Republic</i></p> <p>Structure refinement against precession electron diffraction data</p>	<p>14:30 <b>MS34-02</b> <b>Arkadiy Simonov</b> <i>ETH, Switzerland</i></p> <p>Accessing disorder in single crystals by means of 3D-PDF analysis</p>
	<p>15:00 <b>MS20-03</b> <b>Sven Hovmöller</b> <i>Stockholm University, Sweden</i></p> <p>Solving structures of sub-micron crystals by rotation electron diffraction</p>	<p>15:00 <b>MS34-03</b> <b>Oliver Oeckler</b> <i>Leipzig University, Germany</i></p> <p>Ternary metastable rocksalt-type tellurides</p>
	<p>15:20 <b>MS20-04</b> <b>Holger Klein</b> <i>Institut Néel, CNRS &amp; Univ. J. Fourier, France</i></p> <p>The structure of nano-twinned rhombohedral <math>\text{YCuO}_{2.66}</math> solved by electron crystallography</p>	<p>15:20 <b>MS34-04</b> <b>Valentina F. Degtyareva</b> <i>Institute of Solid State Physics, Russia</i></p> <p>Low melting point of alkali metals under pressure: electronic origin</p>
	<p>15:40 <b>MS20-05</b> <b>Mahmud Kazimov</b> <i>Institute of Physics of Academy of Sciences, Azerbaijan</i></p> <p>New electron diffraction rotation methods</p>	<p>15:40 <b>MS34-05</b> <b>Maciej Zubko</b> <i>University of Silesia, Poland</i></p> <p>Model of short range order in 5,6-dichlorochinolino-5,8-dion organic compound</p>
16:00 – 17:00	<b>Poster session 2 with Coffee break</b>	

## Scientific programme Friday, 10<sup>th</sup> August 2012 • morning

08:30 – 09:30	Peer Gynt	Scene
	<b>KN13 Randy J Read</b> <i>University of Cambridge, United Kingdom</i> Extending the reach of molecular replacement Chair: Elisabeth Sauer-Eriksson	<b>KN14 Mark A Spackman</b> <i>University of Western Australia, Australia</i> Charge Densities and Crystal Engineering Chair: Peter Luger
09:30 – 10:00	<b>Coffee Break</b>	
10:00 – 12:00	Peer Gynt	Scene
	<b>MS 6: Bioinformatics informs MX</b> Chairs: Eugene Krissinel, Thomas Lütke	<b>MS 12: Molecular recognition</b> Chairs: Maria Carrondo, Annabelle Varrot
	10:00 <b>MS6-01 Jonathan M Diprose</b> <i>University of Oxford, United Kingdom</i> Bioinformatics at OPPF-UK	10:00 <b>MS12-01 Elisabeth Sauer-Eriksson</b> <i>Umeå University, Sweden</i> Structural basis of signal peptide recognition by the signal recognition particle
	10:30 <b>MS6-02 Gabor Bunkoczi</b> <i>University of Cambridge, United Kingdom</i> Applying bioinformatics to improve models for molecular replacement	10:30 <b>MS12-02 Mirjam Czjzek</b> <i>Station Biologique de Roscoff CNRS-UPMC, France</i> Structural determinants for the specific recognition of algal cell wall polysaccharides: examples of agarases and alginate lyases
	11:00 <b>MS6-03 Tim Wiegels</b> <i>EMBL Hamburg, Germany</i> Structural bioinformatics incorporated into ARP/wARP model building	11:00 <b>MS12-03 Isabel Bento</b> <i>ITQB, Portugal</i> Mapping conformational changes of the transcription factor AraR
	11:20 <b>MS6-04 Robbie P. Joosten</b> <i>Netherlands Cancer Institute, Netherlands</i> PDB_REDO: from bioinformatics data bank to crystallographic tool	11:20 <b>MS12-04 Ulrich Baumann</b> <i>University of Cologne, Germany</i> Structure of the Hsp47-Collagen Complex
	11:40 <b>MS6-05 William Duax</b> <i>Hauptman-Woodward Institute, United States</i> Fungal Ribosomal Proteins Trace Evolution from Bacteria to Metazoa and Archaea	11:40 <b>MS12-05 Julie Elisabeth Heggelund</b> <i>Norway</i> Molecular basis of cholera blood group dependence
12:00 – 13:30	<b>Lunch (C11, C12)</b>	

## Scientific programme Friday, 10<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Troldtog	Klokkeklang
	<b>MS 49: Crystallographic teaching</b> <b>Chairs: Santiago Garcia-Granda, Carl Henrik Görbitz</b>	<b>MS 40: Structure prediction for crystalline and amorphous molecular solids</b> <b>Chairs: Martin Schmidt, Aurora Cruz-Cabeza</b>
	<b>10:00 MS49-01 Annalisa Guerri</b> <i>Chemistry Department, University of Florence, Italy</i> Crystallography in Erice: Past, Present and Future	<b>10:00 MS40-01 Jacco van de Streek</b> <i>University of Copenhagen, Denmark</i> Crystal structure prediction of Pyridine with four molecules in the asymmetric unit
	<b>10:30 MS49-02 Eugen Libowitzky</b> <i>Institute of Mineralogy and Crystallography, Austria</i> The 10 two-dimensional crystallographic point groups - an interactive PowerPoint exercise	<b>10:30 MS40-02 Graeme M. Day</b> <i>University of Cambridge, United Kingdom</i> Towards the computation-led design of porous molecular crystals
	<b>11:00 MS49-03 Carlo Mealli</b> <i>CNR ICCOM, Italy</i> The European Crystallographic School (ECS): a permanent initiative to celebrate the IYCr	<b>11:00 MS40-03 Ogaga G Uzoh</b> <i>University College London, United Kingdom</i> A Computational Investigation of the Polymorphophore Concept
	<b>11:20 MS49-04 Laura Torre-Fernández</b> <i>Universidad de Oviedo, Spain</i> Cinema and Crystallography	<b>11:20 MS40-04 Mark D Eddleston</b> <i>University of Cambridge, United Kingdom</i> A novel approach to crystal structure determination for organic compounds
	<b>11:40 MS49-05 Fermín Otálora</b> <i>CSIC-UGr, Spain</i> Boosting Crystallography teaching from Spain	<b>11:40 MS40-05 Philipp Mörschel</b> <i>Goethe-University Frankfurt, Germany</i> Quantumcrystca: A new approach for the prediction of molecular crystal structures by a crystallographic QM-MM-shell-model
12:00 – 13:30	Lunch (C11, C12)	

C11: ECA Council Meeting 3, 12:00 – 13:30 in R4.

C12: GIG2-SC meeting 12:00 – 14:00 in R3.

## Scientific programme Friday, 10<sup>th</sup> August 2012 • morning

09:30 – 10:00	Coffee Break	
10:00 – 12:00	Gjendine	Salong Nina
	<b>MS 38:</b> Structure solution of minerals and inorganics by electron crystallography <b>Chairs:</b> Mauro Gemmi, Enrico Mugnaioli	<b>MS 36:</b> Towards megabar pressures: complex and geo-materials <b>Chairs:</b> Leonid Dubrovinsky, Wilson Crichton
	<b>10:00</b> <b>MS38-01</b> <b>Joke Hadermann</b> <i>University of Antwerp, Belgium</i> Different approaches to solving&refining inorganic structures from electron diffraction	<b>10:00</b> <b>MS36-01</b> <b>Hubert Huppertz</b> <i>University of Innsbruck, Austria</i> Borates under extreme conditions
	<b>10:30</b> <b>MS38-02</b> <b>Xiaodong Zou</b> <i>Stockholm University, Sweden</i> Solving 3D structures of nano- and intergrown porous silicates by combining electron crystallography and powder X-ray diffraction	<b>10:30</b> <b>MS36-02</b> <b>Alexei Bosak</b> <i>ESRF, France</i> Inelastic x-ray scattering: phonon spectroscopy under the extreme conditions
	<b>11:00</b> <b>MS38-03</b> <b>Chen Hong</b> <i>Stockholm University, Sweden</i> Crystal Structure Study for Nano-sized Zeolites With Rotation Electron Diffraction	<b>11:00</b> <b>MS36-03</b> <b>Eran Greenberg</b> <i>Tel-Aviv University, Israel</i> Pressure-induced structural and related electronic transitions in $\text{CaFe}_2\text{O}_4$ and $\text{Fe}_2\text{O}_3$
	<b>11:20</b> <b>MS38-04</b> <b>Iryna Andrusenko</b> <i>Johannes Gutenberg University, Germany</i> Vaterite structure from electron diffraction data – a definitive answer for an old question?	<b>11:20</b> <b>MS36-04</b> <b>Nadine Rademacher</b> <i>Goethe University Frankfurt, Germany</i> High pressure diamond anvil cell studies of carbon monoxide – viscosity, photochemical polymerization and laser heating
	<b>11:40</b> <b>MS38-05</b> <b>Stavros Nikolopoulos</b> <i>Nanomegas SPRL, Belgium</i> Precession coupled orientation / phase mapping on nanomaterials with TEM Cs microscopes	<b>11:40</b> <b>MS36-05</b> <b>Thomas Tschentscher</b> <i>European XFEL, Germany</i> High pressure research using dynamic compression at the European XFEL
12:00 – 13:30	Lunch (C11, C12)	

C11: ECA Council Meeting 3,12:00 – 13:30 in R4.

C12: GIG2-SC meeting 12:00 – 14:00 in R3.

## Scientific programme Friday, 10<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Peer Gynt	Scene
	MS 45: MX- Difficult problems and how to tackle them Chairs: Randy Read, Maryn Winn	MS 16: Crystal chemistry and phase transitions in materials at non-ambient conditions Chair: Fernando Camara
	13:30 <b>MS45-01</b> <b>Linda Reinhard</b> <i>Aarhus University, Denmark</i> New structural insights into the sodium pump	13:30 <b>MS16-01</b> <b>Santiago Garcia-Granda</b> <i>University Oviedo, Spain</i> Light-emitting lanthanide based organic-inorganic hybrids
	14:00 <b>MS45-02</b> <b>Daniel J Rigden</b> <i>University of Liverpool, United Kingdom</i> A cluster and truncate approach to processing ab initio models for Molecular Replacement	14:00 <b>MS16-02</b> <b>Serena C. Tarantino</b> <i>Universita di Pavia, Italy</i> Exotic unmixing processes in columbite-tapiolite minerals from the Nordic countries
	14:30 <b>MS45-03</b> <b>Kevin Pröpper</b> <i>Georg August University, Germany</i> DNA - Protein Complex Structure Prediction	14:30 <b>MS16-03</b> <b>Simon Welzmler</b> <i>Universität Leipzig, Germany</i> Substituted Ge-Sb-Te materials: structure, element distribution and thermoelectric properties
	14:50 <b>MS45-04</b> <b>Robert A Nicholls</b> <i>MRC Laboratory of Molecular Biology, United Kingdom</i> Low Resolution Refinement Tools in REFMAC5	14:50 <b>MS16-04</b> <b>Dean S Keeble</b> <i>University of Warwick, United Kingdom</i> A pair distribution function study of the disorder in a lead-free piezoelectric
	15:10 <b>MS45-05</b> <b>Sandra Pühringer</b> <i>Helmholtz-Zentrum Berlin, Germany</i> Structure determination by Multiple-wavelength anomalous dispersion (MAD) at the Pr LIII-edge	15:10 <b>MS16-05</b> <b>Irina Makarova</b> <i>Shubnikov Institute of Crystallography RAS, Russia</i> $M_nH_n(XO_4)_{(m+n)/2}$ crystals: structure, phase transitions, hydrogen bonds, conductivity
15:30 – 16:30	<b>Poster session 2 with Coffee break</b>	
16:30 – 17:30	Peer Gynt	Scene
	<b>KN15</b> <b>Neil R Champness</b> <i>University of Nottingham, United Kingdom</i> Metal-Organic Frameworks: Synthesis and Applications Chair: Pascal Dietzel	<b>KN16</b> <b>Björn Winkler</b> <i>Goethe University, Germany</i> Recent advances in Computational Crystallography Chair: Alexei Bosak
17:30 – 17:45	<b>Pause</b>	
17:45 – 18:30	<b>Peer Gynt</b>	
	Closing ceremony Poster prize awards Chair: The new ECA president / ECM27 chair	

