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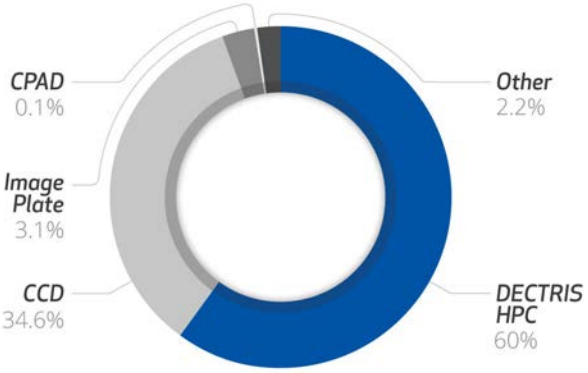

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Organisation and Committees

Date and Venue

18. August – 23. August 2019
University of Vienna, Universitätsring 1, A-1010 Wien, Austria

Scientific Organisation

European Crystallographic Association (ECA), www.ecanews.org

Department of Structural and Computational Biology,
Max Perutz Labs, University of Vienna

X-ray Center (XRC), TU Wien

Institute of Mineralogy and Crystallography,
University of Vienna

Conference Chairs

Kristina Djinovic-Carugo
Klaudia Hradil
Ronald Miletich

Professional Conference Organisation (PCO)

Gerry Schneider, Event Management, University of Vienna

Design / Layout / Print

Content/Design: Ronald Miletich, Manfred Wildner
Layout: Manuela Schmidt (manuschmidt.com)
Print: MAßGEDRUCKT® (www.massgedruckt.at)

Local Organising Committee (LOC)

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Klaudia Hradil (Financial, Social Events, Satellites, ECM32 Chair)
Ronald Miletich (Exhibition, Sponsoring, ECM32 Chair)
Gerry Schneider (Professional Conference Organisator)
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Helga Lichtenegger, (Wien, Austria) Focus Area 3
Michael Reithofer (Wien, Austria), Focus Area 4
Oskar Paris, (Leoben, Austria), Focus Area 5

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Annalisa Guerri (Italy), GIG-3

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Teresa Duarte (Portugal), SIG-13
Anders Østergaard Madsen (Denmark), SIG-14

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Wulf Depmeier (IUCr Executive Committee)
Jan Dohnálek (ECA Executive Committee)
Berthold Stöger (Chair of Bursary Committee)
Santiago Garcia-Granda (ECM31)
Chairs of ECM32
GIG and SIG Representatives
National Representatives of Focus Areas

[1] The entire programme committee is composed from delegates including the national representatives of the focal areas and the representatives of the GIGs and SIGs in addition to delegates with designated functions (see also https://ecm2019.org/home/committees).

Welcome Note ECM32

Dear Participant of ECM32, dear Crystallographers and Friends!

On behalf of the entire team of local organizers it is our pleasure to welcome all participants of ECM32 to Vienna.

The local organizers and programme committee set up an attractive programme covering the latest advances in crystallography and in all fields of applications within the scope of almost 800 scientific contributions. Together with the pre-conference satellite events, various workshops, the second ECM Science Slam and the Young Crystallographer's Mixer, many other social events such as the Conference Concert in the Votivkirche, the Conference Dinner at Schönbrunn, and touristic and scientific excursions will complete a vibrant six-days programme of ECM32.

It is important for us to express our gratitude to all sponsors, exhibitors, institutions and foundations for their generous support, to all our volunteers and numerous helping hands for their time and effort, as well as to the organisers of previous ECMs for sharing their valuable experiences. Last but not least we would like to thank in particular you for coming to Vienna and for making this conference a success with your participation.

Wishing you a pleasant and scientifically fruitful meeting, and make also sure to enjoy the amenities of the city of Vienna and the famous Austrian hospitality.

Klaudia Hradil
Kristina Djinovic-Carugo
Ronald Miletich

Chairs of the ECM32 Organisation Committee



Welcome Note Rectors of the Host Universities

The Vice Rectors for Research of the University of Vienna and the TU Wien are pleased to welcome you to the *European Crystallographic Meeting (ECM32)* held at the University of Vienna, Austria.

Within the scope of visible joint activities, Kristina Djinovic-Carugo, Klaudia Hradil and Ronald Miletich-Pawliczek from the University of Vienna and the TU Wien took the initiative to organize this meeting jointly by the two main universities in Vienna. This initiative is not only highly supported by the Austrian National Committee for Crystallography, but also endorsed by the Austrian universities and the main research facilities, and in particular by all scientists and colleagues being active in the field of crystallography across our country.

Both universities have defined the field of material science as one of the research focal areas in their research profiles. Crystallography provide considerable contributions to the scientific output in these research fields, both using crystallographic methods for materials characterization and theoretical considerations (concerning symmetry) as principles and foundations for modelling new materials. Therefore, the topics of the congress link chemistry, physics and material sciences. Moreover, crystallographic methods also contribute to the analysis of fine arts objects and thus establish a context with the cultural heritage background of Vienna.

We wish you a very successful and hopefully memorable scientific event in Vienna.

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Jean-Robert Tyran
Vice Rector for Research, University Vienna

Johannes Fröhlich
Vice Rector for Research, TU Wien

Welcome Note ECA President

Fellow crystallographers, dear participants and guests of ECM32

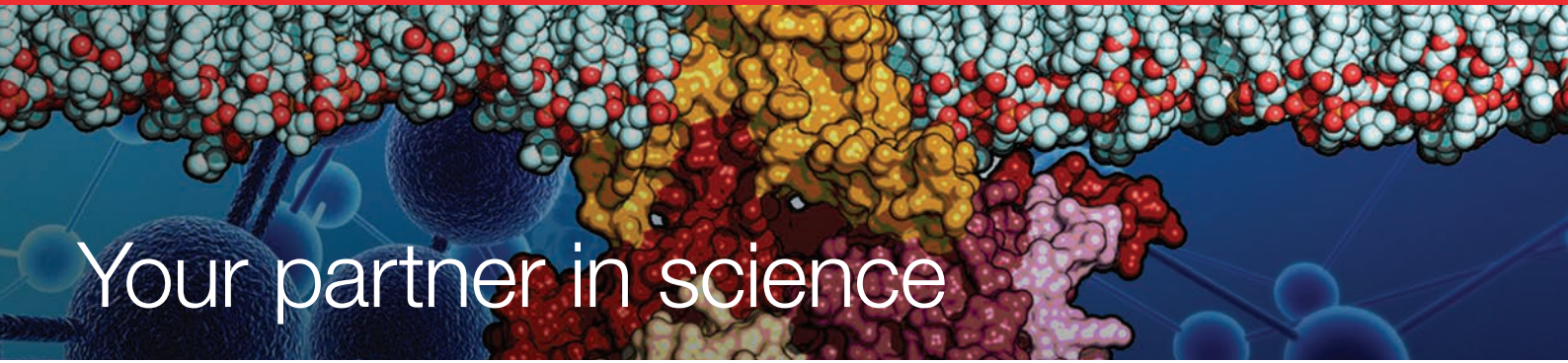
On behalf of the European Crystallographic Association, it is my greatest pleasure to welcome you to the annual gathering of European crystallography in the beautiful city of Vienna.

The European Crystallographic Meetings have a long and cherished tradition dating back to 1973, when ECM1 was held in Bordeaux, France. Since then, the ECMs have expanded considerably, both in attendance and scientific scope. Those of you who participated in some of the earlier ECMs will certainly remember exciting scientific presentations in your narrower field of research, eye-opening keynote and plenary talks as well as meeting old and making new friends. You may be in for more cutting-edge crystallography and stimulating social events at ECM32.

More than thirty years after ECM11 was held in Vienna in 1988, European crystallographers are returning to Austria in the heart of the continent. How much has changed since then in every aspect of science and of everybody's life! I thank you for your continued support of the European Crystallographic Association and its meetings and look forward to meeting all of you in Vienna.

Udo Heinemann
President of the European Crystallographic Association

thermo scientific



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Venue and Exhibition

The Conference Site

Lecture Halls and Meeting Rooms

Poster Area

Exhibition Area and Exhibitors

World's Largest Crystal Structure Model

The Conference Site

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We welcome you to the historic Main Building of the University of Vienna, which will host the venue of the ECM32.

The main building is located within Vienna's historic centre directly on Vienna's most magnificent boulevard, the *Ringstraße*. The building was designed by the Austrian architect *Heinrich Ferstel* in the Historicist style and opened in 1884.

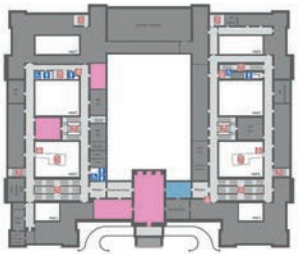
Offering more than 28 lecture halls and impressive ceremonial chamber rooms you can enjoy a unique and historical flair during ECM32. Moreover, the green space of the Arcaded Courtyard will provide a central atmospheric location for our conference with hopefully memorable impressions.

© Universität Wien

Lecture Halls and Meeting Rooms

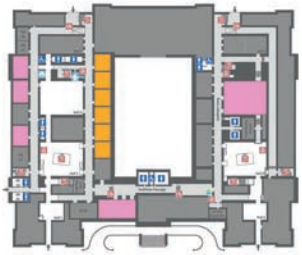
The rooms used for ECM32 are distributed over the **ground floor** (Hochparterre, **HP**), the **semi basement** (Tiefparterre, **TP**), and the **first floor** (1. Obergeschoß, **1.OG**).

Room Name	(abbreviation)	Floor	Purpose of Use at ECM32
Arcaded Courtyard	-	HP	Exhibition, Welcome Reception, Poster Area
Aula	(Aula)	HP	Registration Desk, Meeting Point
Auditorium Maximum	(Audimax)	TP	Opening, Closing, Lectures (PL, KN, MS, Public)
Großer Festsaal	(Gr. FS)	1.OG	Lectures (MS, KN)
Kleiner Festsaal	(Kl. FS)	1.OG	Lectures (MS, KN), Luncheons
BIG Hörsaal	(BIG HS)	TP	Lectures (MS)
Hörsaal 3	(HS3)	TP	Sunday Workshop
Hörsaal 5	(HS5)	TP	ECA Council Meetings, ECA Exec. Comm. Meetings
Hörsaal 6	(HS6)	TP	Sunday Workshop
Hörsaal 7	(HS7)	HP	Lectures (MS)
Hörsaal 16	(HS16)	HP	Wardrobe, Exhibitor supply
Hörsaal 32	(HS32)	1.OG	Lectures (MS)
Hörsaal 33	(HS33)	1.OG	Lectures (MS)
Marietta Blau Saal	-	HP	Child-Care Facility
Seminarraum 1	(SR1)	TP	SIG/GIG Meetings, ECA Executive Comm. Meeting
Seminarraum 2	(SR2)	TP	SIG/GIG Meetings
Seminarraum 3	(SR3)	TP	SIG/GIG Meetings, ECM33 Programme Meeting
Seminarraum 4	(SR4)	TP	SIG/GIG Meetings
Seminarraum 5	(SR5)	TP	SIG/GIG Meetings
Seminarraum 6	(SR6)	TP	Software Fayre
Garderobe Senatssaal	-	1.OG	Viennese Waltz Dancing Course



1.OG

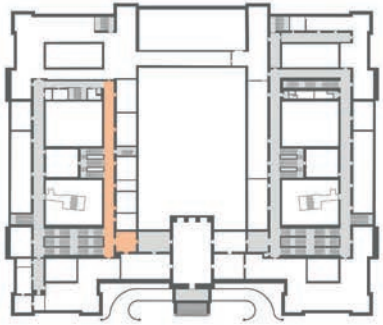
HP



TP

Poster Area

The two poster sessions are organized **on the ground floor** (195 posters in **areas** A, B, C, D) under the arcades and **on the first floor** (81 posters in **area** E) in the south wing of the building next to the Kleiner Festsaal.



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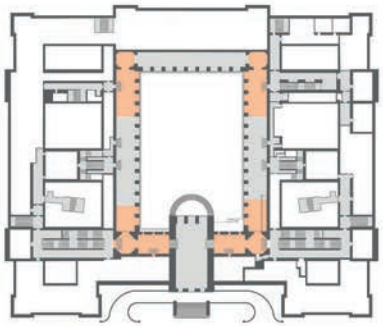
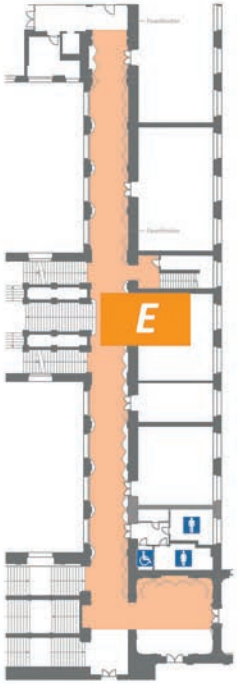
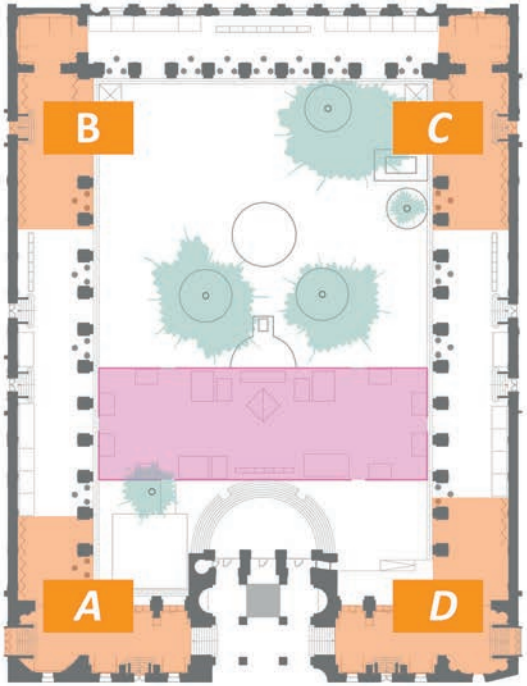


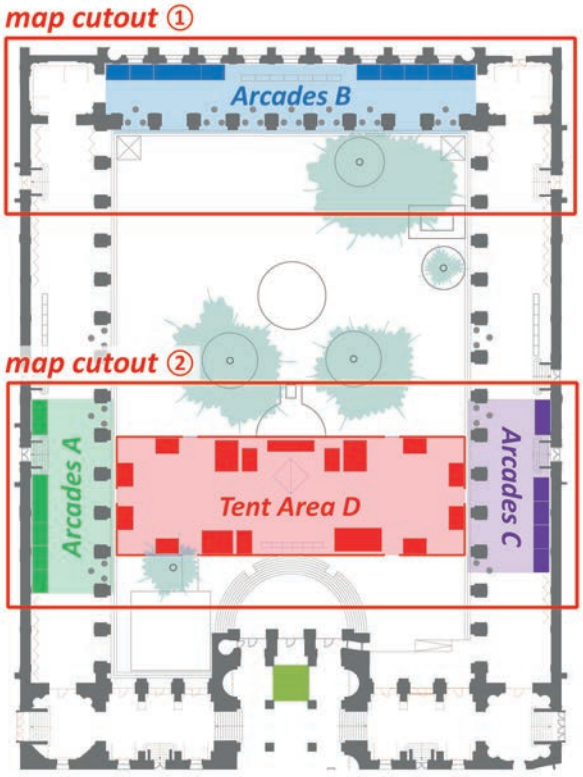
HP





Exhibition Area and Exhibitors

The **Arcaded Courtyard** on the ground floor hosts the commercial exhibition with all booths of in total 35 exhibitors. The exhibition area is open on **Sun 18.08. 16:00–21:00**, and **from Mon 19.08. to Thu 22.08. from 09:30 to 17:00**.



Arcade Areas A, B, and C

- **A01** Oxford Cryosystems Ltd
- **A02** ICDD
- **A03** Arinax Scientific Instrumentation
- **A04** Bruker AXS GmbH
- **A05** Stoe & Cie GmbH

- **B01** ECA
- **B02** ECM – Future Conferences
- **B03** Formulatrix
- **B04** Dunn Labortechnik GmbH
- **B05** Amsterdam Scientific Instruments
- **B06** GE Healthcare – Life Sciences
- **B07** IUCr – Future Conferences
- **B08** HZB and MLZ
- **B09** ELDICO Scientific AG

- **C01** Excillium AB
- **C02** Molecular Dimensions Ltd.
- **C03** Cegitek
- **C04** MarXperts GmbH
- **C05** Wyatt Technologies Europe GmbH

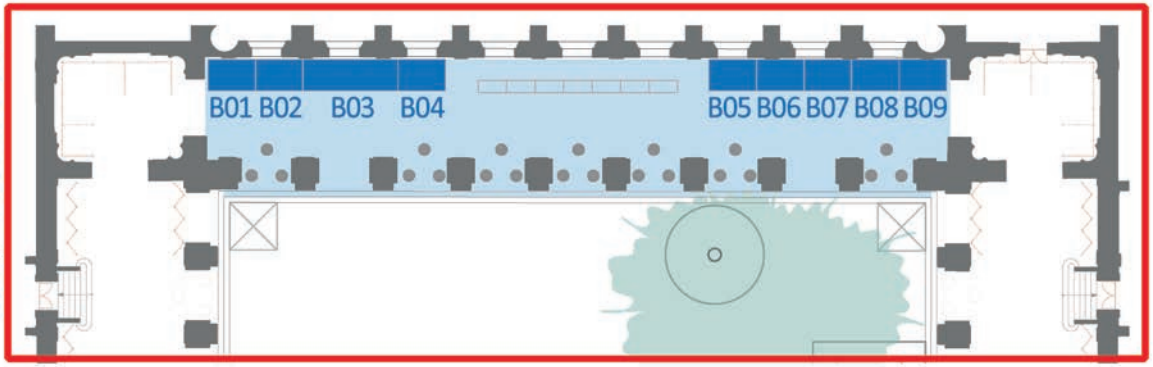
Tent Area D

- **D01** Technobis Crystallization Systems B.V.
- **D02** Malvern Panalytical B.V.
- **D03** Xtal Concepts GmbH
- **D04** Douglas Instruments
- **D05** SmarAct GmbH
- **D06** Huber Diffraktionstechnik / AXO Dresden GmbH
- **D07** Dectris Ltd.
- **D08** CCDC
- **D09** Rigaku Europe SE
- **D10** Anton Paar GmbH
- **D11** Oxford University Press
- **D12** Crystals - MDPI
- **D13** Swissci Scientific Innovation
- **D14** Thermo Fisher Scientific
- **D15** Protein Data Bank in Europe PDBe
- **D16** IUCr

- **CM** *World Largest Crystal Structure Model*

Overview on the exhibitor booths within the exhibition areas A green, B blue, C violet and D red.

map cutout ①



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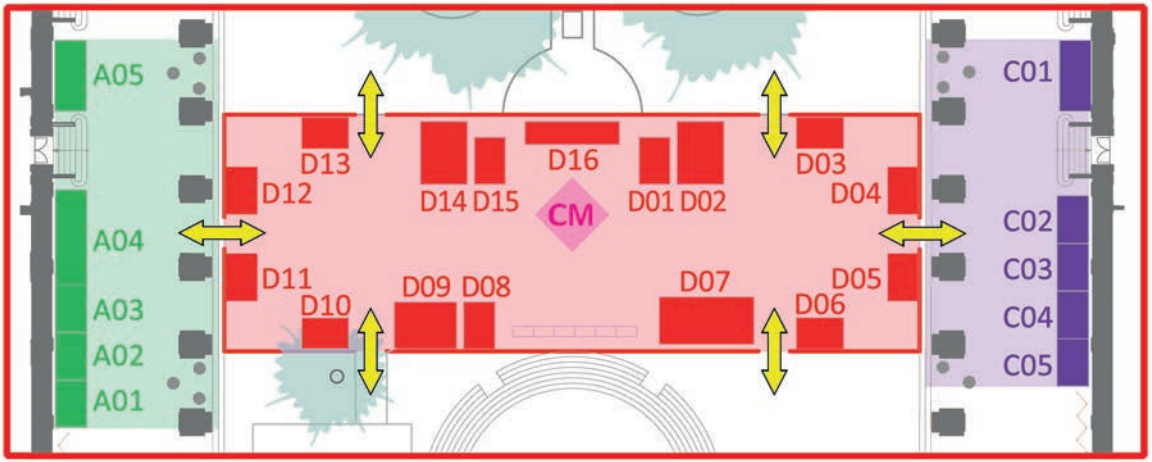


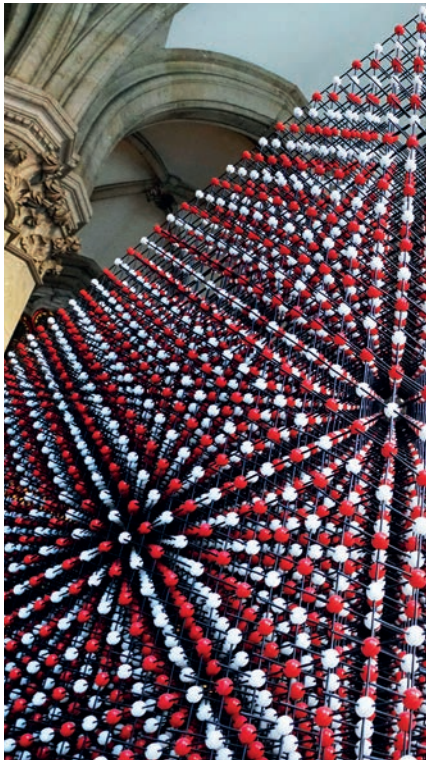
You are kindly invited to our

ECM Luncheon

Tuesday, August 20th, from 12:30 h to 13:30 h
University of Vienna (Hauptgebäude)
1st floor, Kleiner Festsaal

Register via www.bruker.com/ecm2019 and pick up your ticket until Monday evening at our stand.

World's Largest Crystal Structure Model



© Manfred Wildner

38'880 balls and total of more than 10 km sticks are assembled to form the largest crystal structure model in the world. The original of the entire model of a NaCl-type structure, officially registered with Guinness Book of Records, will be displayed on the occasion of the ECM32.

You won't miss the cube measuring 3.1 m in length...

Sun 18.08.2019 to Thu 22.08.2019, exhibition area D (tent)

The ECM32 is grateful to Bruker AXS GmbH and the Faculty of Earth Sciences, Geography and Astronomy (FGGA) for generous sponsorship of this project.

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Scientific Programme

Scientific Programme – Overview

Monday 19. August 2019

08:30-09:30	**Plenary Lecture**	**Jan Löwe (UK)** - Audimax -					
09:30-10:00	**Coffee Break**	**Coffee Break** - Arcaded Courtyard -					
10:00-12:00	**Microsymposia** (6 in parallel)	**MS46** - BIG HS -	**MS02** - HS7 -	**MS05** - HS32 -	**MS16** - Gr. FS -	**MS22** - HS33 -	**MS31** - Audimax -
12:00-14:00	**Lunch Break & Meetings**	**Software Fayre** - SR6 -	**Luncheon** - Kl. FS -	**ECA Council I** - HS5 -	**SIG-1** - SR3 -	**SIG-12** - SR5 -	**SIG-4** - SR4 -
14:00-16:00	**Microsymposia** (6 in parallel)	**MS09** - Audimax -	**MS18** - BIG HS -	**MS23** - HS7 -	**MS25** - HS32 -	**MS37** - Gr. FS -	**MS44** - HS33 -
16:00-17:00	**Coffee Break & Poster Session**	**Coffee Break and Poster Session I** - Arcaded Courtyard and First Floor -					
17:00-18:00	**Keynote Lectures** (2 in parallel)	**Bruce Gaulin (CA)** - Gr FS -			**Kenneth Harris (UK)** - Audimax -		
18:00-19:30	**Science Slam**	**Science Slam** - Audimax -					
19:30-20:00	**Break**						
20:00-21:15	**Conference Concert**	**Conference Concert with the TU Orchestra** - Votivkirche -					

Tuesday, 20. August 2019

08:30-09:30	**Keynote Lectures** (2 in parallel)	**Luca Bindi (IT)** - Gr. FS -			**Donatella Armentano (IT)** - Audimax -			
09:30-10:00	**Coffee Break**	**Coffee Break** - Arcaded Courtyard -						
10:00-12:00	**Microsymposia** (6 in parallel)	**MS06** - HS32 -	**MS10** - HS33 -	**MS14** - Gr. FS -	**MS21** - HS7 -	**MS42** - BIG HS -	**MS30** - Audimax -	
12:00-14:00	**Lunch Break & Meetings**	**Software Fayre** - SR6 -	**Luncheon** - Kl. FS -	**ECA ExCom II** - HS5 -	**ECM33** - SR3 -	**GIG-1** - SR1 -	**GIG-2** - SR2 -	**SIG-2** - SR5 -	**SIG-3** - SR4 -
14:00-16:00	**Microsymposia** (6 in parallel)	**MS47** - BIG HS -	**MS12** - HS33 -	**MS24** - HS7 -	**MS27** - HS32 -	**MS35** - Gr. FS -	**MS41** - Audimax -	
16:00-17:00	**Coffee Break & Poster Session**	**Coffee Break and Poster Session I** - Arcaded Courtyard and First Floor -						
17:00-18:00	**Keynote Lectures** (2 in parallel)	**Martin Noble (UK)** - Gr. FS -			**Anders Mikkelsen (SE)** - Audimax -			
18:00-19:00	**Keynote Lectures** (2 in parallel)	**Elena Bykova (DE)** - Gr. FS -			**Richard Welberry (AU)** - Audimax -			
19:00-19:30	**Break**							
19:30-20:30	**Public Lectures**	**Elspeth Garman (UK), Koen Janssens (BE)** - Audimax -						
20:00-22:00		**Young Crystallographer's Mixer** - TU Wien, Gußhausstraße 25-29 -						

Wednesday 21. August 2019

08:30-09:30	**Keynote Lectures** (2 in parallel)	**Luca Jovine (SE)** - Gr. FS -			**Suzanna Ward (UK)** - Audimax -			
09:30-10:00	**Coffee Break**	**Coffee Break** - Arcaded Courtyard -						
10:00-12:00	**Microsymposia** (6 in parallel)	**MS48** - HS7 -	**MS01** - Gr. FS -	**MS15** - HS33 -	**MS20** - HS32 -	**MS38** - Audimax -		**MS36** - BIG HS -
12:00-14:00	**Lunch Break & Meetings**	**Software Fayre** - SR6 -	**Luncheon** - Kl. FS -	**ECA Council II** - HS5 -	**GIG-3** - SR2 -	**SIG-11** - SR3 -	**SIG-13** - SR4 -	**SIG-6** - SR5 -
14:00-16:00	**Microsymposia** (6 in parallel)	**MS08** - BIG HS -	**MS11** - HS33 -	**MS19** - HS32 -	**MS17** - Audimax -	**MS32** - Gr. FS -		**MS43** - HS7 -
16:00-17:00	**Coffee Break & Poster Session**	**Coffee Break and Poster Session II** - Arcaded Courtyard and First Floor -				*Kálmán* Prize Ceremony - Gr. FS -		
17:00-18:00	**Keynote Lectures** (2 in parallel)	**Naomi Chayen (UK)** - Gr. FS -			**Muriel Véron (FR)** - Audimax -			
18:00-19:30	**Break**							
19:30-22:30	**Conference Dinner**	**Conference Dinner** - Orangerie Schönbrunn -						

Thursday 22. August 2019

08:30-09:30	**Keynote Lectures**	**Martin Caffrey (IE)** - Kl. FS -			**Katherine Page (US)** - Audimax -			
09:30-10:00	**Coffee Break**	**Coffee Break** - Arcaded Courtyard -						
10:00-12:00	**Microsymposia** (6 in parallel)	**MS45** - BIG HS -	**MS04** - Audimax -	**MS13** - HS33 -	**MS29** - HS32 -	**MS34** - HS7 -	**MS33** -Kl. FS -	
12:00-14:00	**Lunch Break & Meetings**	**Software Fayre** - SR6 -	**ECA Council III** - HS5 -		**SIG-7** - SR3 -	**SIG-5** - SR5 -	**SIG-14** - SR4 -	**SIG-9** - SR1 -
14:00-16:00	**Microsymposia** (6 in parallel)	**MS07** - HS32 -	**MS03** - HS7 -	**MS26** - BIG HS -	**MS28** - HS33 -	**MS39** - Kl. FS -	**MS40** - Audimax -	
16:00-17:00	**Coffee Break & Poster Session**	**Coffee Break and Poster Session II** - Arcaded Courtyard and First Floor -						
17:00-18:00	**Plenary Lecture**	**Bo Brummerstedt Iversen (DK)** - Audimax -						
18:00-19:00	**Keynote Lectures**	**David Stuart (UK)** - Kl. FS -			**Françoise Damay (FR)** - Audimax -			
19:00-20:00	**Closing Ceremony**	**Closing Ceremony** - Audimax -						

Introduction to Scientific Programme

The scientific programme covers the latest advances in crystallography and related sciences, which are promoted by the General and Special Interest Groups (GIGs and SIGs).

General Interest Groups (GIGs)

GIG-1: Young Crystallographers
GIG-2: Senior Crystallographers
GIG-3: Education in Crystallography

Special Interest Groups (SIGs)

SIG-1: Macromolecular Crystallography
SIG-2: Quantum Crystallography
SIG-3: Aperiodic Crystals
SIG-4: Electron Crystallography
SIG-5: Mineral and Inorganic Crystallography
SIG-6: Instrumentation and 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 and Chemical Properties
SIG-14: Dynamic Disorder and Diffuse Scattering

The scientific programme is divided into the following 48 microsymposia (MS) as promoted by the SIGs and GIGs. They will take place on the following days (Mon-19, Tue-20, Wed-21, or Thu-22), either in the morning (am) or afternoon (pm).