## Scientific programme Friday, 10<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Troldtog	Klokkeklang
	<b>MS 29:</b> Likely to be useful: Statistical software packages <b>Chairs:</b> James Foadi, Gleb Bourenkov	<b>MS 33:</b> Neutrons and high-resolution X-ray diffraction for bio-crystallography <b>Chairs:</b> John Helliwell, Matthew Blakeley
	<b>13:30</b> <b>MS29-01</b> <b>Garib N Murshudov</b> <i>MRC Laboratory of Molecular Biology, United Kingdom</i> Statistics package R for prototyping in Macromolecular Crystallography	<b>13:30</b> <b>MS33-01</b> <b>Alberto D. Podjarny</b> <i>IGBMC, France</i> Protein Neutron Crystallography with “tiny” crystals of fully deuterated proteins
	<b>14:00</b> <b>MS29-02</b> <b>Manfred W. Baumstark</b> <i>Uniklinik Freiburg, Germany</i> R as a tool to check data quality in the context of low resolution crystallography	<b>14:00</b> <b>MS33-02</b> <b>Esko Oksanen</b> <i>ESS, Sweden</i> Surprising Protonation States in Urate Oxidase - Combining X-ray and Neutron Crystallography with QM/MM
	<b>14:30</b> <b>MS29-03</b> <b>Fabio Dall'Antonia</b> <i>European Molecular Biology Laboratory, Germany</i> Implementation of a B-factor validation protocol for macromolecular structures	<b>14:30</b> <b>MS33-03</b> <b>Stuart J. Fisher</b> <i>University of Salzburg, Austria</i> Determining protonation states in proteins using high-resolution X-ray crystallography
	<b>14:50</b> <b>MS29-04</b> <b>Oleg V. Sobolev</b> <i>Institute of Mathematical Problems of Biology RAS, Russia</i> Atomic shifts in unrestrained refinement can indicate alternative conformations	<b>14:50</b> <b>MS33-04</b> <b>Melina Haupt</b> <i>Institut Lave Langevin, France</i> Neutrons on the Loose: Tracking Down Weaknesses in the Hydrogen-Network of Tranthyretin
	<b>15:10</b> <b>MS29-05</b> <b>Michael Wedel</b> <i>MPI CPFS Dresden, Germany</i> Better data – proper redundancy	<b>15:10</b> <b>MS33-05</b> <b>Salyha Ali</b> <i>ILL, France</i> A joint neutron/X-ray crystallographic study on the mechanism of pectate lyase
15:30 – 16:30	<b>Poster session 2 with Coffee break</b>	



## Scientific programme Friday, 10<sup>th</sup> August 2012 • afternoon

13:30 – 15:30	Gjendine	Salong Nina
	<p><b>MS 19:</b> The importance of low temperature in charge density studies: history and future  <b>Chairs:</b> Hans-Beat Bürgi, Anders Madsen</p>	<p><b>MS 32:</b> Optimizing the use of Databases  <b>Chairs:</b> Peter Wood, Simon J. Coles</p>
	<p>13:30 <b>MS19-01</b> <b>Peter Luger</b>  <i>Institute for Chemistry, Free University Berlin, Germany</i>                      Synchrotron radiation and extremely low temperatures, best conditions for charge density work</p>	<p>13:30 <b>MS32-01</b> <b>Cheryl L Doherty</b>  <i>Pfizer, United Kingdom</i>                      Solid Form Design of Pharmaceutical Products</p>
	<p>14:00 <b>MS19-02</b> <b>Bartolomeo Civalleri</b>  <i>Department of Chemistry, University of Torino, Italy</i>                      Ab-initio lattice dynamics of molecular crystals and related properties with the CRYSTAL code</p>	<p>14:00 <b>MS32-02</b> <b>Clemens Vornheim</b>  <i>Global Phasing Ltd., United Kingdom</i>                      Improving the quality of protein-ligand complex structures</p>
	<p>14:30 <b>MS19-03</b> <b>Regine Herbst-Irmer</b>  <i>University of Göttingen, Germany</i>                      Resolution dependent scaling – a solution for problems in a multipole refinement?</p>	<p>14:30 <b>MS32-03</b> <b>Aurora J. Cruz-Cabeza</b>  <i>University of Amsterdam, Netherlands</i>                      Conformational bias in small-molecule crystal structures is rare (and explicable)</p>
	<p>14:50 <b>MS19-04</b> <b>Katarzyna N. Jarzemska</b>  <i>University of Warsaw, Poland</i>                      Interrelations between crystal architecture, charge density and energy of uracil derivatives</p>	<p>14:50 <b>MS32-04</b> <b>Sameer Velankar</b>  <i>Protein Data Bank in Europe, EBI, EMBL, United Kingdom</i>                      PDBe - Bringing Structure to Biology</p>
	<p>15:10 <b>MS19-05</b> <b>Konstantin V. Kamenev</b>  <i>University of Edinburgh, United Kingdom</i>                      Tiny diamond anvil cell for high-pressure crystallography at low temperature</p>	<p>15:10 <b>MS32-05</b> <b>Susanne Coles</b>  <i>United Kingdom</i>                      250 Structures later – Friendly Relationships in a Compound Family</p>
15:30 – 16:30	<b>Poster session 2 with Coffee break</b>	

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## Poster presentations

The poster sessions are split up into two parts scheduled on:

### Part 1 (Odd numbers)

Tuesday 7th August 2012 15:30 - 16:30

Wednesday 8th August 2012 16:00 - 17:00

### Part 2 (Even numbers)

Thursday 9th August 2012 16:00 - 17:00

Friday 10th August 2012 15:30 - 16:30

## MS-1: Protein crystallization and sample preparation

- MS1-P1**      **Cultivation at 6-10 is Effective to Overcome the Insolubility of Recombinant Proteins**  
Young Jun An (Korea Ocean Research & Development Institut, Republic of Korea)
- MS1-P2**      **Towards the Co-crystallization of Dihydroorotate dehydrogenase in Plasmodium falciparum and Plasmodium vivax with novel inhibitors**  
Rhawnie Carlsson (Gothenburg University, Sweden)
- MS1-P3**      **Structure-function studies of proteins operating on nucleic acids**  
Jan Dohnalek (Institute of Macromolecular Chemistry, Czech Republic)
- MS1-P4**      **The high resolution structure of the assembly domains of the S-layer protein SbsC**  
Andela Dordic (Karl Franzens University, Austria)
- MS1-P5**      **Additives changing the adhesion properties of macromolecules during crystallization process**  
Jindrich Hasek (Institute of Macromolecular Chemistry, Czech Republic)
- MS1-P6**      **Norwegian Structural Biology Centre**  
Ronny Helland (University of Tromso, Department of Chemistry, Norway)
- MS1-P7**      **Microseed it! A Theoretical and Practical Exploration of Seed Stability and Seeding Techniques for Successful Protein Crystallization**  
Stefan Kolek (Douglas Instruments, United Kingdom)
- MS1-P8**      **Structure of UvrA nucleotide excision repair protein in complex with modified DNA.**  
Elzbieta Nowak (IIMCB, Poland)
- MS1-P9**      **Fyn, Fab, Xap: Evaluation of different protein binders as crystallization facilitators.**  
Armin Ruf (F. Hoffmann-La Roche AG, Switzerland)
- MS1-P10**     **Mixing high oligomerization with low resolution, winding way! What's Key in Invertases?**  
Maria-Angela Sainz-Polo (Spanish National Research Council (CSIC), Spain)
- MS1-P11**     **Structure of eukaryotic 2'-O-ribose methyltransferase in complex with mRNA cap analogue**  
Mirosław Śmietaniński (IIMCB, Laboratory of Protein Structure, Poland)

- MS1-P12**     **Structural and functional studies of FNE, a bacterial adhesion protein of *Streptococcus equi***  
Mounira Tiouajni (IBBMC, Université Paris-sud 11, France)
- MS1-P13**     **Protein crystallization in gels: the better choice to grow crystals for structural determination**  
Alexander E.S. Van Driessche (LEC, IACT, CSIC-Univ.Granada, Spain)
- MS1-P14**     **Insulin Analogues for Insulin Receptor Studies and Medical Applications**  
Christopher J Watson (YSBL, University of York, United Kingdom)

## **MS-2: MX at Synchrotron Sources, including X-FELs and time-resolved crystallography**

- MS2-P1**     **Structural basis of the protein-protein interactions among ISC proteins involved in de novo Fe-S clusters biosynthesis**  
Kei Hirabayashi (Dept. of Biol. Sci., Grad. Sch. of Sci., Osaka Uni, Japan)
- MS2-P2**     **Terahertz Absorption change in Photosynthetic Reaction Center from *Rhodobacter sphaeroides* upon photoactivation**  
Ida V Lundholm (Department of Chemistry and Molecular Biology, Sweden)
- MS2-P3**     **BioMAX, a multipurpose high-throughput crystallography beamline at MAX IV**  
Thunnissen Marjolein (MAX IV laboratories, Lund University, Sweden)
- MS2-P4**     **The Cassiopeia suite of beamlines at the MAX IV Laboratory**  
Thunnissen Marjolein (MAX IV laboratories, Lund University, Sweden)
- MS2-P5**     **EMBL beamlines for life-science applications at PETRA III**  
Thomas R. Schneider (EMBL c/o DESY, Germany)
- MS2-P6**     **Structural biology beamlines at the Photon Factory**  
Yusuke Yamada (High Energy Accelerator Research Organization, Japan)

## **MS-3: Getting the best data from your crystal(s)**

- MS3-P1**     **Crystal Shape Recognition Software**  
Vaclav Eigner (Czech Republic)
- MS3-P2**     **New Tools for Biological Crystallography in the Home Lab**  
Severine Freisz (Bruker AXS, Germany)
- MS3-P3**     **Key metrics for single crystal 2D X-ray area detector systems.**  
Zoltan A. Gal (Agilent Technologies Ltd., United Kingdom)
- MS3-P4**     **XDSAPP - A graphical user interface for processing diffraction data using XDS**  
Uwe Mueller (Helmholtz-Zentrum Berlin, Germany)
- MS3-P5**     **PHOTON 100 CMOS Detecor for Crystallography**  
Holger Ott (Bruker AXS GmbH, Germany)
- MS3-P6**     **G-Rob: a flexible, multitask 6-axis robotic-arm based systems for crystallography**  
Xavier Vernede (IBS, France)

## MS-5: Advances in refinement and validation. Ligand chemistry

- MS5-P1 **Shelxle – a GUI for SHELXL**  
Christian B. Hubschle (Georg-August-University Goettingen, Germany)
- MS5-P2 **Using Partial Observations, Partial Models and Partial Residuals in Least Squares Refinement.**  
A. David Rae (the Australian National University, Australia)