The microsymposia given in the time tables follow the colours of the focus area as stated below:

	sponsored by:	
Focus Area 1 Biological and Macromolecular Crystallography (SIG-1)		
MS01: Serial Approaches in Crystallography	* DECTRIS *	Wed 21 am
MS02: Fragment/Ligand Binding: Tools Development		Mon 19 am
MS03: Crystallisation and Biophysical Characterisation		Thu 22 pm
MS04: Progress Methods in High Resolution Cryo-EM	* Thermo Fisher *	Thu 22 am
MS05: Proteins in Signalling (Including Membrane Proteins)		Mon 19 am
MS06: Proteins-Nucleic-Acid Interactions		Tue 20 am
MS07: Structural Enzymology		Thu 22 pm
MS08: Hot Structures	* BRUKER *	Wed 21 pm
MS09: Low Resolution Software Development		Mon 19 pm
MS10: Validation, Errors and Noise in Macromolecular Crystallography		Tue 20 am
MS11: Big Data at Facilities and Cloud Computing in Crystallography		Wed 21 pm
MS12: Structural Bioinformatics		Tue 20 pm
Focus Area 2 Materials and Minerals (SIG-5, 11, 12)		
MS13: Biomineralogy and Bioinspired Materials		Thu 22 am
MS14: Mineralogical and Inorganic Crystallography		Tue 20 am
MS15: Minerals and Materials Under Extreme Conditions		Wed 21 am
MS16: Structural Characterization of Functional Materials	* Malvern Panalytical *	Mon 19 am
MS17: Pressure and Mechanical Stress Induced Phase Transition and Polymorphism in [...] Compounds		Wed 21 pm
MS18: Materials for Energy Storage and Conversion	* Thermo Fisher *	Mon 19 pm
MS19: Quantum Materials		Wed 21 pm

Focus Area 3 Physical Including Fundamental Crystallography (SIG-2, 3, 4, 14)

MS20: Combined Approaches for Structure Characterization of Complex Materials at Multiple Length Scales . . . Wed 21 am
MS21: Modern Quantum Crystallography * BRUKER * Tue 20 am
MS22: Structure-Property Relationships via Charge Density Methods . . . Mon 19 am
MS23: Aperiodic and Modulated Structures . . . Mon 19 pm
MS24: Magnetic Order: Methods and Properties . . . Tue 20 pm
MS25: Electron Crystallography as a Tool for Structure Solution and Refinement * ELDICO * Mon 19 pm
MS26: Complex Metallic Alloys: Periodic and Non Periodic . . . Thu 22 pm
MS27: Structural Dynamics, Disorder and Physical Properties . . . Tue 20 pm
MS28: Dynamics and Disorder Probed by Diffuse Scattering . . . Thu 22 pm
MS29: Accurate Treatment of Hydrogen Atoms . . . Thu 22 am

Focus Area 4 Chemical Crystallography (SIG-7, 13)

MS30: Chirality and Polarity in Crystals . . . Tue 20 am
MS31: Single-Crystal Transformations * STOE * Mon 19 am
MS32: New Insights into Non-Covalent Bondings . . . Wed 21 pm
MS33: Tuning Crystalline Frameworks and Their Applications Through Structural Design and Polymorphism . . . Thu 22 am
MS34: Computer Simulation of Molecular Interactions and Crystal Structures . . . Thu 22 am
MS35: From Synthon Engineering to Property Engineering . . . Tue 20 pm
MS36: Amorphous Solids, Solid Solutions, Cocrystal Alloys and Cocrystals . . . Wed 21 am
MS37: NMR Crystallography . . . Mon 19 pm

Focus Area 5 Experimental and Computational Techniques (SIG-6, 8, 9)

MS38: New Detectors for High Energy X-Ray Applications * DECTRIS * Wed 21 am
MS39: Time-Resolved Diffraction and Scattering Techniques . . . Thu 22 pm
MS40: The Use of X-Rays and Neutrons for Experiments in Nanoscience . . . Thu 22 pm
MS41: Crystallisation of Small and Large Molecules (Challenges and developments in Crystallisation Techniques) . . . Tue 20 pm
MS42: In Situ and In Operando Analysis of Functional Materials * Malvern Panalytical * Tue 20 am
MS43: Total Scattering Studies and Disorder * Rigaku * Wed 21 pm
MS44: Solving Structures Through Combination of Reciprocal and Direct Space Methods . . . Mon 19 pm

General Interest (GIG-1, 2 3)

MS45: How to… Successfully Collaborate as a Crystallographer		Thu 22 am
MS46: Status and New Activities at Large Scale Facilities		Mon 19 am
MS47: Women in Crystallography	* sponsored by IUCr *	Tue 20 pm
MS48: Teaching New Dogs Old Tricks	* sponsored by Rigaku *	Wed 21 am

Sponsors of Microsymposia

Invited Talks and Contributed Talks

The individual MS are organized with five speakers each (2 **invited** talks – 30 minutes, 3 **contributed** – 20 minutes). Sponsorships of dedicated microsymposia have been taken over for the respective MS as stated above.

We thank **Thermofisher Scientific, Dectris, Bruker, Rigaku, Malvern Panalytical, STOE, ELDICO** and **IUCr** for taking over the sponsorship of in total 13 microsymposia (as indicated in the list above).

Plenary Lectures, Keynote Lectures and Public Lectures

In addition, **two plenary lectures** (PL) on Mon 19.08., 08:30-09:30 (given by **Jan Löwe**/UK) and on Thu 22.08., 17:00-18:00 (given by **Bo Brummerstedt Iversen**/DK), are scheduled together with **sixteen keynote lectures** (KL) spread out over the four days (Mon 17:00-18:00, Tue 08:30-09:30 and 17:00-19:00, Wed 08:30-09:30 and 17:00-18:00, Thu 08:30-09:30).

According to generous support of **Boehringer Ingelheim** and **European Molecular Biology Organization** (EMBO) we are glad to announce the sponsorship of the following dedicated lectures:

Jan Löwe	**19.08.2019, 08:30-09:30**	**Boehringer Ingelheim sponsored Plenary Lecture**
Luca Jovine	**21.08.2019, 08:30-09:30**	**The EMBO Keynote Lecture**

On Tue 20.08.2019, 19:30-20:30, two **public lectures** given by **Elspeth Garman**/UK and **Koen Janssens**/BE complete the scheduled programme of scientific lectures:

Elspeth Garman	**19:30-20:00**	*More than a century of X-ray crystallography: What has it taught us and where will it lead?*
Koen Janssens	**20:00-20:30**	*Examining old paintings with new X-ray methods: A fresh look at and below the surface*

Sponsors of Keynote and Plenary Lectures

Boehringer Ingelheim

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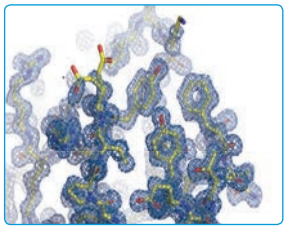
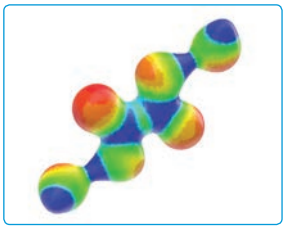


Density maps from a ten minute thaumatin dataset solved by S-SAD phasing



Electron density from a 0.37 Å quantum crystallography measurement of oxalic acid

Rigaku

Rigaku Europe SE | Hugenottenallee 167 | 63263 Neu Isenburg | Germany | www.rigaku.com | info@rigaku.com

Monday, 19. August 2019 – morning (1/3)

08:30-09:30	Audimax	
	PL01 * Boehringer Ingelheim Plenary Lecture * **Jan Löwe** (UK) Prokaryotic Cytoskeletons. Chair: Kristina Djinovic-Carugo (AT)	
10:00-12:00	BIG HS	HS7
	MS46 *Status and new activities @ large scale facilities.* Chairs: Jean Susini (FR), Sandor Brockhauser (DE)	MS02 *Fragment/ligand binding tools and development.* Chairs: Christoph Mueller-Dieckmann (FR), Melanie Vollmar (UK)
10:00-10:30	MS46-01 **Harald Reichert** (FR) The ESRF-EBS and the Next Chapter in X-Ray Science	MS02-01 **Bernhard Rupp** (AT) How not to Shoot Yourself into the Foot
10:30-11:00	MS46-02 **Romain Letrun** (DE) Megahertz Rate Serial Crystallography at the European XFEL	MS02-02 **Dorothee Liebschner** (US) Polder Maps: Improving OMIT Maps for Ligand Building and Validation
11:00-11:20	MS46-03 **Gleb Bourenkov** (DE) EMBL Beamlines for Macromolecular Crystallography at PETRA III	MS02-03 **Uwe Mueller** (SE) FragMAX - The New Fragment Screening Facility of MAX IV Laboratory
11:20-11:40	MS46-04 **Ana Gonzalez** (SE) Macromolecular Crystallography at MAX IV	MS02-04 **Irina Cornaciu** (FR) Automated, Remote-Controlled Ligand Screening Pipelines for Drug Discovery
11:40-12:00	MS46-05 **Anita D'Angelo** (AU) Facility upgrades at the Australian Synchrotron: Extending the powder diffraction capabilities	MS02-05 **Helena Taberman** (DE) Structure-Based Fragment Screening on Dynamin GTPase Domain
12:00-14:00	ECA Council Meeting 1 (HS5), Dectris Luncheon (Kl. FS), Viennese Waltz Dancing Course (Garderobe Senatssaal)	

Monday, 19. August 2019 – morning (2/3)

08:30-09:30	Audimax
	PL01 * Boehringer Ingelheim Plenary Lecture * **Jan Löwe** (UK) Prokaryotic Cytoskeletons. Chair: Kristina Djinovic-Carugo (AT)

10:00-12:00	HS32	Großer Festsaal (Gr. FS)
	MS05 *Proteins in signalling (Including Membrane Proteins).* Chairs: Thomas Leonard (AT), Anastassis Perrakis (NL)	MS16 *Structural characterization of functional materials.* Chairs: Virginia Monteseguro-Padron (FR), Simona Galli (IT)
10:00-10:30	MS05-01 **Bert Janssen** (NL) Protein Conformational and Oligomeric Rearrangements Control Intercellular Signalling	MS16-01 **Juan Ángel Sans** (ES) Polymorphism in Sesquioxides of Late Group-15: Work under Pressure
10:30-11:00	MS05-02 **Daniel Panne** (UK) Structural Insights into Signal Processing to Chromatin	MS16-02 **Claudia Weidenthaler** (DE) In Situ Methods for the Analysis of Functional Materials
11:00-11:20	MS05-03 **Albert Guskov** (NL) Transport of Enantiomeric Neurotransmitters by SLC1A Family of Proteins	MS16-03 **Marco Scavini** (IT) Impact of Intense Electric Fields on the Structure of Centrosymmetric Relaxor Ferroelectric $Sr_{0.85}Pr_{0.15}TiO_3$
11:20-11:40	MS05-04 **Gabrielle Watson** (AU) Structural Basis for CD96 Immune Receptor Recognition of Nectin-like Protein-5, CD155	MS16-04 **Marie Münchhalfen** (DE) Structural Control of thermomechanical Properties of Monoclinic Rare-Earth Calcium Oxoborates
11:40-12:00	MS05-05 **Ivana Nemcovicová** (SK) Analysis of Cytomegalovirus Immune Evasion Protein UL144 Glycosylation Profile Revealed its Role in Immune Recognition	MS16-05 **Daniel Többens** (DE) MEAD, Salt, and Sunshine: Cation Distribution in CZTSe, CFTS, and CZSiSe

12:00-14:00	SIG-1 Meeting (SR3) SIG-12 Meeting (SR5)

Monday, 19. August 2019 – morning (3/3)

08:30-09:30	Audimax
	PL01 * Boehringer Ingelheim Plenary Lecture * **Jan Löwe** (UK) Prokaryotic Cytoskeletons. Chair: Kristina Djinovic-Carugo (AT)

10:00-12:00	HS33	Audimax
	MS22 *Structure-property relationships via charge density methods.* Chairs: Anna Krawczuk (PL), Lilianna Checinska (PL)	MS31 *Single-Crystal Transformations.* Chairs: Giancarlo Terraneo (IT), Elena Boldyreva (RU)
10:00-10:30	MS22-01 **Delia Haynes** (ZA) 'Pancake' Bonding - A Charge Density Perspective	MS31-01 **Pance Naumov** (AE) Mechanical Properties of Molecular Crystals: The Bigger Picture
10:30-11:00	MS22-02 **Jacob Overgaard** (DK) Elucidating the Mechanisms of Single Molecule Magnets using Diffraction Methods	MS31-02 **Espallargas Guillermo Mínguez** (ES) Dynamic MOFs with Breathing-Dependent Redox Behavior
11:00-11:20	MS22-03 **Peter Luger** (DE) Electron Densities of two Nonapetides from Invariom Application	MS31-03 **Consiglia Tedesco** (IT) Energy Studies of Single Crystal to Single Crystal Transformations in Cyclic Peptoids
11:20-11:40	MS22-04 **Urszula Budniak** (PL) The Role of Electrostatic Interactions in IFIT Proteins Complexed with RNA with Different 5' End Predicted by the UBDB+EPMM Method	MS31-04 **Sajesh Thomas** (DK) Insights from High-Pressure Crystallography and X-Ray Charge Density Analysis into Mechanical Flexibility of Metal-Organic Complex Crystals
11:40-12:00	MS22-05 **Francesco Caruso** (US) Using Crystal Structure, an Improved Electrochemical Method and Computational DFT Studies to Understand the Medicinal Properties of Celastraceae Species of Plants	MS31-05 **Philippe Guionneau** (FR) Single-Crystal to Single-Crystal Transformations in Spin-Crossover Compounds. An Incredible Zoology!