## MS-7: Pharmaceutical crystallography - Drug design: success and failures

- MS7-P1 **Discovery of Novel Inhibitors of Bacterial beta-Lactamases using ARP/wARP-based Drug Design**  
Ciaran G Carolan (European Molecular Biology Laboratory, Germany)
- MS7-P2 **Structure determination of 9-[E]-2-(substituted-phenyl)ethenyl]-3,4,5,6,7,9-hexahydro-2H-xanthen-1,8-dione.**  
Joo Hwan Cha (Korea Institute of Science and Technology, Republic of Korea)
- MS7-P3 **Meformium guanyleurea salt of decavanadate, (HMet<sup>+</sup>)<sub>2</sub>(HGU<sup>+</sup>)<sub>4</sub>(V100286-) • 2H<sub>2</sub>O**  
Aungkana Chatkon (Suranaree University of Technology, Thailand)
- MS7-P4 **XRD, Vibrational, and Thermal Characterization of Theophylline:Carboxylic Acid Adducts**  
Kenneth Haller (Suranaree University of Technology, Thailand)
- MS7-P5 **Structural studies of cisplatin and carboplatin binding to histidine in a protein upto 1 year**  
John R Helliwell (University of Manchester, United Kingdom)
- MS7-P6 **Supramolecular Structure of Flavanone.**  
Nongnaphat Khosavithikul (Suranaree University of Technology, Thailand)
- MS7-P7 **Conformation and hydrogen bonding in amine salts of diclofenac**  
Carl H. Schwalbe (Aston University, United Kingdom)
- MS7-P8 **Crystal packing in methoxybenzyl and methoxyphenethyl-1,3,4-oxadiazole-2(3H)-thiones**  
Jim Simpson (University of Otago, New Zealand)
- MS7-P9 **Structural Characterization of Trypanosomatids Kinases: Targets to Drug Discovery**  
Tatiana A C B Souza (Brazil)
- MS7-P10 **Structural evidence for the specificity of anti-HIV lectin actinohivin in binding to the target alpha(1,2)-mannobiose**  
Akio Takenaka (Iwaki Meisei University, Japan)



## MS-8: Membrane proteins

- MS8-P1**      **Conformational changes in the Calcium Pump**  
Maïke Bublitz (Aarhus University, Denmark)
- MS8-P2**      **Nearly there: The structure of human aquaporin 2**  
Anna Frick (University of Gothenburg, Sweden)
- MS8-P3**      **SAXS analysis of membrane proteins reconstituted into nanodiscs**  
Michael Järva (Sweden)
- MS8-P4**      **Cardiotonic Steroids and the Na/K-ATPase**  
Jonas Lindholt (PUMPKIN, University of Aarhus, Denmark)
- MS8-P5**      **Crystal structure of Acid-sensing ion channel 1 in complex with the gating modifier Psalmotoxin 1.**  
Armin Ruf (F. Hoffmann-La Roche AG, Switzerland)
- MS8-P6**      **Glycosylation increases the thermostability of human aquaporin 10**  
Jennie A. Sjöhamm (university of Gothenburg, Sweden)
- MS8-P7**      **Towards the Structural Characterization of MgtA, a Magnesium transporter.**  
Saranya Subramani (UIO, Norway)
- MS8-P8**      **Proton translocating Pyrophosphatase**  
Yuh-Ju Sun (National Tsing Hua University, Taiwan)

## MS-10: Infection and Disease

- MS10-P1**      **Crystal structure of the human IgG4 CH3 dimer reveals the role of Arg409 in Fab-arm exchange**  
Anna Marie Davies (King's College London, United Kingdom)
- MS10-P2**      **Crystal Structure of Filamentous Aggregates of Human DJ-1**  
Min-Kyu Kim (Korea Ocean Research and Development Institute, Korea, Republic Of)
- MS10-P3**      **Structural studies of sarsin**  
Guennadi Kozlov (McGill University, Canada)
- MS10-P4**      **HP0315 from *Helicobacter pylori* as a VapD protein with an endoribonuclease activity**  
Ae-Ran Kwon (Daegu Haany University, Republic of Korea)
- MS10-P5**      **Auto-inhibitory assembly of protein kinase CK2 revealed by X-ray crystallography**  
Graziano Lolli (Università di Padova, Italy)
- MS10-P6**      **Crystal structure of Staphylococcal enterotoxin B in complex with two human immunoreceptors**  
Karin Rödström (Lund University, Sweden)
- MS10-P7**      **Structural details for the disassembly of the AAA-ATPase VCP/p97 by ASPL**  
Yvette Roske (MDC, Germany)
- MS10-P8**      **Structural and Functional Insights into Mycobacterium tuberculosis and Mycobacterium smegmatis Enhanced intracellular survival protein**  
Hye-Jin Yoon (Seoul National University, Korea, Republic Of)

- MS10-P9**      **Damaged guanine residue relevant to gastrointestinal cancer allows thymine residue to be flexible between Watson-Crick type pairing and large wobbling**  
Fang Zhang (Japan)

### MS-11: Frontiers in Structural Enzymology

- MS11-P1**      **Structure-function studies on the proteolytic activity of the *Marasmius oreades* agglutinin (MOA), a cytotoxic lectin**  
Gabriele Cordara (University of Oslo, Norway)
- MS11-P2**      **Crystallization and Structure Determination of *A. C. Sativus* Cysteine Protease**  
Sadaf Iqbal (ICCBS, University of Karachi, Pakistan)
- MS11-P3**      **Structural determinants of substrate specificity in a nitrilase superfamily amidase**  
Serah W Kimani (University of Cape Town, South Africa)
- MS11-P4**      **Crystal Structure of Enzyme-Substrate Complex of Protein-Glutaminase Obtained by the Mutant of Pro-Enzyme**  
Bunzo Mikami (Kyoto University, Japan)
- MS11-P5**      **Structural basis for the cytidylyltransferase reaction catalyzed by yeast ECT.**  
Jun Ohtsuka (University of Tokyo, Japan)
- MS11-P6**      **Identification and structure of a novel archaeal HypB for [NiFe] hydrogenase maturation**  
Daisuke Sasaki (Japan)
- MS11-P7**      **The 1-Cys Prx protein from cyanobacteria is a peroxidase and a chaperone**  
Uwe H. Sauer (Umea University, Sweden)
- MS11-P8**      **Hpy1881-DNA structures-snapshots of the GIY-YIG nuclease mediated catalysis.**  
Monika Sokolowska (International Institute of Molecular and Cell Biol, Poland)
- MS11-P9**      **Crystal structure and functional characterization of *Helicobacter pylori* DsbG**  
Hye-Jin Yoon (Seoul National University, Korea, Republic Of)

### MS-12: Molecular recognition

- MS12-P1**      **Structural Studies on the Metastasis associated S100A4 using X-ray Crystallography and small Angle X-ray Scattering (SAXS)**  
Annette Duelli (University of Gothenburg, Sweden)
- MS12-P2**      **The N-terminal domain of the CI repressor from bacteriophage TP901-1 in complex with DNA**  
Kristian H. Frandsen (Denmark)
- MS12-P3**      **Interaction Surface of Get3/Get4/Get5, a Complex Involved in Tail-Anchored Proteins Targeting**  
Chwan-Deng Hsiao (Academia Sinica, Taiwan)
- MS12-P4**      **Crystal structure of Lon protease**  
Chang-Sook Jeong (Korea Ocean Research and Development Institute, Republic of Korea)

- MS12-P5**     **Structural analysis of Nur and Zur from *Streptomyces coelicolor*.**  
Sangmin Lee (KORDI, Republic of Korea)
- MS12-P6**     **Structure, electrostatics and complexation of immune receptors and ligands.**  
Tereza Skalova (Institute of Macromolecular Chemistry AS CR, v.v.i, Czech Republic)
- MS12-P7**     **Mechanism for DNA recognition by transcriptional factor AdpA from *Streptomyces griseus***  
Masaru Tanokura (University of Tokyo, Japan)
- MS12-P8**     **The relevance of cyanobacterial Tic22 to plant and malarial protein transport**  
Ivo Tews (University of Southampton, United Kingdom)

### MS-13: Energy related materials

- MS13-P1**     **Title: Li-oxide garnet " $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ " doped with Fe: Chemical and structural properties and potential use as cathode materials in batteries**  
Georg Amthauer (University of Salzburg, Austria)
- MS13-P2**      **$\text{LiCoO}_2$ : from the precursors to the oxide**  
Jean-Pierre Brog (University of Fribourg, Switzerland)
- MS13-P3**     **Reactions of the  $2\text{LiBH}_4\text{-Mg}_2\text{FeH}_6$  assemblage for hydrogen storage**  
Michele Catti (University of Milano Bicocca, Italy)
- MS13-P4**     **Mixed-metal precursors for mixed-metal oxides**  
Claire-Lise Chanez (University of Fribourg, Switzerland)
- MS13-P5**     **Mg/Zn Mixed-Metal Borohydride for hydrogen storage: ab-initio periodic computational study of the phase stability and decomposition**  
Bartolomeo Civalieri (Department of Chemistry, University of Torino, Italy)
- MS13-P6**     **Structural and functional analysis of a GH12 from *Aspergillus terreus***  
Bruno A Dias (CTBE, Brazil)
- MS13-P7**     **Volatile heterometallic precursors for lithium ion battery cathodes**  
Evgeny V. Dikarev (University at Albany, SUNY, United States)
- MS13-P8**     **XRD analysis of superconducting  $\text{MgB}_2$  prepared by Reactive Mg Liquid Infiltration process**  
Giovanni Giunchi (EDISON S.P.A., Italy)
- MS13-P9**     **Crystal Structure Analysis of Layered Compounds  $\text{Cr}_x\text{TiS}_2$**   
Ken-ichi Ohshima (University of Tsukuba, Japan)
- MS13-P10**    **Proton conduction in geometrically frustrated lanthanum tungstate**  
Tobias Scherb (Helmholtz-Zentrum Berlin, Germany)
- MS13-P11**    **Structural richness of  $\text{Cr}^{6+}$  and  $\text{Cr}^{5+}$  oxysalt materials: new insights and trends**  
Oleg I. Siidra (Saint-Petersburg State University, Russia)
- MS13-P12**    **Crystal and twin structure in LSGMn crystals**  
Taras Tataryn (State Scientific-Research Control Institute, Ukraine)
- MS13-P13**    **Structure and morphology of nanosized  $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{1.9}/\text{Ni}$  infiltrate in a ceramic anode of a solid oxide fuel cell**  
Wei Zhang (Technical University of Denmark, Denmark)



## MS-14: Materials in operando and in situ crystallography of materials

- MS14-P1 **Crystal structure behaviour in the La(Pr)AlO<sub>3</sub>-TbAlO<sub>3</sub> systems**  
Tetyana Basyuk (Institute for Superhard Materials of NASU, Ukraine)
- MS14-P2 **High Pressure Crystallography on the CRISTAL beamline at SOLEIL synchrotron**  
Pierre Fertey (Synchrotron Soleil, France)
- MS14-P3 **Characterization of ceramics from Inner Mongolia using complementary diffraction techniques**  
Ralph Gilles (TU München, Germany)
- MS14-P4 **Novel rehydration mechanism of iron based Layered Double Hydroxides**  
Dorthe Haase (MAX-IV laboratory, Lund University, Sweden)
- MS14-P5 **G-Rob with Crystal Listing function for automated in situ diffraction and with robotic Crystal Harvesting.**  
Mohammad Yaser Heidari Khajepour (Institut de Biologie Structurale, France)
- MS14-P6 **Surface modification of calcium hydroxyapatite by etidronic acid**  
Masseoud Othmani (Faculty of science of Monastir, Tunisia)
- MS14-P7 **High pressure X-ray single-crystal and powder diffraction of SF6 up to 14 GPa.**  
Nadine Rademacher (Goethe University Frankfurt, Germany)
- MS14-P8 **High resolution electron microscopy study of the early stages of calcium sulfate formation**  
Alexander E.S. Van Driessche (LEC, IACT, CSIC-Univ.Granada, Spain)