12:00-14:00	SIG-4 Meeting (SR4) Software Fayre (SR6)

Monday, 19. August 2019 – afternoon (1/3)

14:00-16:00	Audimax	BIG HS
	MS09 *Low resolution software development.* Chairs: Alexandre Urzhumtsev (FR), Victor Lamzin (DE)	MS18 *Materials for energy storage and conversion.* Chairs: Yaroslav Filinchuk (BE), Manuel Hinterstein (DE)
14:00-14:30	MS09-01 **Robert Nicholls** (UK) Tools to Aid Macromolecular Refinement at Low Resolution	MS18-01 **Helmut Ehrenberg** (DE) Electrochemical Energy Storage beyond Lithium
14:30-15:00	MS09-02 **Vladimir Lunin** (RU) Mask-Based Approach to Restoring and Phasing Single-Particle Diffraction Data	MS18-02 **Dorthe Bomholdt Ravnsbæk** (DK) Order-Disorder Transitions in Battery Electrodes Studied by Operando X-Ray Scattering
15:00-15:20	MS09-03 **Helen Ginn** (UK) Vagabond: Redefining the Model for Macromolecular Refinement	MS18-03 **Artem Abakumov** (RU) Defects, Disorder and Electrochemistry in Phosphate-Based Metal-Ion Battery Cathodes
15:20-15:40	MS09-04 **Rafael Borges** (ES) ARCIMBOLDO Towards Low Resolution: Recent Updates	MS18-04 **Junji Akimoto** (JP) Crystal Growth and Structural and Electrochemical Properties of Garnet-type Lithium Ion Conducting Oxides
15:40-16:00	MS09-05 **Ronan Keegan** (UK) Molecular Replacement Model Preparation and its Automation in MoRDa and MrBUMP	MS18-05 **Nils Prinz** (DE) Structural Insights into Methanation Catalysts from MOF-Precursors via PDF
16:00-16:20		MS18-06 **Simon Welzmiller** (Thermo Fisher Scientific) Increase your Energy with XRD

16:00-17:00	Coffee Break & Poster Session I

17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN01 **Bruce Gaulin** (CA) Ground State Selection in Quantum Pyrochlore Magnets. Chair: Oksana Zaharko (CH)	KN02 **Kenneth Harris** (UK) New Experimental Techniques for Exploring Crystallization Pathways and Structural Properties of Solids. Chair: Maria Teresa Duarte (PT)

Monday, 19. August 2019 – afternoon (2/3)

14:00-16:00	HS7	HS32
	MS23 *Aperiodic and Modulated Structures.* Chairs: Kirsten E. Christensen (UK), Marc de Boissieu (FR)	MS25 *Electron crystallography as a tool for structure solution and refinement.* Chairs: Xiaodong Zou (SE), Tatiana Gorelik (DE)
14:00-14:30	MS23-01 **Leila Noohinejad** (DE) Chemical vs Conformational Entropies at the Incommensurate and Lock-In Phase Transitions of Morpholinium Tetrafluoroborate	MS25-01 **Louisa Meshi** (IL) Structure Determination of Nano-Precipitates in Metallic Alloys using Electron Crystallography Methods
14:30-15:00	MS23-02 **Elen Duverger-Nédellec** (CZ/FR) Evidencing of Charge Density Wave instabilities in even members of the Monophosphate Tungsten Bronzes Family	MS25-02 **Tim Gruene** (AT) Electron Crystallography is a Powerful and Feasible Extension to Every X-Ray Facility
15:00-15:20	MS23-03 **Shelomo Ben-Abraham** (IL) Multidimensional Aperiodic Structures from BGU	MS25-03 **Tsumoru Shintake** (JP) How Can We Directly See the Molecule Array in 3D Protein Crystal under TEM?
15:20-15:40	MS23-04 **Caroline Röhr** (DE) The 1D Modulated Structure of the Mixed-Valent Chain Sulfido Ferrate $K_{7.09}[FeS_2]_4$	MS25-04 **Robert Bücker** (DE) Serial Protein Crystallography in a S/TEM
15:40-16:00	MS23-05 **Morgan Poupon** (CZ) New Tools in Jana2006/Jana2020 to Study and Characterization of Pi-Pi Stacking of Incommensurate Modulated Structures: a & ß-Mn(dmp)Cl_2	MS25-05 **Claudia Lucía Millán Nebot** (ES) Using ARCIMBOLDO's Fragment-Based MR for Solving microED Data from Macromolecular Structures
16:00-17:00	Coffee Break & Poster Session I	
17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN01 **Bruce Gaulin** (CA) Ground State Selection in Quantum Pyrochlore Magnets. Chair: Oksana Zaharko (CH)	KN02 **Kenneth Harris** (UK) New Experimental Techniques for Exploring Crystallization Pathways and Structural Properties of Solids. Chair: Maria Teresa Duarte (PT)

Monday, 19. August 2019 – afternoon (3/3)

14:00-16:00	Großer Festsaal (Gr. FS)	HS33
	MS37 *NMR Crystallography.* Chairs: Paul Hodgkinson (UK), Luís Mafra (PT), Kenneth Harris (UK)	MS44 *Solving structures through combination of reciprocal and direct space methods.* Chairs: Amin Sadeghpour (CH), Ute Kolb (DE)
14:00-14:30	MS37-01 **Giulia Mollica** (FR) New Sensitivity-Enhanced NMR Crystallography Approaches to Investigate Crystallization and Polymorphism in Organic Materials	MS44-01 **Mauro Gemmi** (IT) Crystal Structure of New and Highly Complex Organic Molecules Solved by 3D Electron Diffraction
14:30-15:00	MS37-02 **Yaroslav Khimyak** (UK) Understanding Self-Assembly of Molecular Organic Solids using NMR Crystallography: From Multicomponent Solids to Supramolecular Hydrogels	MS44-02 **Tatiana Latychevskaia** (CH) Collecting and Phasing of Single Molecule Electron Diffraction Data
15:00-15:20	MS37-03 **Lara Sulcek** (DE) ^{1}H, ^{19}F and ^{29}Si MAS NMR Investigations of Synthetic Lepidolite Samples with Variable OH/F Ratios	MS44-03 **Alan David Rae** (AU) The Need for Correlation Coefficients in the Modelling of Stacking Faulted Crystal Structures
15:20-15:40	MS37-04 **Marta Dudek** (PL) Determination of Elusive Crystal Structure of Solvate-Hydrate of Catechin by Crystal Structure Prediction and NMR Crystallography	MS44-04 **Jingjing Zhao** (SE) Structure Study of a Disordered Zeolite by cRED and HRTEM
15:40-16:00	MS37-05 **Karol Nartowski** (UK) Understanding the Role of Molecular Mobility in Phase Transitions of Bulk and Confined Pharmaceuticals	MS44-05 **Simone Dolabella** (CH) Direct and Fourier Space Traveling: Multi-Dimensional Mapping of Lattice Strain and Tilt of a Suspended Silicon Nanowire in a Monolithic System
16:00-17:00	Coffee Break & Poster Session I	
17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN01 **Bruce Gaulin** (CA) Ground State Selection in Quantum Pyrochlore Magnets. Chair: Oksana Zaharko (CH)	KN02 **Kenneth Harris** (UK) New Experimental Techniques for Exploring Crystallization Pathways and Structural Properties of Solids. Chair: Maria Teresa Duarte (PT)

Tuesday, 20. August 2019 – morning (1/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN03 **Luca Bindi** (IT) Solar System Secrets Hidden in Quasicrystals. Chair: Ronan McGrath (UK)	KN04 **Donatella Armentano** (IT) Metal-Organic Frameworks as Chemical Reactors: X-Ray Crystallographic Snapshots of the Confined State. Chair: Carolyn P. Brock (UK)

10:00-12:00	HS32	HS33
	MS06 *Proteins-nucleic-acid interactions.* Chairs: Ralf Ficner (DE), Bohdan Schneider (CZ)	MS10 *Validation, errors and noise in macromolecular crystallography.* Chairs: Gerard Bricogne (UK), Kay Diederichs (DE)
10:00-10:30	MS06-01 **Erik Johansson** (SE) Structural Studies of the Leading Strand DNA Polymerase in Eukaryotes	MS10-01 **Gwyndaf Evans** (UK) Combatting MX Measurement Errors at Source
10:30-11:00	MS06-02 **Markus Wahl** (DE) Structural Basis of Ribosomal RNA Synthesis in Bacteria	MS10-02 **Isabel Uson** (ES) Errors in Electron Scattering and Validation of Experimental Maps through Combination of MicroED and CryoEM
11:00-11:20	MS06-03 **Florian Hamann** (DE) RNA Translocation Mechanism of Spliceosomal DEAH-box ATPases	MS10-03 **Ian Tickle** (UK) STARANISO: Use of a WebGL-based 3-D Interactive Graphical Display to Represent and Visualise Data Quality Metrics for Anisotropic Macromolecular Diffraction Data
11:20-11:40	MS06-04 **Yu-Yuan Hsiao** (TW) Molecular Mechanisms of TREX1 in DNA Repair and Immune Silencing	MS10-04 **Piotr Neumann** (DE) Assessment of Model Bias in Crystallographic Maps and its Implications for Validation of Crystal Structures
11:40-12:00	MS06-05 **Jiri Cerny** (CZ) Structural Alphabets for Conformational Analysis of Nucleic Acids	MS10-05 **Mariusz Jaskolski** (PL) Stereochemical Restraints for Nucleic Acids Revisited

12:00-14:00	ECA Executive Committee Meeting II (HS5), Bruker Luncheon (Kl. FS) GIG-1 Meeting (SR1)

Tuesday, 20. August 2019 – morning (2/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN03 **Luca Bindi** (IT) Solar System Secrets Hidden in Quasicrystals. Chair: Ronan McGrath (UK)	KN04 **Donatella Armentano** (IT) Metal-Organic Frameworks as Chemical Reactors: X-Ray Crystallographic Snapshots of the Confined State. Chair: Carolyn P. Brock (UK)

10:00-12:00	Großer Festsaal (Gr. FS)	HS7
	MS14 *Mineralogical and Inorganic Crystallography.* Chairs: Frédéric Hatert (BE), Marie Colmont (FR)	MS21 *Modern Quantum Crystallography.* Chairs: Sajesh P. Thomas (DK), Piero Macchi (CH)
10:00-10:30	MS14-01 **Nicolas Barrier** (FR) Search for New Tellurium and Selenium Oxides with Potential Ferroelectric and Multiferroic Properties	MS21-01 **Jean-Michel Gillet** (FR) Possible Quantum Crystallography Solutions for N-Representable One-Electron Reduced Density Matrices Reconstruction
10:30-11:00	MS14-02 **Sergey Aksenov** (RU) New Data about Topology and Modularity of Heteropolyhedral Frameworks in Minerals and Inorganic Compounds	MS21-02 **Martin Rahm** (SE) Electron Configuration and Electronegativity of the Atoms Under Compression
11:00-11:20	MS14-03 **Biljana Krueger** (AT) Kahlenbergite, a New Potassium ß-Alumina Mineral	MS21-03 **Kasper Tolborg** (DK) Interactions between Stereo Chemically Active Lone Pairs in $MnSb_2O_4$
11:20-11:40	MS14-04 **Massimo Nespolo** (FR) Modularity in Minerals: the Example of Biopyriboles-Palysepioles	MS21-04 **Alessandro Genoni** (FR) Quantum Crystallography for Macromolecules: the HAR-ELMO Method
11:40-12:00	MS14-05 **Daniel Guenther** (DE) The Structure of the Lanthanum Oxonitridophosphate $La_{21}P_{40}O_{46}N_{57}$	MS21-05 **Claude Lecomte** (FR) Spin-Resolved Atomic Orbital Model Refinement for Combined Charge and Spin Density Analysis: Application to the Perovskite

12:00-14:00	GIG-2 Meeting (SR2), SIG-2 Meeting (SR5) Viennese Waltz Dancing Course (Garderobe Senatssaal)

Tuesday, 20. August 2019 – morning (3/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN03 **Luca Bindi** (IT) Solar System Secrets Hidden in Quasicrystals. Chair: Ronan McGrath (UK)	KN04 **Donatella Armentano** (IT) Metal-Organic Frameworks as Chemical Reactors: X-ray Crystallographic Snapshots of the Confined State. Chair: Carolyn P. Brock (UK)

10:00-12:00	BIG HS	Audimax
	MS42 *In Situ and In Operando Analysis of Functional Materials.* Chairs: Antonia Neels (CH), Bridget Murphy (DE)	MS30 *Chirality and Polarity in Crystals.* Chairs: Dario Braga (IT), Tim Gruene (AT)
10:00-10:30	MS42-01 **Uta Hejral** (SE) High Energy Surface X-Ray Diffraction from Surfaces and Nanoparticles in Operando Catalysis	MS21-01 **Fabrizia Grepioni** (IT) Solid-State Chiral Resolution via Metal Complexation
10:30-11:00	MS42-02 **Stephen Hull** (NL) Neutron Diffraction Studies of Energy Materials	MS21-02 **Peter Oleynikov** (CN) Electron Crystallography for Determining the Handedness of Chiral Crystals
11:00-11:20	MS42-03 **Monique van der Veen** (NL) Morphology and Structure of Metal-Organic Framework ZIF-8 during Crystallisation Measured by a New Technique: Dynamic Angle Resolved Second-Harmonic Scattering (AD-SHS).	MS21-03 **Petr Brazda** (CZ) Absolute Configuration of Pharmaceutical Molecules Determined from a Nanocrystal by Electron Diffraction
11:20-11:40	MS42-04 **Manuel Wilke** (CH) In Situ Mechanochemistry of Hybrid Materials	MS21-04 **Laura Bereczki** (HU) Optical Resolution of 2- and 4-Chloromandelic Acids with Cyclohexylethylamine Resolving Agent–Crystal Structures of the Diastereomers and the Double Salt
11:40-12:00	MS42-05 **Semen Gorfman** (IL) Inspecting Piezoelectricity in $PbZr_{1-x}Ti_xO_3$ Single Crystals with Ferroelastic Domains	MS21-05 **Linda Shimon** (IL) Highly Versatile Metal-Organic Frameworks

12:00-14:00	SIG-3 Meeting (SR4), Software Fayre (SR6) ECM33 Programme (SR3)

Tuesday, 20. August 2019 – afternoon (1/3)

14:00-16:00	BIG HS	HS33
	MS47 *Women in Crystallography.* Chairs: Kamil Dziubek (IT), Alessia Bacchi (IT)	MS12 *Structural Bioinformatics.* Chairs: Eugene Krissinel (UK), Oliviero Carugo (IT)
14:00-14:30	MS47-01 **Elspeth Garman** (UK) 32 Years of Travels in Crystallography	MS12-01 **Anna Panchenko** (US) Exploring Cancer Heterogeneity: From DNA Mutability to Protein Dysfunction
14:30-15:00	MS47-02 **Delia Haynes** (ZA) Women in Science – An African Perspective	MS12-02 **Birgit & Frank Eisenhaber** (SG) Darkness in the Human Gene and Protein Function Space Despite Big Omics Data and Decline in Molecular Mechanism Discovery after 2000
15:00-15:20	MS47-03 **Biserka Kojic-Prodic** (HR) Modest Recognition for High Achievements	MS12-03 **Massimo D. Sammito** (UK) Phaser.Voyager: Data-Guided Model Generation and Visualization
15:20-15:40	MS47-04 **Andrea Thorn** (DE) "It's just Like Planning a Dinner..." - Women in Crystallographic Computing	MS12-04 **Daniel Rigden** (UK) Molecular Replacement Using Structure Predictions from new Generation Databases
15:40-16:00	MS47-05 **Delphine Cabaret** (FR) Women in a Historical French Laboratory of Crystallography	MS12-05 **Ana Medina** (ES) ALEPH: A New Software for Structural Analysis and Generation of Fragment Libraries for Molecular Replacement

16:00-17:00	Coffee Break & Poster Session I

17:00-19:00	Großer Festsaal (Gr. FS)	Audimax
17:00-18:00	KN05 **Martin Noble** (UK) 40 years of CCP4: Where we are, How we Got Here and Where we are Going. Chair: Marjolein Thunnissen (SE)	KN06 **Anders Mikkelsen** (SE) Crystal Phase Control in Nanostructures as a Platform for Atomic Scale Tailoring of Electronic, Optical and Chemical Properties. Chair: Antonia Neels (CH)
18:00-19:00	KN07 **Elena Bykova** (DE) Chemistry and Crystallography at Ultra-High Pressures. Chair: Daniel Többens (DE)	KN08 **Richard Welberry** (AU) Diffuse Scattering - Past, Present and Future. Chair: Stephan Rosenkranz (US)

Tuesday, 20. August 2019 – afternoon (2/3)

14:00-16:00	HS7	HS32
	MS24 *Magnetic order: Methods and Properties.* Chairs: Pascal Manuel (UK), Manuel Perez Mato (ES)	MS27 *Structural Dynamics, Disorder and Physical Properties.* Chairs: Dmitry Chernyshov (FR), Ruggero Frison (CH)
14:00-14:30	MS24-01 **Mark Senn** (UK) A Symmetry Motivated Approach for Enumerating Magnetoelectric Couplings in Perovskites	MS27-01 **Alexeï Bosak** (FR) Combining Diffuse and Inelastic Scattering in the Exploration of Phase Transitions
14:30-15:00	MS24-02 **Oksana Zaharko** (CH) Spiral Spin-Liquid, Multi-Step Order and the Emergence of a Vortex-Like State in $MnSc_2S_4$	MS27-02 **Stephan Rosenkranz** (US) Recent Developments in the Use of Single Crystal Diffuse Scattering to Study Materials Properties
15:00-15:20	MS24-03 **Vladimir E. Dmitrienko** (RU) High Symmetry Dictates a Vortex Magnetic Structure for the Mysterious Hidden Order in URu_2Si_2	MS27-03 **Thomas Weber** (CH) Understanding Two-Dimensional Polymerisation Using Bragg and Diffuse X-Ray Scattering
15:20-15:40	MS24-04 **Jose Luis Garcia-Munoz** (ES) Magnetic Inversion Symmetry Breaking and Spin Reorientation in Tb_2MnNiO_6: A Polar Strong Ferromagnet	MS27-04 **Paulus Werner** (FR) Sub-Mesoscale Oxygen Ordering in Non-Stoichiometric Oxygen Ion Conductor Pr_2NiO_{4+d}
15:40-16:00	MS24-05 **Vladimir Pomjakushin** (CH) Superspace Magnetic Structure and Topological Charges in Weyl Semimetal CeAlGe	MS27-05 **Daria Andronikova** (RU) Phase Transitions in Zr-Rich Lead Zirconate-Titanate Studied by Single Crystal Diffuse and Inelastic X-Ray Scattering

16:00-17:00	Coffee Break & Poster Session I

17:00-19:00	Großer Festsaal (Gr. FS)	Audimax
17:00-18:00	KN05 **Martin Noble** (UK) 40 years of CCP4: Where we are, How we Got Here and Where we are Going. Chair: Marjolein Thunnissen (SE)	KN06 **Anders Mikkelsen** (SE) Crystal Phase Control in Nanostructures as a Platform for Atomic Scale Tailoring of Electronic, Optical and Chemical Properties. Chair: Antonia Neels (CH)
18:00-19:00	KN07 **Elena Bykova** (DE) Chemistry and Crystallography at Ultra-High Pressures. Chair: Daniel Többens (DE)	KN08 **Richard Welberry** (AU) Diffuse Scattering - Past, Present and Future. Chair: Stephan Rosenkranz (US)

Tuesday, 20. August 2019 – afternoon (3/3)

14:00-16:00	Großer Festsaal (Gr. FS)	Audimax
	MS35 *From Synthon Engineering to Property Engineering.* Chairs: Katharina Edkins (UK), Christian Lehmann (DE)	MS41 *Crystallisation of Small and Large Molecules (Challenges and Developments in Crystallisation Techniques).* Chairs: Naomi E. Chayen (UK), May Marsh Sharpe (CH)
14:00-14:30	MS35-01 **Dejan-Kresimir Bucar** (UK) Synthons: Through the Looking-Glass, and What We Have Yet to Find There	MS41-01 **Isabel Moraes** (UK) Crystallisation for Serial Crystallography in Lipidic Cubic Phase (LCP) Made Simple
14:30-15:00	MS35-02 **Marijana Dakovic** (HR) Flexible Crystalline Coordination Polymers with Tunable Responses to Mechanical Stimuli	MS41-02 **Soneya Majumdar** (SE) Four for the Price of One: Cross-Seeding to Obtain Crystals of Ancestral Elongation Factor Tus
15:00-15:20	MS35-03 **Aida Samigullina** (RU) Crystallization of Chiral 2,4-Dinitrophenyl Pyridoxine Derivatives in «no Zonk» Groups: Regularity or Randomness?	MS41-03 **Bernhard Spingler** (CH) Nano-crystallization: Applying the Methods of Macromolecular Crystallography for Small Molecules
15:20-15:40	MS35-04 **Nikoletta Bathori** (ZA) Direct Proportionality between Structural Features and Property in Multicomponent Crystals of Salicylic Acid	MS41-04 **Roland Resel** (AT) Substrate Induced Polymorphism of Organic Electronic Molecules
15:40-16:00	MS35-05 **Jasper Van de Velde** (BE) Surface Properties of Organic Crystals Based on a Guantum Chemical Treatment of Crystal Facets	MS41-05 **Sophie Janbon** (AstraZeneca) Shaping Drug Process Development with Crystal Structure Databases
16:00-17:00	Coffee Break & Poster Session I	

17:00-19:00	Großer Festsaal (Gr. FS)	Audimax
17:00-18:00	KN05 **Martin Noble** (UK) 40 years of CCP4: Where we are, How we Got Here and Where we are Going. Chair: Marjolein Thunnissen (SE)	KN06 **Anders Mikkelsen** (SE) Crystal Phase Control in Nanostructures as a Platform for Atomic Scale Tailoring of Electronic, Optical and Chemical Properties. Chair: Antonia Neels (CH)
18:00-19:00	KN07 **Elena Bykova** (DE) Chemistry and Crystallography at Ultra-High Pressures. Chair: Daniel Többens (DE)	KN08 **Richard Welberry** (AU) Diffuse Scattering - Past, Present and Future. Chair: Stephan Rosenkranz (US)

Wednesday, 21. August 2019 – morning (1/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN09 * The EMBO Keynote Lecture * **Luca Jovine** (SE) Fertilization at the Atomic Level: Marrying Basic Science and Reproductive Medicine. Chair: Daniel Panne (UK)	KN10 **Suzanna Ward** (UK) One Million Structures and Counting: The Journey, the Insights, and the Future of the Cambridge Structural Database. Chair: Hans-Beat Bürgi (CH)

10:00-12:00	HS7	Großer Festsaal (Gr. FS)
	MS48 *Teaching New Dogs Old Tricks.* Chairs: Fernando J. Lahoz (ES), Sine Larsen (DK)	MS01 *Serial Approaches in Crystallography.* Chairs: Thomas Schneider (DE), Gisela Brandén (SE)
10:00-10:30	MS48-01 **William Clegg** (UK) Some Reflections on Symmetry	MS01-01 **Takehiko Tosha** (JP) Elucidation of NO Reduction Mechanism in Soluble NO Reductase by Time-Resolved Crystallography with Photosensitive Caged Compound
10:30-11:00	MS48-02 **Anthony Linden** (CH) Seeing is Believing: Model Finalisation and Interpretation of Results	MS01-02 **Robin Owen** (UK) A Tale of two Sources: Serial Crystallography at Synchrotrons and XFELs
11:00-11:20	MS48-03 **Ton Spek** (NL) The Difference Electron Density Map as a Crystal Structure Validation Tool	MS01-03 **Isabelle Martiel** (CH) SwissMX: a New, Versatile Instrument for Fixed Target Femtosecond Macromolecular Crystallography at SwissFEL
11:20-11:40	MS48-04 **Andrew Malony** (UK) Crystal Structure Exploration – I didn't Know Mercury Could Do That!	MS01-04 **Martin R. Fuchs** (US) Ultra-Fast Raster-Scanning Synchrotron Serial Micro-Crystallography
11:40-12:00	MS48-05 **Gemma de la Flor** (DE) Resolution of Crystallographic Problems Using the Bilbao Crystallographic Server	MS01-05 **Selina Storm** (UK) Measuring the Dose: Photoelectron Escape in Micro-Crystals

12:00-14:00	ECA Council Meeting II (HS5), Rigaku Luncheon (Kl. FS) GIG-3 Meeting (SR2)

Wednesday, 21. August 2019 – morning (2/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN09 * The EMBO Keynote Lecture * **Luca Jovine** (SE) Fertilization at the Atomic Level: Marrying Basic Science and Reproductive Medicine. Chair: Daniel Panne (UK)	KN10 **Suzanna Ward** (UK) One Million Structures and Counting: The Journey, the Insights, and the Future of the Cambridge Structural Database. Chair: Hans-Beat Bürgi (CH)
10:00-12:00	HS33	HS32
	MS15 *Minerals and Materials under Extreme Conditions.* Chairs: Paul Attfield (UK), Hubert Huppertz (AT)	MS20 *Combined Approaches for Structure Characterization of Complex Materials at Multiple Length Scales.* Chairs: Artem Abakumov (RU), Lukas Palatinus (CZ)
10:00-10:30	MS15-01 **Chrystèle Sanloup** (FR) Reactivity of Heavy Noble Gases Under High Pressures	MS20-01 **Alexander M. Korsunsky** (UK) Combined Analysis of Structure and Strain in Engineering Materials by Neutron and Synchrotron X-Ray Diffraction, and Electron Microscopy
10:30-11:00	MS15-02 **Sergey V. Ovsyannikov** (DE) High-Pressure Synthesis and Properties of Iron Oxides	MS20-02 **Ehrenfried Zschech** (DE) X-Ray Characterization of Morphology and Structure of Materials at Multiple Length Scales
11:00-11:20	MS15-03 **Ross J. Angel** (IT) The True Structural Relationship between Zircon and Scheelite Structure Types, and a New Polymorph of Zircon	MS20-03 **Philippe Boullay** (FR) Characterization of Aperiodic Bi-based Layered Oxides Thin Films by TEM Multiscale Approaches
11:20-11:40	MS15-04 **Katharina Scheidl** (NO) Structural Behavior of the sII Clathrasil Chibaite at Low Temperatures and High Pressures	MS20-04 **Martin U. Schmidt** (DE) Orientional Disorder in Monomethyl-Quinacridone Investigated by Rietveld Refinement, Pair-Distribution Function Analysis and Lattice-Energy Minimisations
11:40-12:00	MS15-05 **Xiaojiao Liu** (UK) Crystallisation Studies of Biodiesel and Methyl Stearate at Extreme Conditions	MS20-05 **Yue Zhao** (JP) Small-angle Scattering Study for Developing Alkaline Durable Imidazolium-Based Grafted Anion Exchange Membranes for Pt-Free Fuel Cells
12:00-14:00	SIG-11 Meeting (SR3) SIG-13 Meeting (SR4)	

Wednesday, 21. August 2019 – morning (3/3)

08:30-09:30	Großer Festsaal (Gr. FS)	Audimax
	KN09 * The EMBO Keynote Lecture * **Luca Jovine** (SE) Fertilization at the Atomic Level: Marrying Basic Science and Reproductive Medicine. Chair: Daniel Panne (UK)	KN10 **Suzanna Ward** (UK) One Million Structures and Counting: The Journey, the Insights, and the Future of the Cambridge Structural Database. Chair: Hans-Beat Bürgi (CH)

10:00-12:00	Audimax	BIG HS
	MS38 *New Detectors for High Energy X-Ray Applications.* Chairs: Ulli Pietsch (DE), David Pennicard (DE)	MS36 *Amorphous Solids, Solid Solutions, Cocrystal Alloys and Cocrystals.* Chairs: Enrique Espinosa (FR), Fabrizia Grepioni (IT), Bathori Nikoletta (ZA)
10:00-10:30	MS38-01 **Marie Ruat** (FR) Recent Advances in High-Z Pixel Detectors	MS36-01 **Dario Braga** (IT) Ionic Co-Crystals
10:30-11:00	MS38-02 **Mohammad Shokr** (DE) Subpixel Spatial Resolution at 122 keV of an Spectroscopic Imager Composed of a pnCCD Coupled to a Columnar CsI(Tl) Scintillator	MS36-02 **Frédéric Affouard** (FR) Manipulation of the Crystalline and Amorphous Physical States of Pharmaceutical Materials: Possibilities, Limits and Challenges
11:00-11:20	MS38-03 **Martin Adam** (DE) Photon Counting with Mixed Mode Detection	MS36-03 **Paul Hodgkinson** (UK) Characterisation of "Polyamorphism" and the Molecular Origins of Disorder using Complementary Methods
11:20-11:40	MS38-04 **Stefan Brandstetter** (CH) EIGER2 CdTe Detectors: Tools for hard X-Ray Studies	MS36-04 **Matteo Lusi** (IE) Pharmaceutical Solid Solutions from Non-Soluble Components
11:40-12:00	MS38-05 **Catherine Dejoie** (FR) Combining a Nine-Crystal Multianalyser Stage with a Hybrid CdTe Photon Counting Detector for High-Resolution X-Ray Powder Diffraction at ESRF-ID22	MS36-05 **Tatiana Timofeeva** (RU) Charade transfer donor-acceptor complexes of several polycyclic aromatic molecules

12:00-14:00	SIG-6 Meeting (SR5) Software Fayre (SR6)

Wednesday, 21. August 2019 – afternoon (1/3)

14:00-16:00	BIG HS	HS33
	MS08 *Hot Structures.* Chairs: Luca Jovine (SE), Martin Caffrey (IE)	MS11 *Big Data at Facilities and Cloud Computing in Crystallography.* Chairs: Ana Gonzalez (SE), Sameer Velankar (UK)
14:00-14:30	MS08-01 **Junko Yano** (US) Capturing Reaction Intermediates of the Water Oxidation Reaction in Photosystem II at X-Ray Free Electron Lasers	MS11-01 **Anastassis Perrakis** (NL) Recalculating all X-Ray Structures in the PDB by PDB_REDO: Going Cloud
14:30-15:00	MS08-02 **Jessica Thomaston** (US) Structural Basis of Adamantane Resistance in the Influenza A M2 Proton Channel	MS11-02 **Eugene Krissinel** (UK) CCP4 Cloud for Distributed Crystallographic Computations
15:00-15:20	MS08-03 **Chwan-Deng Hsiao** (TW) Structural Analysis of Chloroplast Tail-Anchored Membrane Protein Recognition by ArsA1	MS11-03 **Gianluca Santoni** (FR) EXI, the EXtended ISPyB Interface
15:20-15:40	MS08-04 **Joan Lopez Arolas** (AT) Structural Basis of A-Actinin-2/Titin Interaction in the Z-Disk	MS11-04 **Natalie Johnson** (UK) Keeping Things 'N Synch: Analysing the Content and Completeness of CIF Metadata in the CSD
15:40-16:00	MS08-05 **Antonio Sponga** (AT) Structure of A-Actinin-2/FATZ-1 Fuzzy Complex and Implications in Z-Disk Formation via Phase Separation	MS11-05 **Melanie Vollmar** (UK) Machine Learning for Experimental Phasing in MX

16:00-17:00	Coffee Break & Poster Session II *Kálmán* Prize Ceremony

17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN11 **Naomi E. Chayen** (UK) Enhancing the Success of Macromolecular Crystallization. Chair: Elspeth Garman (UK)	KN12 **Muriel Véron** (FR) Application to E-Precession in Transmission Electron Microscope: Phase and Orientation Map. Chair: Luisa Meshi (IL)

Wednesday, 21. August 2019 – afternoon (2/3)