## MS-15: Structural complexity of minerals and inorganic materials

- MS15-P1 **Crystal structure features of christofschäferite-(Ce) a new mineral of chevkinite-group**  
Sergey M. Aksenov (Shubnikov Institute of Crystallography of RAS, Russia)
- MS15-P2 **Crystal Structure of the Fluorite-like Nd<sub>5</sub>Mo<sub>3</sub>O<sub>16</sub> Compound**  
Olga Alekseeva (Shubnikov Institute of Crystallography RAS, Russia)
- MS15-P3 **A topological method for classification of entanglements in crystal networks**  
Evgeny V. Alexandrov (Samara State University, Russia)
- MS15-P4 **3D mapping of reciprocal space and structural complexity of A<sub>x</sub>Fe<sub>2-y</sub>Se<sub>2</sub> superconductor (A = Rb, Cs).**  
Alexei Bosak (ESRF, France)
- MS15-P5 **X-ray structure investigation of the minerals from lake-marsh ores**  
Anton A. Chuev (Cherepovets State University, Russia)
- MS15-P6 **Crystal structure of ~RCu<sub>3</sub>S<sub>3</sub> and ~RCuTe<sub>2</sub> (R = Gd-Lu) compounds**  
Marek Daszkiewicz (ILT&SR, Polish Academy of Sciences, Poland)
- MS15-P7 **Towards the solution of challenging crystal structures using Laue Microdiffraction**  
Catherine Dejoie (ETH Zurich, Switzerland)
- MS15-P8 **Progress in the Calcium-Palladium-Germanium system**  
Isa Doverbratt (Lund university, Sweden)

- MS15-P9** Relationship between structure of graphene layers and electrical properties of natural nanostructured carbon compounds  
Yevgeny A. Golubev (Institute of Geology of Komi SC of RAS, Russia)
- MS15-P10** Crystal structures of  $\text{NaLnF}_4$  (Ln = La, Ce, Pr, Nd, Sm, and Gd) studied with synchrotron single-crystal and powder diffraction  
Andrzej Grzechnik (RWTH Aachen, Germany)
- MS15-P11** Mineralogical composition of atmospheric dust in Pilsen studied by X-ray powder diffraction  
David Havlicek (Faculty of Science, Charles University in Prague, Czech Republic)
- MS15-P12** Number-theoretic Approaches to the Description of Crystal Structures  
Wolfgang Hornfeck (German Aerospace Center, Germany)
- MS15-P13** A systematic crystal chemical study of mixed stannides/germanides  
Michael Jehle (Institut für Anorganische und Analytische Chemie, Germany)
- MS15-P14** Crystal chemistry and electronic structures of oxidosulphido metallates  
Anna J. Lehner (Albert-Ludwigs-Universität Freiburg, Germany)
- MS15-P15** Boron in Mullites  
Hanna Luehrs (Universität Bremen, Germany)
- MS15-P16** Crystal structure and spectroscopic characterization of the 1D coordination polymer.  
Anissa Mansour (Université de Monastir, Faculté des Sciences de M, Tunisia)
- MS15-P17** Systematic investigation of the structure and the electronic requirements of the  $\text{Na}_{36}\text{Cd}_{24}\text{Ga}_{56}$  type.  
Viktoria Mihajlov (Albert-Ludwigs-Universität Freiburg, Germany)
- MS15-P18** Lattice thermal expansion of mullite-type  $\text{PbMBO}_4$  for M = Al, Ga, Fe and Mn  
Mangir Murshed (Germany)
- MS15-P19** Novel Hg-rich mercurides  $\text{BaHg}_6$  and  $\text{Ba}_{20}\text{Hg}_{103}$  and their ternary derivatives  
Caroline Röhr (Universität Freiburg, Germany)
- MS15-P20** Experimental and theoretical Electron Density in  $\text{MgB}_7$   
Vaness Sagawe (Germany)
- MS15-P21** Theoretical analysis of  $\text{MB}_2$ ,  $\text{M}_3\text{B}_4$  and  $\text{M}_5\text{B}_6$  (M=V, Nb, Ta, Cr)  
Vaness Sagawe (Germany)
- MS15-P22** Rumseyite,  $[\text{Pb}_2\text{OF}]\text{Cl}$ -fluoroxychloride mineral with the parent crystal structure for layered lead oxychlorides  
Oleg I. Siidra (Saint-Petersburg State University, Russia)
- MS15-P23** Diopside-titanian pargasite intergrowth: crystallography and formation mechanism  
Serena C. Tarantino (Universita di Pavia, Italy)
- MS15-P24** In situ high temperature study of structural transformation of cronstedtite-IT  
Serena C. Tarantino (Universita di Pavia, Italy)
- MS15-P25** Structure change and Peierls mechanism of metal-insulator transition in ferromagnetic  $\text{K}2\text{Cr}8\text{O}16$   
Yutaka Ueda (ISSP, University of Tokyo, Japan)
- MS15-P26** New chain diborate  $\text{TmH}[\text{B}_2\text{O}_5]$  and its relation to  $\text{GdH}[\text{B}_2\text{O}_5]$ : group-subgroup relation.  
Anastasya P. Zorina (Lomonosov Moscow State University, Russia)
- MS15-P27** Metasideronatrite-1M,  $\text{Na}_2\text{Fe}(\text{SO}_4)_2(\text{OH}) \cdot \text{H}_2\text{O}$ : a new polytype from Mezica (Slovenia).  
Fernando Camara (Universita di Torino, Italy)

## MS-16: Crystal chemistry and phase transitions in materials at non-ambient conditions

- MS16-P1** Studies of structural changes in  $K_9H_7(SO_4)8 \cdot H_2O$  single crystals with temperature.  
Tatiana Chernaya (Shubnikov Institute of Crystallography, RAS, Russia)
- MS16-P2** Synthesis and high-temperature characterization of mullite-type  $(Al_{1-x}Ga_x)_4B_2O_9$ .  
Thorsten M. Gesing (Inorganic Chemistry, University Bremen, Germany)
- MS16-P4** Temperature dependence of local structure change in lithium peroxide  
Yoshitaka Matsushita (NIMS, Japan)
- MS16-P5** Structure, elasticity, thermodynamics and high pressure behavior of  $ZnB_4O_7$  and  $CdB_4O_7$ .  
Leonore Wiehl (Institut für Geowissenschaften, Uni Frankfurt, Germany)
- MS16-P6** Phase transitions in  $KIO_3$   
Leonore Wiehl (Institut für Geowissenschaften, Uni Frankfurt, Germany)
- MS16-P7** HT behaviour of orthorhombic amphiboles: ferroholmquistite  
Michele Zema (University of Pavia, Italy)

## MS-18: New perspectives for charge density analysis: materials properties from inorganics to macromolecules

- MS18-P1** Electronic structure of the nickel(II) complex of the Schiff base and glycine  
Marek Fronc (FCHFT, Slovak Univ. of Technology, Slovakia)
- MS18-P2** Electrostatic interactions and sequence recognition by Zinc Fingers  
Anna M. Goral (University of Warsaw, Poland)
- MS18-P3** MoProViewer: a molecule viewer for the MoPro charge density analysis program  
Benoit Guillot (CRM2 Université de Lorraine, France)
- MS18-P4** Mosaic Structure of Single Crystals: Investigation of Mosaicity and Anisotropy of Pyrite.  
Anne K. Hüsecken (Universität Siegen / DELTA, Germany)
- MS18-P5** Physicochemical properties of hybrid organic-inorganic complexes via the charge density studies  
Radoslaw Kaminski (Department of Chemistry, University of Warsaw, Poland)
- MS18-P6** Charge Density Distribution of Diborides  
Boris N. Kodess (VNIIMS-ICS&E, Russia)
- MS18-P7** Charge Density Study on the Quinazoline Derivative Crystals  
Akmaljon Tojiboev (Namangan State university, Uzbekistan)

## MS-19: The importance of low temperature in charge density studies: history and future

- MS19-P1 **Dithiazyl Radicals - Structures and Charge Densities of their Crystals and Co-Crystals**  
Krzysztof Wozniak (Chemistry Department, University of Warsaw, Poland)

## MS-21: Crystal chemistry of aperiodic crystals and frustrated systems

- MS21-P1 **Structural impact of Pt on a  $\beta$ -brass related composite structure in the Zn-Pd system: a guided view by (3+1)-dimensional space description**  
Partha Pratim Jana (Lund University, Sweden)
- MS21-P2 **Multidimensional crystallography applied to critical phenomena**  
Céline Mariette (Institute of Physics of Rennes, France)
- MS21-P3 **Structure modulation and charge ordering in selfdoped  $M_xCuO_2$  crystals**  
Ognjen Milat (Institute of Physics, Croatia)
- MS21-P4 **Standard and non-standard settings of superspace groups**  
Sander van Smaalen (University of Bayreuth, Germany)

## MS-22: Quasicrystals, their approximants and surfaces: from the atomic to the nanoscale

- MS22-P1 **Ab initio structure analysis of hexagonal MnO using X-ray powder diffraction data**  
Yongil Kim (Korea Research Institute of Standards and Science, Republic of Korea)

## MS-23: Intermolecular interactions at ambient and extreme conditions

- MS23-P1 **Structural relations between particular and double brucinium diastereomeric salts**  
Agata Bialonska (Faculty of Chemistry, University of Wrocław, Poland)
- MS23-P2 **High Pressure Studies of a Trio of Polymorphs with Conformational Variability**  
Alexander J. Blake (University of Nottingham, United Kingdom)
- MS23-P3 **Charge density studies of halogen bond in crystals of chloro-nitrobenzene derivatives**  
Teresa Borowiak (Poland)
- MS23-P4 **Structural and energetic landscape of diboronic acids**  
Krzysztof Durka (Warsaw University of Technology, Poland)
- MS23-P5 **High pressure crystallography 2.0: harnessing the power of the crystallographers' community**  
Kamil F. Dziubek (Adam Mickiewicz University, Faculty of Chemistry, Poland)
- MS23-P6 **Supramolecular structure of an unusual Nevirapine derivative**  
Joao Ferreira da Silva (Centro Quimica Estrutural, IST, U Tecnica Lisboa, Portugal)
- MS23-P7 **Study of pressure-induced structural transformations in bis(glycinium)oxalate**  
Anna Ivanova (Shubnikov Institute of Crystallography, RAS, Russia)

- MS23-P8**     **Single crystal X - ray structure analysis of the complex  $[\text{Fe}(\text{btr})_3](\text{ClO}_4)_y(\text{BF}_4)_{2-y}$ .**  
Joachim Kusz (Institute of Physics, University of Silesia, Poland)
- MS23-P9**     **Contribution of weak S-H...X H-bonds to phase transitions in crystals of cysteine, its salts and derivatives under high pressures and low temperatures**  
Vasily S. Minkov (Institute of Solid State Chemistry and Mechanochem, Russia)
- MS23-P10**    **Chiral aggregation hierarchy in high-pressure resolved 2-butanol and 2,3-butanediol**  
Marcin Podsiadlo (Poland)
- MS23-P11**    **Challenges in small molecule XRD – Alkali Metal Organics from Ammonia**  
Dietmar Stalke (Georg-August University Goettingen, Germany)
- MS23-P12**    **Anion- $\pi$  interactions in pentafluorobenzyl-substituted ammonium salts**  
Arto Valkonen (University of Jyväskylä, Finland)
- MS23-P13**    **Molecular interactions in complexes of 4,4'-Dinitrophenyl**  
Petrus H van Rooyen (University of Pretoria, South Africa)
- MS23-P14**    **Non-covalent interactions in crystals of some heterocyclic compounds**  
Julia K. Voronina (Russia)
- MS23-P15**    **Amide hydrogen bonding vs. coordination?**  
Marijana Đaković (University of Zagreb, Faculty of Science, Croatia)