14:00-16:00	HS32	Audimax
	MS19 *Quantum Materials.* Chairs: Manuel Angst (DE), Bruce Gaulin (CA)	MS17 *Pressure and Mechanical Stress Induced Phase Transition and Polymorphism in Inorganic, Metalorganic and Organic Compounds.* Chairs: Karen Appel (DE), Boris Zakharov (RU)
14:00-14:30	MS19-01 **Paul Attfield** (UK) Orbital Molecules in Oxides	MS17-01 **Hauke Marquardt** (UK) Dynamic Compression of Materials at Pressures of Earth's Interior Using the dDAC
14:30-15:00	MS19-02 **Christianne Beekman** (US) Torque Magnetometry, a Tool for Magnetic Crystallography in Thin Films of Frustrated Magnets	MS17-02 **Anna Olejniczak** (PL) High-Pressure Polymorphs of Organic Compounds with Interactions Involving Nitrogen Atoms
15:00-15:20	MS19-03 **Linda Kerkhoff** (DE) Crystal Growth Investigations of Lithium Iridate, Li_2IrO_3, and Lithium Ruthenates, Li_2RuO_3 and Li_3RuO_4	MS17-03 **Alexandra Friedrich** (DE) Crystal Structure Compression and Pressure-Induced Polymerization of Arene-Perfluoroarene Co-Crystals Leading to Columnar Hydrofluorocarbons
15:20-15:40	MS19-04 **Alexandra Gibbs** (UK) Crystal Structure and Isotope Effect in Quantum Liquid $H_3LiIr_2O_6$	MS17-04 **Martin Ende** (AT) Pressure Induced Phase Transition in $CoSO_4 \cdot H_2O$
15:40-16:00	MS19-05 **Natalija van Well** (DE) Structure and Magnetic Phases in the $Cs_2CuCl_{4-x}Br_x$ Mixed System	MS17-05 **Piero Macchi** (CH) Pressure-Induced Polymerization and Electrical Conductivity of a Polyiodide
16:00-17:00	Coffee Break & Poster Session II *Kálmán* Prize Ceremony	
17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN11 **Naomi E. Chayen** (UK) Enhancing the Success of Macromolecular Crystallization. Chair: Elspeth Garman (UK)	KN12 **Muriel Véron** (FR) Application to E-Precession in Transmission Electron Microscope: Phase and Orientation Map. Chair: Luisa Meshi (IL)

Wednesday, 21. August 2019 – afternoon (3/3)

14:00-16:00	Großer Festsaal Gr. FS)	HS7
	MS32 *New Insights into Non-Covalent Bondings.* Chairs: Pierangelo Metrangolo (IT), Tom Roseveare (UK)	MS43 *Total Scattering Studies and Disorder.* Chairs: Matteo Leoni (IT), Mirijam Zobel (DE)
14:00-14:30	MS32-01 **Giuseppe Resnati** (IT) Chalcogen Bonding in Crystal Engineering	MS43-01 **Andrew Goodwin** (UK) Hidden Vacancy-Network Polymorphism of Prussian Blue Analogues
14:30-15:00	MS32-02 **Sławomir J. Grabowski** (ES) Interactions Involving 13-17 Groups' Elements Acting as the Lewis Acid Centres – Comparison with the Hydrogen Bond	MS43-02 **Federica Bertolotti** (IT) Characterizing Structure, Microstructure and Morphology of Nanomaterials through Reciprocal Space Total Scattering Methods
15:00-15:20	MS32-03 **Mladen Borovina** (HR) Can MEP Values Be Used to Predict the Supramolecular Connectivity in the Crystal Structure?	MS43-03 **Hassan Khoder** (FR) Study of the Confinement Effect of Water in Bioactive Glasses Using Atomic Pair Distribution Function
15:20-15:40	MS32-04 **Eugenia Peresypkina** (DE) Phosphorus Can Do More: p-p Stacking of Planar Aromatic P5-rings	MS43-04 **Anna-Lena Hansen** (DE) Using Nuclear Magnetic Resonance Spectroscopy, Neutron and X-Ray Pair Distribution Function
15:40-16:00	MS32-05 **Aidar Gubaidullin** (RU) Supramolecular Synthons Orientation Rule in the Crystals of Benzodiazepines, Quinoxalines and Benzimidazoles as a Predictive Tool in the Material Design	MS43-05 **Antonio Cervellino** (CH) Texture Correction for Total Scattering Functions

16:00-17:00	Coffee Break & Poster Session II *Kálmán* Prize Ceremony

17:00-18:00	Großer Festsaal (Gr. FS)	Audimax
	KN11 **Naomi E. Chayen** (UK) Enhancing the Success of Macromolecular Crystallization. Chair: Elspeth Garman (UK)	KN12 **Muriel Véron** (FR) Application to E-Precession in Transmission Electron Microscope: Phase and Orientation Map. Chair: Luisa Meshi (IL)

Thursday, 22. August 2019 – morning (1/3)

08:30-09:30	Kleiner Festsaal (Kl. FS)	Audimax
	KN13 **Martin Caffrey** (IE) Mesophase Mirabilis. The Lipid Cubic Phase as a System for Investigating Membrane Proteins. Chair: Kay Diederichs (DE)	KN14 **Katharine Page** (US) Capturing Functional Nanostructures and their Interfaces with Neutron Total Scattering. Chair: Mirjiam Zobel (DE)

10:00-12:00	BIG HS	Audimax
	MS45 *How to… Successfully Collaborate as a Crystallographer.* Chairs: Filip Topić (CA), Galina Kiriukhina (RU)	MS04 *Progress of Methods in High Resolution Cryo-EM.* Chairs: Holger Stark (DE), Thomas Marlovits (DE)
10:00-10:30	MS45-01 **Massimo Nespolo** (FR) Fighting the Wind Mills: Are Crystallographers the Successors of Don Quixote?	MS04-01 **Bonnie Murphy** (DE) Mechanisms of C-Ring Protonation and Flexible F1-Fo Coupling in a Mitochondrial ATP Synthase
10:30-11:00	MS45-02 **Isabel Moraes** (UK) Secrets to a Successful Collaboration	MS04-02 **Jürgen Plitzko** (DE) Recent Advances in Cryo-Electron Tomography for In Situ Structural Biology
11:00-11:20	MS45-03 **Elena Boldyreva** (RU) Education for New Synchrotron Sources. An Interdisciplinary Master Program of the Novosibirsk State University	MS04-03 **Hongyi Xu** (SE) A New and Simple Method for Cryo-EM Specimen Preparation
11:20-11:40	MS45-04 **John Helliwell** (UK) How, and When, to Effect Collaborations	MS04-04 **Andrea Thorn** (DE) Automated Interpretation of Cryo-EM Density Maps with Convolutional Neural Networks
11:40-12:00	MS45-05 **Lauren Agnew** (UK) Using Crystal Structures to Guide Pharmaceutical Drug Substance Development	MS04-05 **Alevtyna Yakushevska** (Thermo Fisher Scientific) Micro Electron Diffraction is a Quick and Versatile Tool for Structure Determination of Macromolecules and Small Molecules

12:00-14:00	ECA Council Meeting III (HS5) SIG-7 Meeting (SR3)

Thursday, 22. August 2019 – morning (2/3)

08:30-09:30	Kleiner Festsaal (Kl. FS)	Audimax
	KN13 **Martin Caffrey** (IE) Mesophase Mirabilis. The Lipid Cubic Phase as a System for Investigating Membrane Proteins. Chair: Kay Diederichs (DE)	KN14 **Katharine Page** (US) Capturing Functional Nanostructures and their Interfaces with Neutron Total Scattering. Chair: Mirjiam Zobel (DE)

10:00-12:00	HS33	HS32
	MS13 *Biomineralogy and Bioinspired Materials.* Chairs: Wolfgang Schmahl (DE), Linda Pastero (IT)	MS29 *Accurate Treatment of Hydrogen Atoms.* Chairs: Horst Puschmann (UK), Matteo Lusi (IE)
10:00-10:30	MS13-01 **Elisa Boanini** (IT) Bioinspired Calcium Phosphates: Structural Modifications Induced by Functionalization	MS29-01 **Anders Østergaard Madsen** (DK) Modelling of Hydrogen Atoms in Crystallography – An Overview
10:30-11:00	MS13-02 **Helga Lichtenegger** (AT) Alteration of Human Bone Mineralization in a Sclerosing Osteosarcoma	MS29-02 **Anna Krawczuk** (PL) Influence of a Hydrogen Bond on Optical Properties of Materials
11:00-11:20	MS13-03 **Lilianna Checinsk** (PL) New Complexes of Silver(I) with Azoles	MS29-03 **Birger Dittrich** (Novartis Pharma) Structure Specific Restraints for Least-Squares Refinement from Tight Binding Quantum Chemistry
11:20-11:40	MS13-04 **Markus Eder** (AT) Surface Layer Proteins of Lactobacilli – Determining the Cell Wall Binding and their Antibacterial Effect	MS29-04 **Molly Lightowler** (SE) Hydrogen Positions in Small Organic Molecules Determined by 3D Electron Diffraction
11:40-12:00	MS13-05 **Iracema Caballero** (ES) Dealing with Modulated Macromolecular Structures With Translational Non-Crystallographic Symmetry	MS29-05 **Regine Herbst-Irmer** (DE) Anisotropic Hydrogen Atoms in Charge Density Analysis
12:00-14:00	SIG-5 Meeting (SR5) SIG-14 Meeting (SR4)	

Thursday, 22. August 2019 – morning (3/3)

08:30-09:30	Kleiner Festsaal (Kl. FS)	Audimax
	KN13 **Martin Caffrey** (IE) Mesophase Mirabilis. The Lipid Cubic Phase as a System for Investigating Membrane Proteins. Chair: Kay Diederichs (DE)	KN14 **Katharine Page** (US) Capturing Functional Nanostructures and their Interfaces with Neutron Total Scattering. Chair: Mirjiam Zobel (DE)

10:00-12:00	HS7	Kleiner Festsaal (Kl. FS)
	MS34 *Computer Simulation of Molecular Interactions and Crystal Structures.* Chairs: Martin Schmidt (DE), Sally Price (UK)	MS33 *Tuning Crystalline Frameworks and Their Applications Through Structural Design and Polymorphism.* Chairs: Jia Min Chin (UK), Anthony Linden (CH), George Ferguson (UK)
10:00-10:30	MS34-01 **Jan Gerit Brandenburg** (DE) Towards the Design of Molecular Materials	MS33-01 **Wendy L. Queen** (CH) Understanding the Structure-Derived Function of Metal-Organic Frameworks and their Application in Separations
10:30-11:00	MS34-02 **Dragica Prill** (DE) Towards Crystal Structure Solution of Organic Compounds by fit to the Pair Distribution Function without Prior Knowledge of Space Group and Lattice Parameters	MS33-02 **Ross Forgan** (UK) Modulated Self-Assembly of Hard and Soft Porous Crystals
11:00-11:20	MS34-03 **Leonardo Lo Presti** (IT) CLPdyn: A Cheap and Reliable Tool for Molecular Dynamics Studies of Organic Molecules in Condensed Phase	MS33-03 **Ekaterina Vaganova** (RU) Rules for Designing Rod Metal-Organic Frameworks: A Topological Approach
11:20-11:40	MS34-04 **Andrea Ienco** (IT) Computational Protocol for Simulating the Anisotropic Lattice Expansion in Organic Crystals	MS33-04 **Rene de Gelder** (NL) The Crystalline Sponge Method: Pitfalls, Challenges and Solutions
11:40-12:00	MS34-05 **Ioana Sovago** (UK) Analysing Aromatic Interactions: Clarity out of Complexity	MS33-05 **Thomas Roseveare** (UK) Exploring the Dynamic Gas Adsorption Behaviour of a Family of Coordination Polymers through in situ Diffraction Techniques

12:00-14:00	SIG-9 Meeting (SR1) Software Fayre (SR6)

Thursday, 22. August 2019 – afternoon (1/3)

14:00-16:00	HS32	HS7
	MS07 *Structural Enzymology.* Chairs: Maria Solà (ES), Irmi Sinning (DE)	MS03 *Crystallisation and Biophysical Characterisation.* Chairs: Isabel Moraes (UK), Melanie Vollmar (UK)
14:00-14:30	MS07-01 **Ivo Tews** (UK) Taking Crystallographic Snapshots of Vitamin B6 Biosynthesis and Treating Specific Radiation Damage	MS03-01 **Emmanuel Saridakis** (GR) Protein Thermodynamic Parameters to Understand and Guide Crystallisation
14:30-15:00	MS07-02 **Thomas Schneider** (DE) Crystallographic Enzymology: Using Synchrotroton Radiation for High Resolution in Space and Time	MS03-02 **Maria Garcia** (DE) High-Throughput Stability Screening of Integral Membrane Proteins
15:00-15:20	MS07-03 **Eike Schulz** (DE) Watching an Enzyme at Work: Breaking the Strongest Single Bond in Organic Chemistry	MS03-03 **Fabrice Gorrec** (UK) In Numbers: Initial Screening at the MRC-LMB Protein Crystallization Facility
15:20-15:40	MS07-04 **Esko Oksanen** (SE) The Neutron Structure of Leishmania Mexicana Triose Phosphate Isomerase with Transition State Mimics Reveals General Base Catalyst	MS03-04 **Linda Oester** (UK) Biophysical Methods to Aid Protein Crystallization in a Pharmaceutical Setting
15:40-16:00	MS07-05 **Simona Fermani** (IT) Arabidopsis and Chlamydomonas Phosphoribulokinase Crystal Structures Complete the Redox Structural Proteome of the Calvin-Benson Cycle	MS03-05 **Georg Mlynek** (AT) High-Throughput Thermal Stability Approaches for Sample Optimization

16:00-17:00	Coffee Break & Poster Session II

17:00-18:00	Audimax	
	PL02 **Bo Brummerstedt Iversen** (DK) Quantum Crystallographic Studies of Advanced Materials. Chair: Helmut Ehrenberg (DE)	
18:00-19:00	Kleiner Festsaal (Kl. FS)	Audimax
	KN15 **David Stuart** (UK) Changing Times in Structural Virology. Chair: Walter Keller (AT)	KN16 **Françoise Damay** (FR) Unusual Magnetic Orderings from the Interplay of Triangular Topology and Magnetic Anisotropy. Chair: Manuel Perez-Mato (ES)

Thursday, 22. August 2019 – afternoon (2/3)

14:00-16:00	BIG HS	HS33
	MS26 *Complex Metallic Alloys: Periodic and Non-Periodic.* Chairs: Louisa Meshi (IL), Radoslaw Strzalka (PL)	MS28 *Dynamics and Disorder Probed by Diffuse Scattering.* Chairs: Anders Ø. Madsen (DK), Arkadiy Simonov (DE)
14:00-14:30	MS26-01 **Ronan McGrath** (UK) Some Recent Advances in the Surface Science of Complex Metallic Alloys	MS28-01 **Nozomi Ando** (US) Challenges in Measurement and Interpretation of Scattering from Protein Crystals
14:30-15:00	MS26-02 **Ron Lifshitz** (IL) The Power of Analogy in Physics: From Faraday Waves through Soft Matter to Complex Metallic Alloys	MS28-02 **Hans-Beat Bürgi** (CH) Beyond the Average Bragg Structure - Dynamics, Disorder and Diffuse Scattering
15:00-15:20	MS26-03 **Wolfgang Hornfeck** (CZ) Nucleation and Growth of Tenfold Twins of NiZr during Non-Equilibrium Solidification	MS28-03 **Ella Mara Schmidt** (DE) A Disordered Superspace Approach to Understand Highly Structured Diffuse Scattering
15:20-15:40	MS26-04 **Kazuki Nozawa** (JP) Theoretical Study of Single-Element Quasi-Periodic Thin Films Formed on Ag-In-Yb Quasicrystal	MS28-04 **Stefano Canossa** (NL) The Secret Life of MOFs' Functional Groups: Should we Trust Random Disorder?
15:40-16:00	MS26-05 **Marc de Boissieu** (FR) Three Dimensional Local Atomic Configurations of Decagonal AlNiCo Quasicrystal Studied by X-Ray Fluorescence Holography	MS28-05 **Marek Pasciak** (CZ) Unravelling Local Correlations in Heavily Disordered Ferroelectric $Sr_xBa_{1-x}Nb_2O_6$

16:00-17:00	Coffee Break & Poster Session II

17:00-18:00	Audimax
	PL02 **Bo Brummerstedt Iversen** (DK) Quantum Crystallographic Studies of Advanced Materials. Chair: Helmut Ehrenberg (DE)

18:00-19:00	Kleiner Festsaal (Kl. FS)	Audimax
	KN15 **David Stuart** (UK) Changing Times in Structural Virology. Chair: Walter Keller (AT)	KN16 **Françoise Damay** (FR) Unusual Magnetic Orderings from the Interplay of Triangular Topology and Magnetic Anisotropy. Chair: Manuel Perez-Mato (ES)

Thursday, 22. August 2019 – afternoon (3/3)

14:00-16:00	Kleiner Festsaal (Kl. FS)	Audimax
	MS39 *Time-Resolved Diffraction and Scattering Techniques.* Chairs: Semen Gorfman (IL), Michael Wulff (FR)	MS40 *The Use of X-Rays and Neutrons for Experiments in Nanoscience.* Chairs: Helga Lichtenegger (AT), Rainer Timm (SE)
14:00-14:30	MS39-01 **Tim van Driel** (US) Ultrafast Dynamics of Chemistry in Solution Studied by Time-Resolved X-Ray Diffuse Scattering at LCLS	MS40-01 **Hugh Simons** (DK) Nanoscale In-Situ 3D Imaging of Defect Dynamics in Oxide Ferroelectrics
14:30-15:00	MS39-02 **Mathias Sander** (CH) Application of Ultrafast Strain Fields for X-Ray Pulse Shortening and Pulse Picking	MS40-02 **Gerardina Carbone** (SE) Opportunities with Coherent X-Ray Nanobeams: A Short Perspective from a Beamline
15:00-15:20	MS39-03 **Shinobu Aoyagi** (JP) Time-Resolved Structure Analysis of Piezoelectric Crystals Resonantly Vibrating Under Alternating Electric Field	MS40-03 **Dmitry Dzhigaev** (SE) Nano-Scale Strain Mapping in Complete Nanowire Based Electronic Devices by Bragg Coherent X-Ray Diffraction
15:20-15:40	MS39-04 **Eugenia Peresypkina** (DE) Liquid-Metal-Jet X-Ray Source for Time-Resolved SAXS Studies in the Home Laboratory	MS40-04 **Frederik Søndergaard-Pedersen** (DK) In Situ X-Ray Scattering Study of Hydrothermal Synthesis of Anatase TiO_2 Nanoparticles from Commercial Precursor $TiOSO_4$
15:40-16:00	MS39-05 **Katarzyna Jarzembska** (PL) At the Intersection of Crystallography and Spectroscopy - Studies of Selected Photoactive Coinage Metal Complexes	MS40-05 **Sabrina Thomae** (DE) Atomic Insight into Hydration Shells around Facetted Iron Oxide Nanoparticles

16:00-17:00	Coffee Break & Poster Session II

17:00-18:00	Audimax
	PL02 **Bo Brummerstedt Iversen** (DK) Quantum Crystallographic Studies of Advanced Materials. Chair: Helmut Ehrenberg (DE)

18:00-19:00	Kleiner Festsaal (Kl. FS)	Audimax
	KN15 **David Stuart** (UK) Changing Times in Structural Virology. Chair: Walter Keller (AT)	KN16 **Françoise Damay** (FR) Unusual Magnetic Orderings from the Interplay of Triangular Topology and Magnetic Anisotropy. Chair: Manuel Perez-Mato (ES)

Poster Presentations

Poster Sessions are scheduled every day between 16:00 and 17:00, organized in two sessions (**Poster Session I on Mon+Tue, Poster Session II on Wed+Thu**).

Posters with **odd number** will be presented in Poster Session I, posters with **even numbers** in Poster Session II. Posters are displayed in the respective **area A, B, C, D and E** (Poster contributions listed in this booklet include submissions by 16.07.2019).

Poster Session I

MS01-P01 A **Data Analysis Infrastructure for Serial Crystallography Experiments at the EuXFEL** Dall'Antonia F., et al.

MS01-P03 A **MicroMAX - New Possibilities for Serial Crystallography** Ursby T., et al.

MS01-P05 A **Serial Crystallography at the ESRF Extremely Brilliant Source: The ID29 Upgrade Project** de Sanctis D.

MS01-P07 A **Optimized Design for New Scientific Opportunities in Macro-Molecular Crystallography at the Future Microfocus XAIRA [...]** Juanhuix J., et al.

MS01-P09 A **P11 at PETRA III: A Versatile Beamline for Serial and High-Throughput Crystallography** Burkhardt A., et al.

MS02-P01 A **Structure-Based Drug Design to Tackle Disorders of Haem Biosynthesis** Arruda Bezerra G., et al.

MS02-P03 A **PanDDA: Extracting Ligand-Bound Protein States from Conventionally Uninterpretable Crystallographic Electron Density** Pearce N.

MS02-P05 A **New Fully Automatic Measurement MX Beamline BL45XU at SPring-8** Mizuno N., et al.

MS03-P01 A **Structural Basis of Inactivation of Human Counterpart of Mouse Motor Neuron Degeneration 2 Mutant in Serine Protease HtrA2** Wagh A.

MS03-P03 A **Molecular Investigation of Muscle Z-Disc Assembly Centered on the Complex Human A-actinin Isoform-2 and ZASP** Stefania V., et al.

MS03-P05 A **Invitation to Perform Experiments on High End Instruments: Centre of Molecular Structure in BIOCEV** Stránský J., et al.

MS03-P07 A **Structural and Biophysical Analysis of the Pyridoxal Phosphate Synthase from Plasmodium Vivax** Ullah N., et al.

MS03-P09 A **Crystal Structure of Human AMACR Provides Insight into Substrate Recognition and Catalytic Mechanism** Lin M.H., et al.

MS03-P11 A **A Reliable and Versatile Tool for High-End In-House Structural Studies** Smith V., et al.

MS03-P13 A **Profilins and the Quest for Structure-Based IgE-epitope Mapping** Gottstein N.A., et al.

MS03-P15 A **Novel Biochemical Bases for Nuclear Factor I X (NFIX)** Lapi M.

MS03-P17 A **Crystal and Solution Structures of SH_2 Domain of Signaling Molecule in Complex with the Co-stimulatory Receptor CD28** Inaba-Inoue S., et al.

MS03-P19 A **Structural Determinants of the Interaction Specificity at the G and NC Interfaces of Human Septins** Leonardo D., et al.

MS03-P21 A **The N-terminal Domain of Lactobacillus acidophilus SlpA promotes Self-Assembly of the S-Layer Array** Sagmeister T., et al.

MS03-P23 A **The Crystal Structure of the Major Olive Pollen Allergen Ole e 1** Hofer G., et al.

MS04-P01 A **CCP-EM: The Collaborative Computational Project for Electron Cryo-Microscopy** Winn M., et al.

MS04-P03 A **Efficient Real-Space Refinement for Cryo-EM and Crystallography** Urzhumtsev A., et al.

MS05-P01 A **The Critical Role of the Fourth Position of the VxGFL Motif of PP_2Cs from Oryza sativa in Regulation of ABA Responsiveness** Lee S., et al.

MS06-P01 A **Structural Insights in a Mitochondrial Nucleoid Maintenance Factor** Tarrés-Solé A.

Poster Session I (cont.)

MS06-P03 A **Structural Studies of Temperate Phage Genetic Switches** Varming A., et al.

MS06-P05 A **Molecular Basis of Self-Induced Genomic Degradation Inhibition by the Sub-Nanomolar Interaction of Nin with NucA and NucB […]** Booth S., et al.

MS06-P07 A **Structural Study Two Different Forms of Smap From Halobacterium salinarum Which Have A Different […]** Fando M., et al.

MS07-P01 A **Crystal Structure of the Cell Wall Binding Domain of a Novel Bacteriophage PBC5 Endolysin and its Peptidoglycan Interaction** Suh J.Y.

MS07-P03 A **Structural and Functional Characterization of Phosphoglucomutase 5** Pühringer D.

MS07-P05 A **Studying the Structural Basis for Selectivity in Complexes of Peptide Inhibitors and Serine-Proteases of the Complement System** Dürvanger Z., et al.

MS07-P07 A **Beetle Luciferases and their Color Emission** Rabeh W.

MS07-P09 A **Active Site Evolution in Biomass Degrading Enzymes** Lo Leggio L., et al.

MS07-P11 A **Differences in Crystallization of Several Selected Haloalkane Dehalogenases and their Mutation Variants** Kuta Smatanova I., et al.

MS07-P13 A **Enzyme Activation by a Flavoprotein Redox Network** Hammerstad M., et al.

MS07-P15 A **Structural Insight in Peptidyl Substrate Binding to Cysteine Cathepsins** Loboda J., Tusar L.

MS07-P17 A **Porphyromonas Gingivalis Tpr Protease Zymogen Resembles Calpain-Calpastatin Complex** Staniec D.

MS07-P19 A **Neutron Protein Crystallography at the Heinz Maier-Leibnitz Zentrum (MLZ): New Developments and Recent Application […]** Schrader T.E., et al.

MS07-P21 A **Structure-Function Characterisation of Novel Galactosidases from Lactobacillus Plantarum: Exploring the Link Between Gut […]** Feliciotti I., et al.

MS08-P01 A **Regulation of p97 ATPase Activity by Cofactor-Mediated Remodeling and Post-Translational Modification** Heinemann U., et al.

MS08-P03 A **TraF is an Essential Factor of the pIP501 Type IV Secretion System (T4SS) and Exhibits Structural Homology with the T7SS […]** Keller W., et al.

MS08-P05 A **Atomic Structure of Potato Virus X, the Prototype of the Alphaflexviridae Virus Family** Zanotti G., et al.

MS08-P07 A **Crystal Structures of Streptococcus Pyogenes Cas1 and Cas2 in the Type II-A CRISPR-Cas System** Ka D., et al.

MS08-P09 A **Structural Study for Recognition of Ubiquitylated Histone H3 by DNA Methyltransferase** Arita K., et al.

MS09-P01 A **Improving Density Histogram by Phase Optimisation Using a Genetic Algorithm** Kantamneni S.M., et al.

MS10-P01 A **A New 3D Reflection Data Viewer Based on NGL** Oeffner R., et al.

MS10-P03 A **Improving Identification and Validation of Water Molecules in Protein Crystal Structures with Molecular Dynamics Simulations** Caldararu O., et al.

MS10-P05 A **B-Factors Reflect the Local Dynamics of Proteins and Nucleic Acids** Schneider B., Cerný J.

MS11-P01 A **New ARP/wARP Web Service Integrated into Virtual Computation Frameworks** Sobolev E., et al.

MS11-P03 A **SIMBAD: Structure Based Search Model Identification for Molecular Replacement using the PDB Database** Simpkin A., et al.

MS11-P05 A **PReSTO Integrative Structure Biology Software for all Platforms** Unge J.

MS12-P01 A **Crystallization and Structure Determination of Aldo-keto Reductase 1C3 in Complex with Steroidal Inhibitors Using in situ Proteolysis** Petri E., Celic A.

MS12-P03 B **Symmetry in Structures of Protein Assemblies** Grudinin S., Pages G.

MS12-P05 B **PDBe Knowledge Base (PDBe-KB) – Infrastructure for FAIR Structural and Functional Annotations** Velankar S.

MS12-P07 B **Structural Comparison and Evolutionary Relationships Between Ceruloplasmin, Hephaestin and Blood Coagulation Factor VIII** Zaitsev V., Lindley P.

MS13-P01 B **Brachiopod Shell Calcite Mineralization Occurs by Ion-by-Ion Transport Controlled by the Epithelial Cell Membranes** Schmahl W., et al.

MS13-P03 B **Structure and Microstructure Study of Charonia Lampas Lampas Shell** Salim O., et al.

MS13-P05 B **The Interaction Between Calcium Carbonate and Calcium Phosphate as the Driving Mechanism for […]** Pastero L., et al.

MS14-P01 B **Reassessing Pauling's Rules** George J., et al.

MS14-P03 B **Electron Crystallography of Planetary Materials: Impactites and Micrometeorites** Gemmi M., et al.

MS14-P05 B **Synthesis and Crystal Structures of $Zr_2(OH)_2(XO_4)_3 \cdot 4H_2O$ (X=S,Se) and $Zr(SeO_3)_2$** Giester G., et al.

MS14-P07 B **Steric Effect in Tetracoordinated Ni(II) Complexes with Enamino-Ketone Ligands and Their Reaction Products with Heterocyclic [...]** Zep A.

MS14-P09 B **Crystal Structure and Hirshfeld Surface Analyses of a new Organogold(III) with Thiosemicarbazone** Almeida C., et al.

MS14-P11 B **Synthesis of Calcium and Strontium Rare-Earth Aluminates and Its Use as Host Lattice for LEDs** Otgonbayar C., Poellmann H.

MS14-P13 B **Periodic Trend of Stereochemical Activity of Lone Electron Pairs** Murshed M.M., Gesing T.M.

MS14-P15 B **Crystal Structure and Thermodynamic Behavior of $Bi_6Te_2O_{15}$: the Likely Structure of the Rare Mineral Pingguite** Nenert G., et al.

MS14-P17 B **Preparation, Spectral, Structural, Hirshfeld Surface and Molecular Docking of Tetrakis(pyridine-'N)bis(thiocyanato-'N) [...]** El Hamdani H., et al.

MS14-P19 B **Synthesis, Spectroscopic Properties, Crystal Structure, Antimicrobial Properties and Molecular Docking Studies of [...]** El Hamdani H., et al.

MS14-P21 B **Inverse Crystal Structure Behaviour of $Ca_3Al_4ZnO_{10}$ at High Pressure and High Temperature** Hejny C., et al.

MS14-P23 B **Structural Ordering in the Pyrite-Related Phases: PtSnS, PtSnSe and PtSnTe** Laufek F., Vymazalová A.

MS14-P25 B **A New Polymorph of Trisodium Hexachlororhodate** Etter M.

MS14-P27 B **Doped Single Crystal TiO_2 Series Products by Molten Salt Method Used as Photocatalytic Materials** Zhao Z.

MS14-P29 B **Evidence of Anatase Intergrowths Formed During Slow Cooling of Reduced Ilmenite** D'Angelo A.

MS14-P31 B **Crystal Chemistry of Struvite and its Derivatives** Kiriukhina G., Yakubovich O.