#### MS-24: Polymorphism and chirality in molecular crystals

- MS24-P1**     **Polymorphic behaviour of 5-chloro-3-phenyl-2(1H)-pyrazinone**  
Liliana Dobrzanska (Belgium)
- MS24-P2**     **Hydrogen/deuterium-exchange on small organic molecules and its influence on the molecular aggregation**  
Anna Kupka (Germany)
- MS24-P3**     **Design of Crystal  $Z'=2$  Structures: Obtaining, Search for Polymorphs**  
Olga A. Lodochnikova (A.E. Arbutov Institut of Org and Phys Chemistry, Russia)
- MS24-P4**     **The Exhibition of Isomorphism in Alkylammonium Halides with Rac-1,1'-Bi-2-naphthol**  
Emmanuel K. Owusu-Marfo (Chemistry Department, University of Cape Coast, Ghana)
- MS24-P5**     **Low-temperature & high-pressure polymorphism in a room-temperature ionic liquid**  
Sofiane Saouane (Georg-August-Universität GZG, Abteilung Kristallog, Germany)
- MS24-P6**     **Experimental and theoretical studies of the NLO properties of a chiral crystal**  
Pedro S. Silva (CEMDRX, Physics Department, University of Coimbra, Portugal)

#### MS-25: Design, structure, and function of multi-component crystals

- MS25-P1**     **Pharmaceutical Co-crystals with Isonicotinamide**  
Nikoletta B Bathori (Cape Peninsula University of Technology, South Africa)
- MS25-P2**     **Cocrystal constructed of one component?**  
Petra A Bombicz (DepStructChem InstOrgChem ResCentNatSci HungAcSci, Hungary)

- MS25-P3**     **Pyrazinamide cocrystals with dicarboxylic acids by liquid assisted grinding**  
Duane Choquesillo-Lazarte (Laboratorio de Estudios Cristalograficos, IACT-CSIC, Spain)
- MS25-P4**     **Solid-state Diels-Alder Cycloaddition via Charge-Transfer Complexes: Reaction of N,N'-bis(propylimino)-1,4-dithiin with 2-acetylanthracene**  
Manuel A. Fernandes (University of the Witwatersrand, South Africa)
- MS25-P5**     **New bifunctional thiacalix[4]arenes as potential heteroditopic receptors**  
Bulat M. Gabidullin (Institute of Organic and Physical Chemistry, Russia)
- MS25-P6**     **Metal-organic coordination networks with meso-tetra(3-carboxyphenyl)porphyrin**  
Israel Goldberg (Tel Aviv University, Israel)
- MS25-P7**     **Comparative study of glycine co-crystallization with dicarboxylic acids by various technique.**  
Evgeniy A. Losev (Institute of Solid State Chemistry and Mechanochem, Russia)
- MS25-P8**     **Preparation and characterization of an anti-inflammatory drug ethezamide cocrystals with dicarboxylic acids**  
Inese Sarceva (University of Latvia, Latvia)
- MS25-P9**     **Aminoguanidine and diaminoguanidine as adaptive cationic building blocks in organosulfonate structures**  
Arie van der Lee (France)

## MS-26: Porous materials for gas storage and other applications

- MS26-P1**     **Luminescent proton conducting lanthanide carboxyphosphonate open-framework hybrids**  
Miguel A. G. Aranda (University of Malaga, Spain)
- MS26-P2**     **Mesoporous Zr(IV) and Hf(IV) Metal-Organic Frameworks with reo topology**  
Irena Senkovska (Dresden University of Technology, Germany)
- MS26-P3**     **From Stimuli-Responsive Organic Dye Crystals to Photoluminescent Three-Dimension Open-Framework**  
Yu-Chuan Chang (National Tsing Hua University, Taiwan)
- MS26-P4**     **1D polymeric materials based on Mn(II), Zn(II), and Cd(II) pyridine-2-aldoxime**  
Lilia Croitor (Institute of Applied Physics of AS Moldova, Republic of Moldova)
- MS26-P5**     **Novel hybrid inorganic-organic one-dimensional chain systems tailored with monocarboxylic acids**  
Igor Djerdj (Rudjer Boskovic Institute, Croatia)
- MS26-P6**     **Optical Properties and Doping Effects of Divalent Tin Phosphite Grown from Deep-Eutectic Solvent**  
Hui-Lin Huang (Taiwan)
- MS26-P7**     **Synthesis and Structure Determination of a Highly Porosity Zinc Phosphite**  
Hsin You Lin (National Tsing Hua University, Taiwan)
- MS26-P8**     **New MOFs based on the unexplored linker 4,4'-dimethoxy-3,3'-biphenyldicarboxylic acid**  
Fredrik Lundvall (University of Oslo, Department of Chemistry/SMN, Norway)
- MS26-P9**     **Pressure-Induced Post-Synthetic Modification of a Metal-Organic Framework**  
Scott C McKellar (University of Edinburgh, United Kingdom)

- MS26-P10** **New Zn MOFS, topological relationships**  
Manuela E. Medina (ICMM, Spain)
- MS26-P11** **Solid-State Structural Transformations from 2D Interdigitated Layers to 3D Interpenetrated Structures.**  
Raghavender Medishetty (National University of Singapore, Singapore)
- MS26-P12** **Lanthanide MOFs: searching for efficient solvent-free catalysts.**  
Angeles Monge (ICMM-CSIC, Spain)
- MS26-P13** **Insight into the SBU variety in Alkaline-Earth Metal-Organic Frameworks**  
Ana E. Platero-Prats (Stockholm University, Sweden)
- MS26-P14** **A stable organic radical stacked by in situ coordination to Rare Earth cations.**  
Natalia Snejko (ICMM-CSIC, Spain)
- MS26-P15** **Synthesis, Crystal Characterization, and Luminescent Properties of Mixed Carboxylate Ligand Zn(II) Complexes**  
Weenawan Somphon (Kasetsart University, Thailand)
- MS26-P16** **A supramolecular 2:1 guanidinium-carboxylate-based building block for generation of extensive water channels and tetrameric water clusters.**  
Vitthal N. Yadav (Department of Chemistry, University of Oslo, Norway)

### MS-27: Molecular structures in catalysis and magnetism

- MS27-P1** **Structural Analysis and DFT Calculations of (Z)-1-[(5,6,7,8-tetrahydronaphthalen-1-ylamino)-methylene]naphthalen-2(1H)-one**  
Ahmet Erdönmez (Ondokuz Mayıs University, Turkey)
- MS27-P2** **Antiferromagnetic exchange interactions in a Cu(II) alternated chain**  
Manuela R Silva (University of Coimbra, Portugal)

### MS-28: Imaging using diffraction, spectroscopy or coherent signals

- MS28-P1** **Hyperspectral X-ray imaging using scattered radiation**  
Robert Cernik (University of Manchester, United Kingdom)
- MS28-P2** **Integrated XRD/SONICC/TPE-UVF for Identifying and Centering of Protein Crystals**  
Christopher M Dettmar (Purdue University, United States)
- MS28-P3** **The Nd-Gd chromium borates solid solutions: structures and phase relations.**  
Elena A. Dobretsova (Lomonosov's Moscow State University, Russia)
- MS28-P4** **Isolated Heptanuclear Bi-capped Dicubane SBUs in a Lanthanide-MOF Series : Structural, Topological, and Luminescent Behavior.**  
Enrique Gutierrez-Puebla (ICMM-CSIC, Spain)
- MS28-P5** **Gapless Dispersion Surfaces in Diffraction Physics.**  
Tetsuo Nakajima (Saitama Institute of Technology, Japan)
- MS28-P6** **Atomic ordering in PbMgTaO recovered from the anomalous x-ray scattering.**  
Zbynek Sourek (Institute of Physics, Academy of Sciences, Czech Republic)

## MS-31: "How-to"

- MS31-P1** Importance of hydrogen atoms in small molecules.  
Horst Borrmann (Max Planck Institute for Chemical Physics of Solid, Germany)

## MS-33: Neutrons and high-resolution X-ray diffraction for bio-crystallography

- MS33-P1** Neutron Data Collection at Room Temperature with Tiny Crystals of Perdeuterated Proteins  
Andre Mitschler (France)

## MS-34: Aperiodic, short-range ordered, and non-crystalline materials at ambient and non-ambient conditions

- MS34-P1** In-situ GISAXS study of a nanoparticle Langmuir film formation for plasmonic applications.  
Matej Jergel (Institute of Physics, Slovak Academy of Sciences, Slovakia)
- MS34-P2** Stacking disorder and diffuse scattering in the  $\beta$ -phase of Pigment Red 170 explained by lattice-energy minimizations  
Jaroslav L. Teteruk (Goethe University, Germany)
- MS34-P3** The average structure of disordered  $\beta$ -Pigment Red 170  
Rangana S. Warshamanage (University of Zurich, Switzerland)

## MS-35: Ferroic and multiferroic materials

- MS35-P1** Diffraction methods for detailed studies of the Dzyaloshinskii-Moriya ferroics  
Vladimir E. Dmitrienko (Institute of Crystallography, Russia)
- MS35-P2** Structural phase transitions related to magnetic phenomena in  $\text{CuCrSe}_2$  and  $\text{AgCrSe}_2$  magneto-elastics.  
Anna Gagor (Instytut Niskich Temperatur i Badań Strukturalnych, Poland)
- MS35-P3** Crystal structures and stability of trigonal  $\text{KLnF}_4$  fluorides ( $\text{Ln} = \text{Y, Ho, Er, Tm, and Yb}$ ).  
Andrzej Grzechnik (RWTH Aachen, Germany)
- MS35-P4** Kamiokite: A new multiferroic mineral  
Gwilherm Nénerit (Institut Laue Langevin, France)
- MS35-P5** Panoramic phase diagrams of  $\text{BiFeO}_3$  – based solid solutions  
Pavel Teslenko (Russia)
- MS35-P6** Lead-free piezoelectric composites produced by 3D additive manufacturing  
David I Woodward (University of Warwick, United Kingdom)



### MS-36: Towards megabar pressures: complex and geo-materials

- MS36-P1 **Crystal Chemistry of Fe,Al-bearing Silicate Perovskites at High Pressures and Temperatures**  
Leonid Dubrovinsky (BGI, Germany)
- MS36-P2 **Theoretical Probe on Effect of High Pressure on Thermophysical Properties of Perovskite Rare Earth Manganites**  
Archana S. Srivastava (Sri Sathya Sai College for Women, India)

### MS-37: Electron Crystallography on functional materials

- MS37-P1 **Line Edge Roughness estimation in SEM images of lithographic nanostructures**  
Konrad Bojar (PIAP, Poland)
- MS37-P2 **Study of Na<sub>0.44</sub>MnO<sub>2</sub> by Manual Diffraction Tomography using Beam Precession TEM method**  
Athanasios S Galanis (Department of Biology, University of Patras, Greece)
- MS37-P3 **Oxygen Diffusion and Structural and Properties in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4+d</sub>**  
Jürg Schefer (Paul Scherrer Institut, Switzerland)
- MS37-P4 **Bimodal domain configuration and wedge formation in tetragonal Pb[Zr<sub>1-x</sub>Ti<sub>x</sub>]O<sub>3</sub>**  
Ljubomira Ana Schmitt (TU Darmstadt, Germany)
- MS37-P5 **Surface Structural Inhomogeneities and Fractal Properties of MnO<sub>2</sub> Semiconductor Thin Films**  
Leonid Skatkov (Israel)

### MS-39: Electron diffraction and X-ray powder diffraction: getting the best of both worlds

- MS39-P1 **Peak broadening effects from nanocrystallite material: modeling of average shape.**  
Lars F Lundegaard (Haldor topsoe, Denmark)
- MS39-P2 **Nanostructured metal-polymeric catalysts**  
Marina A. Zaporozhetc (Shubnikov Institute of Crystallography of the RAS, Russia)

### MS-41: Dynamics in crystals: experimental techniques and software

- MS41-P1 **Symmetry analysis of IR, Raman and high-order Raman scattering phenomena on the Bilbao Crystallographic Server**  
Gemma de la Flor Martin (Universidad del Pais Vasco (UPV/EHU), Spain)
- MS41-P2 **Thermal motion in the Crystals of Octamethylanthracene, its Molecular Complexes and Ion-Radical Salts from Multi-Temperature Data.**  
Sergey V. Lindeman (Marquette University, United States)
- MS41-P3 **How to measure the Dynamics of Solid-Gas reactions**  
Luigi R Nassimbeni (University of Cape Town, South Africa)

## MS-42: Big "small molecules" and small "macromolecules" – learning techniques from each other

- MS42-P1 **Copper(I) Complexes of Bipyridine and Terpyridine with Fluorous Tails and the Formation of Crystalline Materials with Fluorous Layers.**  
Yael Diskin-Posner (Weizmann Institute of Science, Israel)
- MS42-P2 **Structure Solution and Refinement of "Small" Molecules**  
Yael Diskin-Posner (Weizmann Institute of Science, Israel)
- MS42-P3 **Zn(II) coordination in human and bovine bromo- and iodo-insulin hexamers**  
Dubravka Matkovic-Calogovic (Faculty of Science, University of Zagreb, Croatia)
- MS42-P4 **Multipolar refinement of amino acids with anisotropic H atoms treatment**  
Aleksandra E. Pazio (University of Warsaw, Poland)

## MS-43: Hot topics and structures in molecular chemistry

- MS43-P1 **Unusual Ligand Coordination Effects: Crystallographic Study of  $[\text{Re}(\text{CO})_3]^+$  Complexes.**  
Alice Brink (University of the Free State, South Africa)
- MS43-P2 **Theoretical Modeling And Experimental Studies On (E)-2-chloro-N-((5-nitrothiophen-2-yl)methylene)aniline.**  
Ümit Ceylan (Ondokuz Mayıs University, Turkey)
- MS43-P3 **Synthesis and Characterization of Diborane Compounds**  
Alexander A. Damme (University of Würzburg, Germany)
- MS43-P4 **Experimental and DFT Studies on Poly[okta- $\mu$ -3-acesulfamato-0,0:N,O';0',N:0,0-tetraquatetrabarium(II)] Complex.**  
Güneş Demirtaş (Ondokuz Mayıs University, Turkey)
- MS43-P5 **Selenium? Oxygen and Selenium? Bromine Contacts in a Hypervalent bis-(2-Selanyl-imidazolium)-benzene derivative.**  
Eberhardt Dr. Herdtweck (Technische Universität München, Germany)
- MS43-P6 **A proton transfer compound: pyridinium- fumarate**  
Wahiba Falek (Algeria)
- MS43-P7 **Synthesis, Crystal Structure and Thermal Behavior of Coordination Polymers Based on Zinc(II)**  
Eva Fernández-Zapico (Universidad de Oviedo, Spain)
- MS43-P8 **Understanding hybrid polymeric materials with N-salicylidene aniline derivatives: a structural approach**  
Pierre-Loïc Jacquemin (Université catholique de Louvain, Belgium)
- MS43-P9 **Trans-keto\* form emission in non photochromic N-salicylidene aminomethylpyridines: a structural study**  
Pierre-Loïc Jacquemin (Université catholique de Louvain, Belgium)
- MS43-P10 **Perpendicular versus coplanar conformation of  $\text{SeCl}_2$  moiety in hypervalent T-shaped adducts.**  
Victor N. Khrustalev (Nesmeyanov Institute of Organoelement Compounds, Russia)

- MS43-P11**    **Synthesis and Characterization of Novel Tantalum(V) and Niobium(V) Complexes containing N,O- and O,O'-Bidentate Ligands**  
Renier Koen (University of the Free State, South Africa)
- MS43-P12**    **Structures of Fischer multi-carbene complexes of furan and thiophene.**  
David C. Liles (University of Pretoria, South Africa)
- MS43-P13**    **Carbamates I: Structural and conformational study of eight methoxyphenyl-N-pyridinylcarbamates.**  
Pavle Mocijac (Dublin City University, Ireland)
- MS43-P14**    **(E)-2-[(2,4-dimethylphenylimino)methyl]-6-ethoxyphenol and (E)-2-[(2,4-dichlorophenyl imino)methyl]-6-ethoxyphenol**  
Hakki Yasin Odabasoglu (Pamukkale University, Turkey)
- MS43-P15**    **2,3-Dibromo-3aH,5H-4-oxa-9b-aza-cyclopenta[a]naphthalene-1-one**  
Mustafa Odabasoglu (Pamukkale University, Turkey)
- MS43-P16**    **Solid-State Photochromism of Chromenes**  
Keiichiro Ogawa (The University of Tokyo, Japan)
- MS43-P17**    **An Imidazolium-Substituted Pd<sub>3</sub>-Cycloheptatrienyl-Sandwich Complex**  
Alexander Pöthig (TU München, Germany)
- MS43-P18**    **Coordination and separation chemistry of hafnium oxinate complexes.**  
J. Augustinus Viljoen (University of the Free State, South Africa)

#### **MS44: Controlling and Monitoring crystal growth and quality**

- MS44-P1**    **Pb-doped KCl: from adsorption to habit and crystal structure modification**  
Dino Aquilano (University of Torino, Italy)
- MS44-P2**    **Tuning of micro  $\alpha$ -quartz crystals morphology by low hydrothermal synthesis methods**  
Dino Aquilano (University of Torino, Italy)
- MS44-P3**    **New modules for PiMS: data tracking of crystal handling protocols**  
Edward J. Daniel (University of Oulu, Finland)
- MS44-P4**    **X-ray Laue and Bragg diffraction on oxygen precipitates in annealed CZ-Si wafers**  
Mojmir Meduna (Masaryk University, Czech Republic)
- MS44-P5**    **The use of polystyrene organic-based gels for the diffraction quality single crystal growth of small molecules**  
Laura Menéndez-Taboada (University of Oviedo, Spain)
- MS44-P6**    **Broad solvent compatibility of polystyrene functionalised polystyrene gels for single crystal growth of small molecules.**  
Laura Rocas (Universidad de Oviedo, Spain)

## MS-45: MX - Difficult problems and how to tackle them

- MS45-P1** Crystallization of the photosynthetic core complex of *Blastochloris viridis*  
Elin A. Johansson (Sweden)
- MS45-P2** CCP4 6.3 – new and improved software tools for macromolecular crystallography  
Ville Uski (STFC Rutherford Appleton Laboratory, United Kingdom)
- MS45-P3** Setting high resolution limits for anisotropic data  
Melanie Vollmar (University of Oxford, United Kingdom)

## MS-46: Advances in powder diffraction: structure solution and structure-property relationships

- MS46-P1** Quantification of TiO<sub>2</sub> nanoparticles in samples of crystalline TiO<sub>2</sub>.  
Renie Birkedal (National Research Centre for the Working Environment, Denmark)
- MS46-P2** Highly-Oriented and Stressed Nanocrystalline ZnO Films Prepared by Pulsed Laser Deposition  
Radomír Kuzel (Charles University in Prague, Czech Republic)
- MS46-P3** Simulation of X-ray diffraction line broadening caused by stress gradients and determination of surface stress distribution by Fourier analysis  
Vladimir Monine (Polytechnic Institute/RJ State University, Brazil)
- MS46-P4** Effect of Cr-doping on structural, magnetic and electrical transport properties of LaO<sub>6</sub>7BaO<sub>3</sub>33Mn<sub>1-x</sub>Cr<sub>x</sub>O<sub>3</sub> (x<0.1) perovskites manganites  
Marouan Omezzine (Université Of Sciences Of Monastir, Tunisia)
- MS46-P5** Recognizing the better solutions in powder charge flipping runs  
Dubravka Sisak (ETH Zurich, Switzerland)

## MS-47: 3rd Generation Synchrotrons – Radiation Damage/Impact on Crystals

- MS47-P1** X-Ray-Induced Overall Structural Changes in a Protein Molecule at Cryogenic Temperatures  
Tatiana Petrova (Institute Mathematical Problems of Biology, RAS, Russia)

## MS-49: Crystallographic teaching

- MS49-P1** Symmetry groups in moroccan geometric patterns achieved on wood  
Youssef Aboufakil (Faculty of Sciences - Marrakech-Semalia, Morocco)
- MS49-P2** Crystallographic orientations and mechanical properties of metals  
Anton A. Chuev (Cherepovets State University, Russia)
- MS49-P3** The ARP/wARP model building suite and the Arnavigator user interface.  
Saul Hazledine (EMBL, Germany)
- MS49-P4** BioStruct – Norwegian Graduate School in Structural Biology  
Arne O. Smalås (NorStruct, University of Tromsø, Norway)

## MS-50: X-ray or neutron optics and instrumentations

- MS50-P1 Nanopositioning at beamline P11 at PETRA III**  
Pontus Fischer (DESY/HASYLAB, Germany)
- MS50-P2 A variety of techniques to asses particle size using a laboratory X-ray diffractometer**  
Jan A. Gertenbach (PANalytical BV, Netherlands)
- MS50-P3 High-brightness X-ray sources for biological crystallography**  
Juergen Graf (Incoatec GmbH, Germany)
- MS50-P4 The Testing of Modern Diffractometers for Type Approval**  
Boris N. Kodess (VNIIMS-ICS&E, Russia)
- MS50-P5 The Bio-Imaging and Diffraction beamline P11 at PETRA III**  
Alke Meents (DESY, Germany)
- MS50-P6 Two- and three-dimensional analytical X-ray techniques for analysis of crystalline materials**  
Hans te Nijenhuis (PANalytical B.V., Netherlands)





# ECM29

The 29<sup>th</sup> European Crystallographic Meeting  
August 23-28, 2015  
Rovinj, Croatia



*Welcome to Rovinj, Croatia!*

[ecm29.ecanews.org](http://ecm29.ecanews.org)

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## Exhibition

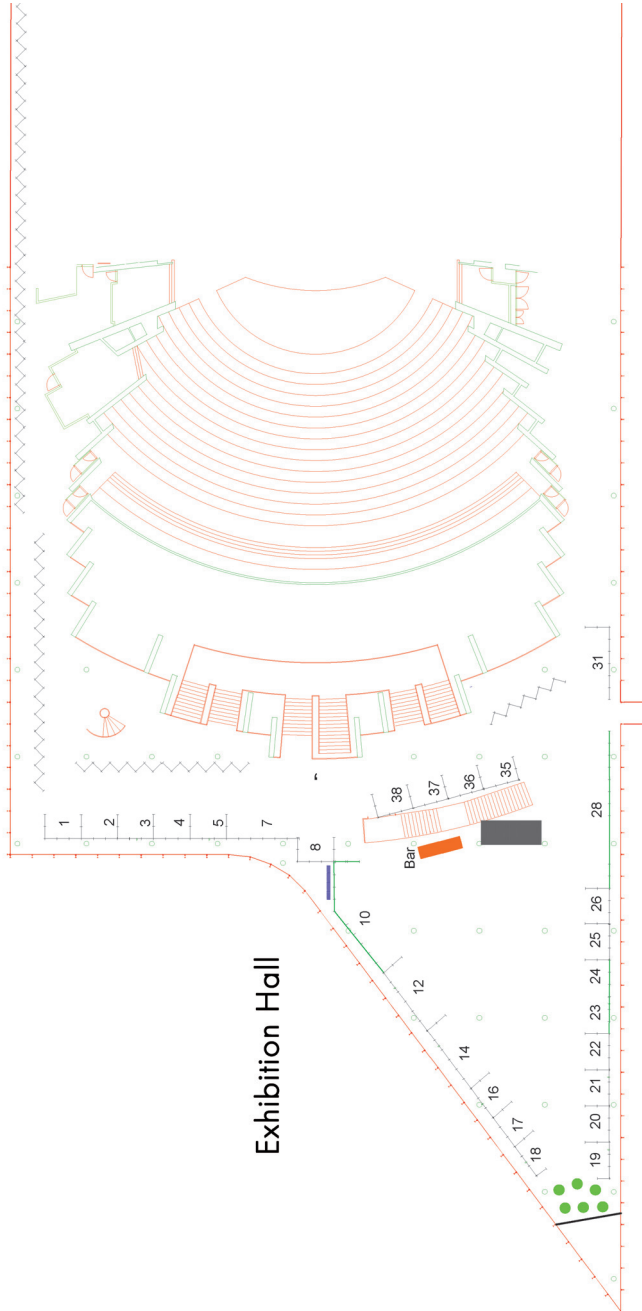
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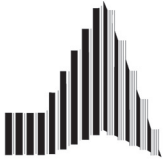
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Art Robbins Instruments (Asbach/DE)	16
AXO Dresden//Huber (Dresden/DE//Rimsting/DE)	38
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International Union of Crystallography (Chester/GB)	5
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MAX IV Laboratory (Lund/SE)	18
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NatX-ray (Saint Martin d ` Heres/FR)	26
Oxford Cryosystems (Long Hanborough/GB)	21
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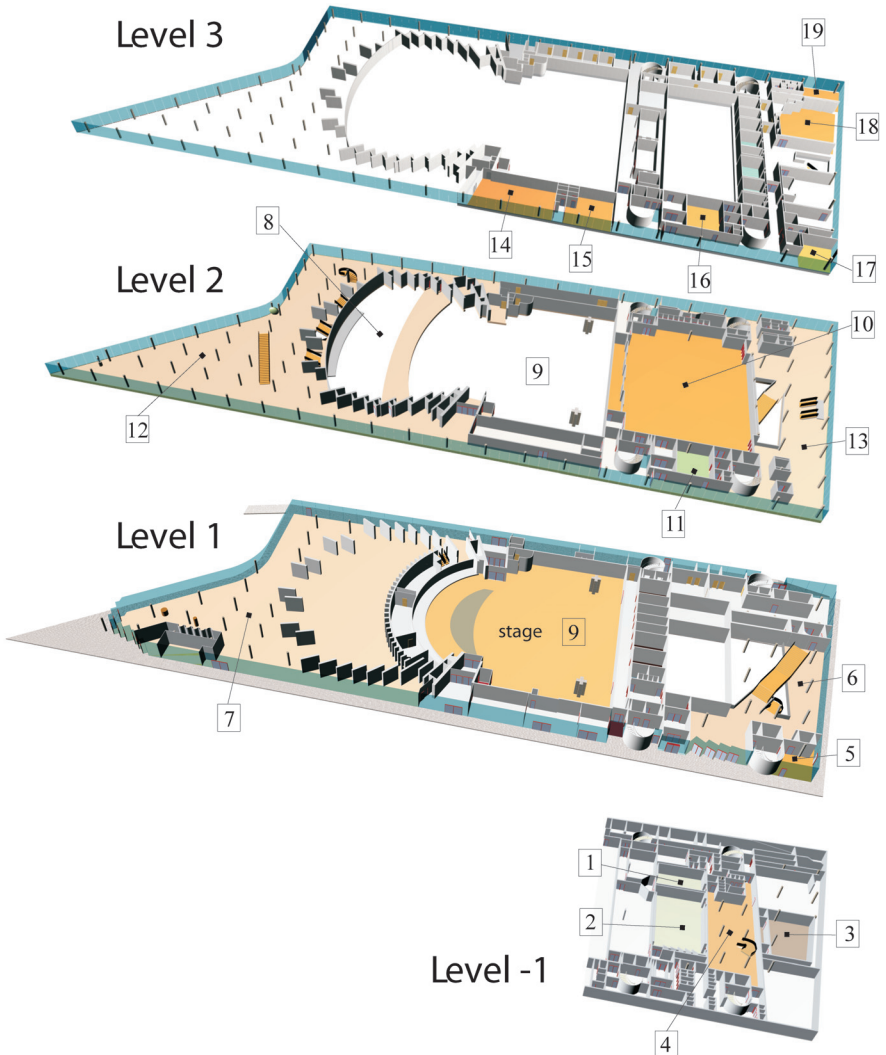


# Exhibition and Poster area





# GRIEG HALL MAP



## Meeting Venue map

### GRIEG HALL ROOM KEY

Level -1	1	Småttroll
	2	<u>Klokkeklang</u>
	3	<u>Gjendine</u>
	4	Foaje
Level 1	5	Glassrommet
	6	Foaje Peer Gynt
	7	Entrance Hall
	9	<u>Scene (Back Stage)</u>
Level 2	8	Grieg Concert hall
	9	Scene (Back stage upper level)
	10	<u>Peer Gynt hall</u>
	11	Bukken
	12	Exhibition Hall ('Spissen')
	13	<u>2PG</u>
Level 3	14	<u>Nina</u>
	15	Edvard
	16	Bøygen - Preview room
	17	Halling
	18	<u>Troldtog</u>
	19	Svane

Seminar rooms are underlined



# BioStruct

The Norwegian PhD network in Structural Biology

Workshops  
Courses  
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The PhD network welcomes all PhD-students and their research groups within molecular/structural biology and offers training in both experimental and theoretical methods for obtaining structural information of biological molecules.

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Courses and workshops are open for international participation.

## BioStruct courses 2012

Membrane proteins; from isolation to crystals  
(5 STP) UiO

Biophysical aspects of protein folding and stability  
(5 STP) UiT

Advanced glycobiology  
(10 STP) UiO

Structure guided drug discovery and design  
(5 STP) UiT

Protein crystal spectroscopy  
(5 STP) UiO

Crystallization of biological macromolecules  
(3 STP) UiT

Protein expression, purification and analysis  
(5 STP) UiB/EMBL

## BioStruct courses 2013

Synchrotron Data Collection  
(3STP) ESRF/UiT

Biomolecular NMR spectroscopy  
(5 STP) UiO

Advanced Biomolecular NMR  
(5 STP) UiO

Biomolecular Modelling  
(10 STP) UiB/UiT

Proteomics Basic  
(5 STP) UiO

Atomic Force Microscopy  
(3 STP) UiB

Biomolecular Structure and Function  
(10 STP) UiO

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## Venue

The Grieg hall

Edvard Griegs Plass 1

5015 Bergen, Norway

Tel. (switchboard): +47 55 21 61 00

<http://www.grieghallen.no/?l=en>

## Conference Dates

6 August–10 August 2012

## Conference Homepage

For latest information please visit <http://ecm27.ecanews.org/home.html>

## The congress registration fee includes

For ECA members, non-ECA members and students: Participation in all scientific sessions, admission to the scientific and commercial exhibition, all congress documentation, coffee and lunch breaks, opening ceremony & City of Bergen reception (first 400 participants).

Accompanying person: name badge, opening ceremony and City of Bergen reception (first 400 participants). Scientific Sessions are not open to accompanying persons.

## Arriving in Bergen

**By air** - You will arrive at the Bergen (Flesland) airport situated 20 km south of the city centre. The airport is small and handy with some 25 meters to walk from the customs exit to reach the outside. Directly by the exit, stands the airport bus that brings you to Bergen city in about 30 minutes, depending on traffic. These buses depart every 15 minutes during most of the day, and every 30 minutes early mornings and late evenings. The airport bus stops at several places in the city centre, the first being the bus and train station, only some five minutes' walk from the conference venue. The current price for a return ticket (valid 30 days) is 160 NOK (21.3 Euro) and a single journey is 100 NOK (13.3 Euro). This can be paid in cash (NOK only) or with MasterCard or Visa cards. Payment can only be made to the bus driver.

Students and senior citizens (+67) are eligible for a discount, for students upon presentation of student identification. Only an International Student Identity Card (ISIC) is accepted. For senior citizen a normal and valid proof of identification is required.

Behind the airport bus is the taxi stand. There are four companies in Bergen, two of which are dominating (Bergen Taxi and Norges Taxi). The price for a ride to the city centre depends on the number of persons, the day of the week and the time of day. As an indication only, a day-fare would amount to about 350-400 NOK for a car with up to 4 persons. Payment can be made with international cards or in cash. Bergen Taxi requires that the credit card be given to the driver before the drive starts. Read more here: <http://www.avinor.no/en/airport/bergen/tofromairport>

**By boat** - The 'proper' way to arrive in Bergen is by boat as this approach is the most scenic possible, as is the journey along the coastline. There is a regular ferry link with Denmark, please follow this link: <http://fjordline.com/> For extended information please read here: <http://www.visitbergen.com/en/TRANSPORT/>

**By train** - The train station is located at the city centre. Most passengers will be able to walk to the hotel, given good weather. Please study the map given under <http://ecm27.ecanews.org/conference-venue.html>

**By car** – Parking in the city centre is best done in parking houses as parking fines are substantial and the official politics is against cars in the city. During the summer season there is however no shortage of such parking space. The closest garage is under the conference venue, and the second closest is by the bus station, within a walk of some 3 minutes. The latter garage charges 10 NOK per 30 minutes or 130 NOK per 24 hours. A weekly card costs 600 NOK, then allowing an unlimited number of passages in and out of the garage during that period. Entering Bergen with a car is subject to a toll (from the registration plate by automatic camera). Rental cars normally have automatic toll transponders. Gasoline is 14.90 NOK and diesel 13.75 NOK per litre (July 2012).

### **Name badges**

Participants and registered accompanying guests will receive a name badge with their registration. Admission and access to the meeting and exhibition area is only allowed with a valid badge. Badges must be worn visibly throughout the congress and at the social activities. Exhibitor's badges will be provided for the staff of the exhibition stands.

### **Check-In & Registration**

Please find the check-in and registration desk in the foyer of the ground floor.

### **Wardrobe**

An (unattended) wardrobe is located next to the conference check-in in the foyer. You can hand in your items free of charge. The organisers accept no responsibility for items deposited.

### **Media check – Preview room**

Please find the media check and preview room “Bøygen” on level 3, room no. 16 in the venue map.

### **Internet**

The Grieg Hall provides free WLAN access to all participants.

### **Language**

The official meeting language is English. English is also generally spoken in hotels, restaurants and touristic areas.

### **Abstract publication**

The abstracts of the 27th European Crystallographic Meeting are published on an USB stick and as a printed book for those that requested it upon registration for the meeting against an extra fee. The abstracts will also be published later on as an online supplement in ActaCrystallographica A.

### **Commercial exhibition**

As part of the conference, an extensive industrial exhibition will take place. Please find an overview and a list of all exhibitors in the programme book. The exhibiting companies are looking forward to welcoming you!

### **Food and Catering**

Lunch and coffee will be served in the exhibition hall during the coffee and lunch breaks as included in the registration fee. A self-cost bar will also be available during daytime.

### **Calling to and from Norway**

The international access code for Norway is 47. International calls from Norway are made by dialling 00 + country code + city code + telephone number.

## Climate and Weather

Bergen has a typical west coast climate, without extreme heat in summer or cold in winter, relative to inland Scandinavia. Instead the mild and humid Atlantic air brings a lot of precipitation all year around as it hits land, albeit with the lowest numbers during the summer months. There is more or less continually a wind mostly from a SE/S/SW direction. In 2011, August gave 109 mm of rain (normal 190 mm) with an average wind of 2.7 m/s and a maximum observation of 10.1 m/s. The average temperature was 15.1 degrees C (normal 14.1). The highest value observed in August 2011 was 25.8, and the lowest 7.3 degrees C.

This calls for clothing that contains a jacket and shoes that tolerate rain. An easily portable umbrella is compulsory albeit it might not survive the trip due to the wind gusts!

You can study the Bergen weather forecast at this page: <http://www.yr.no/place/Norway/Hordaland/Bergen/Bergen/>

## Currency

The currency in Norway is the Norwegian Krona, NOK. The current (July 2012) exchange rate against the Euro is ~7.4, against GBP ~9.50 and against the USD ~6.10.

## Credit Cards

Major credit cards (MasterCard, Visa, Diners Club and American Express) are widely used in almost all major hotels, restaurants, shopping malls and stores. Please note that many smaller restaurants and shops do not accept foreign credit cards – only those issued in Norway! Therefore bring cash on your pocket or ask before ordering. ATM machines generally accept foreign cards for cash withdrawals.

## Electricity

The electric current in Norway is 240V AC.

## Medical emergencies

Medical emergency service operates 24 hours/7 days. Medical emergency telephone: 113. Police: 112. Fire brigade: 110.

## Insurance

The registration or accommodation fees do not include any kind of insurance. The meeting organisers will not assume liability for personal injuries sustained or for the loss or the damage to property belonging to the meeting participants (or their accompanying persons) either during or as a result of the meeting. All participants are invited to arrange for their own insurance. It is recommended to sign an insurance agreement (health, accident, travel) in your country of origin.

## Letter of Participation

A letter of participation will be sent to any individual requesting it after completing registration and acceptance of application by the Organising Committee.

## Time Zone

Time is one hour ahead of Greenwich Mean Time (GMT+1) in Norway



## Instructions for presenting authors

### Instructions on oral presentations

#### Media Check – Preview Room

Speakers are asked to submit their lectures at the Preview Room “Bøyggen” on level 3, room16 in venue map.

In general each speaker is to submit their talk to the Preview Room half a day in advance of the lecture. Hence, e.g. Tuesday morning speakers should do so on Monday afternoon, afternoon speakers on the morning of the same day, etc.

#### Preview Room opening hours:

Monday 6 <sup>th</sup>	14:00-18:30
Tuesday 7 <sup>th</sup>	07:30-17:00
Wednesday 8 <sup>th</sup>	07:30-17:00
Thursday 9 <sup>th</sup>	07:30-17:00
Friday 10 <sup>th</sup>	08:00-17:00

Please prepare your lectures either in PowerPoint format or as a PDF file. If you have special requirements (e.g. animations and/or sound) please contact the Preview Room **well in advance**. The usage of Apple and Open-Office formats as well as the usage of your own laptop are not standard but might be provided if communicated **well in advance**. The final decision on such matters lies with the Preview Room technician.

Video or audio data will in general only be accepted in the following formats: AVI, WMV, and MPG which have to be provided separately. If your presentation includes a video, please ensure that it encloses the right CODEC in order to be played correctly.

#### Speaker's time

To ensure the smooth implementation of all lectures, the speakers are **urged** to keep to the allocated time. Extra time taken by you is taken from a fellow lecturer! The chairs of each session are therefore requested to give due warnings towards the end of a talk and to disrupt the speaker if overriding time. Please advise the chair(s) of your session in advance about any changes or special requests that might occur concerning your presentation. The general speaking time of a lecture is fixed to either of 20 minutes (15 minutes talk plus 5 minutes discussion) and 30 minutes (25+5) for invited MS speakers. Plenary and keynote talks (60 minutes) are recommended to be maximum 50 minutes, allowing for a minimum of 10 minutes for discussions.

### Instructions for poster presentations

Each poster stays up for two days: Posters with **odd** numbers on Tuesday 7<sup>th</sup> and Wednesday 8<sup>th</sup>, posters with **even** numbers on Thursday 9<sup>th</sup> and Friday 10<sup>th</sup>.

#### The poster sessions are scheduled on:

Tuesday 7 <sup>th</sup>	15.30 – 16.30
Wednesday 8 <sup>th</sup>	16.00 – 17.00
Thursday 9 <sup>th</sup>	16.00 – 17.00
Friday 10 <sup>th</sup>	15.30 – 16.30

The poster boards are situated on level 2 in the direct vicinity of the commercial exhibition. The presenting author is expected to attend the official sessions or otherwise find a co-author to attend the session. The size of the posters should not exceed DIN A0 (84.1 \* 118.9 cm). Mounting materials will be provided. Please find the poster number of your poster in the abstract book. The poster number will also be attached to your poster wall by the staff. Posters are to be mounted from Monday 30 August 15.00 on, and should be removed by Friday 17.00.

No responsibility will be taken for posters that are not removed by the time requested. Posters left behind will not be returned. Presenters may also receive information about the exact place of their posters and/or any further details at the registration desk.



## Social events

### City of Bergen Reception



The city of Bergen greets us welcome to Bergen. This reception will follow directly after the ECM27 opening ceremony and Laue Centennial lecture. A brief come-together for drinks and nibble food prior to the scientific conference start. N.B. The number of attendees and time-span is defined by the City Council. Tickets are issued to the first 400 registered participants.

Date: Monday 6th

Place: Grieg Hall, Exhibition hall 'Spissen'

Time: 20:00-21:00

No Fee

Registration required (maximum 400 participants)

### Young Crystallographers Mixer – Sponsored by DECTRIS

# DECTRIS®

The mixer provides a great opportunity for young scientists (students, postgraduates, and early career scientists/teachers) to network and socialise under the auspices of GIG1- Young Crystallographers. This mixer will take place in a Persian restaurant 'Zafran' not far from the conference venue after the plenary lecture of Dan Shechtman. Drinks and a simple buffet style meal will be included. Self-cost drinks are available thereafter. Please note that the restaurant only accepts credit cards issued in Norway. Cash in the pocket is therefore advised.

Date: Wednesday 8th

Place: Restaurant Zafran, <http://zafran-restaurant.com/>

Address: Nygårdsgaten 53, in Bergen city.

Time: 20:30-24:00

No Fee

Registration required (maximum 60 participants)

## ECM27 Conference Dinner



'Fløien folkrestaurant' established in 1925, situated 320 metres above sea level and overlooking Bergen city and the harbour entrance has a spectacular architecture and location. It is reached either by foot up the hill from the city centre or more conveniently using the Floibanen funicular <http://www.floibanen.com/>. The cars can take up to 100 persons and the ride takes 6 minutes. It departs every 15 minutes between 10:00 and 20:30 and is open 07:30-23:00 weekdays. A return ticket is included for participants. **Participants should plan ahead so that all can be present on top for the opening at 19:30.** A great view of the city – or the clouds that cover it are guaranteed! Return rides after 23:00 will leave when a minimum of 30 people are waiting.

Date: Thursday 9th

Place: Fløien folkrestaurant. Departure from the funicular station on the corner of Småskansen & Proms gate.

Time: 19:30-24:00

Fee NOK 750

Registration required (maximum 300 participants)



## Plenary and keynote speakers

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Crystallography 2014**

watch events unfold at [www.iycr2014.org](http://www.iycr2014.org)

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Ratkaj, Marina	ZAGREB	CROATIA	
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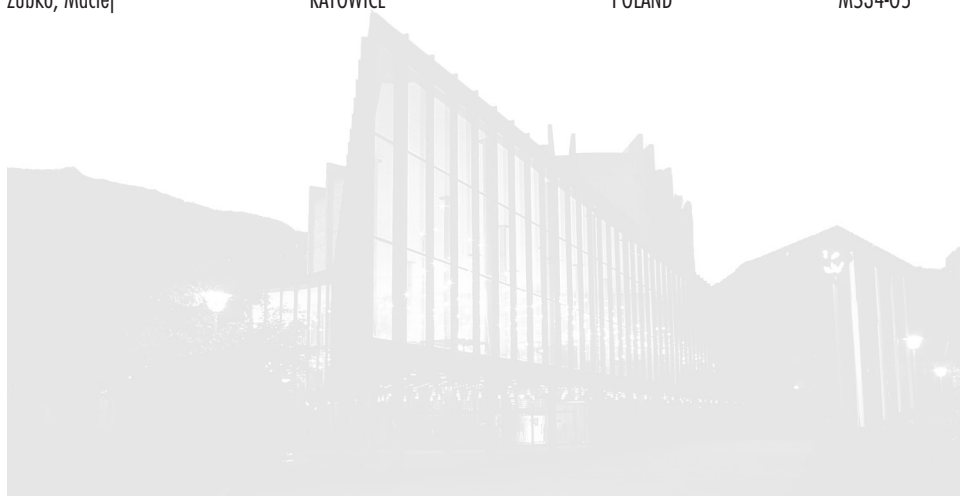
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Wiegels, Tim	HAMBURG	GERMANY	MS6-03
Wiehl, Leonore	FRANKFURT / MAIN	GERMANY	MS16-P5 MS16-P6
Wiesmann, Jörg	GEESTHACHT	GERMANY	MS50-03

Williams, Jane	OXFORD	UNITED KINGDOM	
Wilmanns, Matthias	HAMBURG	GERMANY	MS9-05
Wilson, Keith	DIDCOT	UNITED KINGDOM	
Winkler, Björn	FRANKFURT AM MAIN	GERMANY	KN16
Winn, Martyn	WARRINGTON	UNITED KINGDOM	
Winter, Marcus	OXFORDSHIRE	UNITED KINGDOM	
Wood, Peter	CAMBRIDGE	UNITED KINGDOM	
Woodward, David	COVENTRY	UNITED KINGDOM	MS35-03 MS37-04 MS35-P6
Wozniak, Krzysztof	WARSAWA	POLAND	MS19-P1
Wragg, David S.	OSLO	NORWAY	MS14-03
Xie, Dan	RICHMOND, CA	UNITED STATES	MS46-01
Yadav, Vitthal	OSLO	NORWAY	MS26-P16
Yamada, Kazuhiro	ZURICH	SWITZERLAND	MS3-03
Yamada, Yusuke	IBARAKI	JAPAN	MS2-P6
Yano, Junko	BERKELEY	UNITED STATES	MS2-02
Yoon, Hye-Jin	SEOUL	KOREA, SOUTH	MS10-P8 MS11-P9
Yuan Wahlgren, Weixiao	ÖSTERSUND	SWEDEN	MS42-04
Zakharov, Boris	NOVOSIBIRSK	RUSSIA	MS41-05
Zaporozhetc, Marina	MOSCOW	RUSSIA	MS39-P2
Zema, Michele	PAVIA	ITALY	MS16-P7
Zhang, Fang	IWAKI	JAPAN	MS10-P9
Zhang, Wei	ROSKILDE	DENMARK	MS13-P13
Zorina, Anastasya	MOSCOW	RUSSIA	MS15-P26
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