MS14-P33 B **Crystal Structure and Biological Activities of a New Proton Transfer Material** Hamdi N., et al.

MS14-P35 B **The Crystal Structures of Natural Barium Beryllophosphates** Hatert F., et al.

MS14-P37 B **Crystal Structure of $CaBaFe_4O_7$** Gutmann M.

MS14-P39 B **Stereochemistry of Tl(I) in Inorganic Oxysalts** Markovski M., Siidra O.

MS15-P01 B **Reducing the Background of Ultra-Low Temperature X-Ray Diffraction Data** McMonagle C., Probert M.

MS15-P03 B **Pressure-Induced Spin Transitions in Garnets** Friedrich A., et al.

MS15-P05 B **Ab initio Simulation and X-Ray Diffraction Measurements of Deviatoric Stress in Mineral Inclusions** Morana M., et al.

MS15-P07 B **Toward One-Pot Green Synthesis of Nanoporous Carbon Nitrides** Dziubek K., et al.

MS15-P09 B **New Insights on the High Pressure Behaviour of the $GeSe_xTe_{1-x}$ Solid Solution** Friese K., et al.

MS15-P11 B **Synthesis, Crystal Structures and Thermal Expansion of Novel Lutetium-Barium Borates** Biryukov Y., et al.

MS15-P13 B **High Pressure X-Ray Imaging and Diffraction on the Psiché Beamline: Recent Results and Developments Using Large Volume Presses** Itié J.P., et al.

MS15-P15 B **In-situ Single Crystal X-Ray Diffraction Studies of Proton Transfer Behaviour Under an Applied Electric Field on I19, Diamond [...]** Saunders L., et al.

MS16-P01 B **Short-Range Structure of Zr and Pd Bulk Metallic Glasses Prepared During the Melting and Cooling Process** Frison R., et al.

MS16-P03 B **Structure Design of Novel $Ba_{3-x}Sr_xTeO_6$ Double Perovskites and the Effect of Temperature and Composition on Structure Stability** El Bachraoui F., et al.

MS16-P05 B **Environmental Effect on Titanium Alloy Ti6242S in Air Between 500 and 700°C** Kalienko M.

MS16-P07 B **Crystal Structure and Dehydration Behavior of Ag^+-Exchanged Levyne** Cametti G., et al.

MS16-P09 B **Investigation of Physical Properties of Equiatomic Silver-Rare Earth Compounds Ag-Re (Re=Nd, Ce ,Gd) from First [...]** Abdelhak F.

MS16-P11 B **Moringa Oleifera Waste as Dopants for S, N, C-TiO_2 Photocatalysts Development** Agbahoungbata M.Y., Linden A.

MS17-P01 B **Symmetry Lowering in Natrochalcite $NaCu_2(H_3O_2)(SO_4)_2$ Under Pressure** Miletich R., et al.

MS17-P03 B **Pressure-Induced Modification of Molecular Aggregation in Crystals of Benzocaine** Patyk-Kazmierczak E., et al.

MS17-P05 B **Ex-Situ Study of the Pressure Induced Decomposition of Iron Nitride Fe_4N** Wetzel M.H., et al.

MS17-P07 B **Phase Transitions of Copper(I) Iodide Compounds Under High Pressure** Gonzalez-Platas J., et al.

MS18-P01 B **Prussian Blue Analogues as Cathode Material in Low Cost Aqueous Batteries** Kjeldgaard S., et al.

MS18-P03 B **Phase Evolution During Perovskite Formation - Insight from PDF Analysis** Hua X.

Poster Session I (cont.)

MS18-P05 B **Combination of EXAFS and XRD for Studies of the Orthorhombic-Tetragonal Phase Transformation in $MAPbI_{3-x}Cl_x$ perovskites** Schuck G., et al.

MS18-P07 B **First-Principles Study of Oxygen Adsorption Structure on $Ni_3Al(210)$ Surface** Yamaguchi K., Nozawa K.

MS18-P09 B **Determination of Host and Dopant Ion Distribution in $Mg_2Si_{1-x}Sn_x$ Thermoelectric Materials by Electron Channeling** Delimitis A., et al.

MS18-P11 B **Band Gap Depth Profile of $Cu(In_{1-x}Ga_x)Se_2$ Absorbing Layer in Thin-Film Solar Cell by Glancing Incidence X-Ray Diffraction** Kim Y.I., Kim K.B.

MS18-P13 C **Local Structure of Glass-Ceramic Sodium Sulfidic Solid State Electrolytes** Fritsch C., et al.

MS18-P15 C **Thermochromic Lead-Free Halide Double Perovskites** Ning W., Gao F.

MS18-P17 C **The Influences of Mg Intercalation on the Structure and Supercapacitive Behaviors of MoS_2** Liao L., et al.

MS18-P19 C **Combination of Data Mining and DFT Modeling of Ag^+-Conductivity In S(Se)-Containing Inorganic Compound** Morkhova Y.

MS19-P01 C **High-Pressure Synthesis, Crystal Structure, and Magnetic Properties of $Ba_3CuOs_2O_9$** Chen J., et al.

MS19-P03 C **Magnetism in Double Perovskites Ba_2CrMoO_6** Bouadjemi B., et al.

MS20-P01 C **Discovery of Complex Metal Oxide Materials by Rapid Phase Identification and Structure Determination** Li J., Sun J.

MS20-P03 C **Raman and Surface Analysis Studies of $(CuGaSe_2)_{0.8} – (CuAlSe_2)_{0.2}$ Single Crystals** Rywkin S., et al.

MS20-P05 C **Powder XRD Structure Determination of Nanostructured, Disordered MoS_2-Ethylenediamonium Layered Compound […]** Goloveshkin A., et al.

MS21-P01 C **Structural Investigations on Bridging Stibinidene Complexes with Cu-K_β-radiation: A Comparison** Rummel L., et al.

MS21-P03 C **Accurate Experimental Charge Density Data: Tips & Tricks for Data Collection & Processing** Ott H., et al.

MS22-P01 C **3D-Visualization and -Printing of Molecular Surfaces** Hübschle C.

MS22-P03 C **Phase Transitional Behavior and Charge Density Study of Drug Methimazole** Fayzullin R.R., et al.

MS22-P05 C **Charge Density Analysis of a Series of 4-methylthiostilbene Derivatives** Kubicki M., et al.

MS22-P07 C **Quinoid Dianion Forming a Lone-Pair Pi-Hole Contact** Vukovic V., et al.

MS22-P09 C **Polymorphism and the Role of F…F Interactions in Crystal Packing of Fluorinated Tosylates** Korlyukov A., et al.

MS23-P01 C **Correction for Phonons, Phasons and Multiple Scattering in Quasicrystals** Strzalka R.

MS23-P03 C **From a Single Slit to Periodic, Modulated and Quasiperiodic Crystals – a New Aproach to the Diffraction Analysis of Aperiodic Systems** Wolny J.

MS23-P05 C **Crystal Structure of Incommensurately Modulated ß-$NaBrF_4$** Ivlev S., et al.

MS23-P07 C **Modulated Structure in $Ni_2MnGa_{0.95}In_{0.05}$ Shape-Memory Alloy** Cejpek P., et al.

MS23-P09 C **Incommensurately Modulated Structures in the Series $RETe_{2-d}$** Doert T., Poddig H.

MS24-P01 C **Structural Disorder and Magnetic Correlations Driven by Oxygen Doping in $Nd_2NiO_{4.11}$** Keller L., et al.

MS24-P03 C **Revisiting the Magnetic Structure of $R_{1/3}Sr_{2/3}FeO_3$ (R = La,Pr,Nd) by Neutron Powder and Single Crystal Diffraction Combined […]** Pomjakushina E., et al.

MS24-P05 C **Understanding and Tuning Magnetism of Mesoscopic Hollow Oxide Sphere by Surface Engineering** Chen S., et al.

MS25-P01 C **Electron Crystallography for Studying MOF-Intercalated Guests** Samperisi I.

MS25-P03 C **Automated Electron Diffraction: 3D Structure Determination with Sub-Ångström Resolution** Roslova M., et al.

MS25-P05 C **Continuous Rotational Electron Diffraction Method for Structure Determination of Small Organic Molecules** Ge M., et al.

MS25-P07 C **Dynamical Structure Refinement from Data Obtained with a Dose of Less than 1 $e^-/Å^2$** Klein H., Kodjikian S.

MS25-P09 C **Structure of a Novel R2-Like Ligand-Binding Oxidase Revealed by Electron Diffraction** Clabbers M., et al.

MS26-P01 C **Peculiarities of Solid Solutions with NaTl-Type Structure In Li-Zn-X (X=Al,Ga,In) Systems** Dmytriv G., et al.

MS27-P01 C **Structural and Physical Properties of a 2,2';6',2''-terpyridine Derivative in the Solid State Phase Transition Behavior** Hsu I.J., et al.

MS27-P03 C **Local Order in Co and Mn Prussian Blue Analogues, the 3D-PDF analysis.** Simonov A., et al.

MS27-P05 C **Correlation of High-resolution X-Ray Diffraction with Mechanical Experiments and Finite Element Analysis** Dommann A., et al.

MS27-P07 C **Unique Properties of Geoinspired Nanotubes as Water Nanocontainer** Launois P., et al.

MS28-P01 C **Solving the Disordered Structure of beta-Cu_2Se Using the Three-Dimensional Difference Pair Distribution Function** Roth N.

MS28-P03 C **Understanding Structural Disorder in Nickel Cyanide Using 1D Statistical Mechanical Models** Wolpert E., et al.

MS29-P01 C **KOALA - Routine H-Atom Determinations by Laue Neutron Diffraction** Edwards A., Piltz R.

MS29-P03 C **Comparison of Different Strategies for Modelling Hydrogen Atoms in Charge-Density Analyses** Köhler C., et al.

MS29-P05 C **Comparison of X-Ray Wavefunction Refinement and Multipole Refinement Based on the Energetic Analysis of the [...]** Woinska M., et al.

MS30-P01 C **Features of Crystal Formation of Chiral Derivatives of 1,5-dihydro-2h-pyrrole-2-one** Saifina A., et al.

MS30-P03 C **Crystallization-Induced Stereoisomeric Recognition and Stereochemical Transformations of Chiral Organic Molecules: [...]** Lodochnikova O.

MS30-P05 C **Separation and Resolution of Methylcyclohexanones by Enclathration with Deoxycholic Acid** Bouanga Boudiombo J.S., et al.

MS31-P01 C **Structural Analysis and IR-Spectroscopy of a New Anilinium Hydrogenselenite Hybrid Compound: A Subtle Structural Phase [...]** Takouachet R., et al.

MS31-P03 C **Photocrystallographic Investigations of New Nickel(II) Nitro Complexes** Kutniewska S.E., et al.

MS31-P05 C **Structural and Computational Studies of a Series of New Photoswitchable Nickel Nitro Complexes** Borowski P., et al.

MS31-P07 C **Breathing Metal-Organic Frameworks Based On Flexible Inorganic Building Units** Inge A.K., et al.

MS31-P09 C **Wavelength-Selective Photoisomerisation of NO and NO_2 Ligands** Schaniel D., et al.

MS31-P11 C **Molecular Switches in Nanocontainers** Diskin-Posner Y., et al.

MS31-P13 C **Exceptionally Flexible Coordination Polymers of Cd(II)** Pisacic M., Đakovic M.

MS31-P15 C **Separation of Isomers by Host-Guest Chemistry: Polymorphism, Resolutions and Templating** Nassimbeni L.

MS32-P01 C **In Situ PXRD Monitoring the Mechanosynthesis of Metal-Organic Halogen-Bonded Cocrystals** Lisac K., et al.

MS32-P03 C **Influence of the Basicity of Halogen Bond Acceptors on Stoichiometry of Cocrystals with 1,3,5-triiodo-2,4,6-trifluorobenzene** Bedekovic N., et al.

MS32-P05 D **Insights into Weak C-H...F-C Interactions in C_6F_6:C_6H_6-nMen Co-Crystals Using Variable Temperature Crystallography to Follow [...]** Cockcroft J.

MS32-P07 D **Intermolecular Head-to-Head Interactions of Carbonyl and Thiocarbonyl Groups** Shteingolts S.A., Fayzullin R.R.

MS32-P09 D **Non-Covalent Bonding in Organic Crystals: a Combined X-Ray and DFT Study** Voronina J.

MS32-P11 D **Solid State Structure of Pharmaceutically Important Coumarin Derivatives from in House Collected XRPD Data** Bényei A., et al.

MS32-P13 D **Effect of Localized Non-Bonding/Repulsive Interactions on Distribution of Electron Density in Pi-Conjugated Systems** Lindeman S.

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MS25-P04 C **Dedicated Electron Source for Serial Electron Crystallography** Hogan-Lamarre P., et al.

MS25-P06 C **Low Dose Electron Diffraction Tomography (LD-EDT) Solves the Structure of a New $(Na_{2/3}Mn_{1/3})2Mn_3Ge_3O_{12}$ phase […]** Kodjikian S., et al.

MS25-P08 C **Refinement of Organic Crystal Structure with Multipolar Electron Scattering Factors** Dominiak P., et al.

MS25-P10 C **MicroED, Fast and Furious** Raaijmakers H.

MS26-P02 C **Chemical Bonding and Structural Complexity in Known Intermetallic Compounds o-$Al_{13}Co_4$ and $Al_{2.75}Ir_2$** Grin Y.

MS27-P02 C **New Radiation-Induced Phase of $MAPbI_3$ - an Unexpected Surprise of Synchrotron Experiments** Minns J.

MS27-P04 C **Endohedral Metallofullerene Crystals: Playing with Disorders** Liu F., Popov A.A.

MS27-P06 C **The Benefits of Cu-K_β Radiation in Elucidating the Molecular Structure of Polypnictogen Cations** Riesinger C., et al.

MS28-P02 C **Local Dipole Formation in IV-VI Semiconductors** Holm K., et al.

MS29-P02 C **On Precision and Accuracy of X-Ray and Neutron Diffraction Results for Single Crystals of Glycine** Sutula S., et al.

MS29-P04 C **TAAM: A Reliable and User Friendly Tool for Hydrogen Atom Location Using X-Ray Diffraction Data** Chodkiewicz M., et al.

MS30-P02 C **Absolute Structure assignment Through Interplay of X-Ray Diffraction and EBSD** Borrmann H., et al.

MS30-P04 C **Unexpected Polymorphic Behavior of Four Racemic 3-Pyrrolin-2-One Derivatives** Gerasimova D., et al.

MS30-P06 C **Peculiarities of Supramolecular Organization in Centric, Acentric and Chiral Ketones with Vinylacetylene Fragments** Voronova E., et al.

MS31-P02 C **Triethylphosphine as a Molecular Gear — Phase Transitions in Ferrocenyl–Acetylide–Gold(I)** Makal A.

MS31-P04 C **Probing Spin Crossover in Novel Metal Organic Complexes** Musselle-Sexton J., et al.

MS31-P06 C **Pressure-Induced Polymerization and Electrical Conductivity of a Polyiodide** Poreba T.

MS31-P08 C **Conformational Switching in Single Crystals of a Calix[4] resorcinarene** Lindeman S., et al.

MS31-P10 C **Photoinitiated [2+2] Cycloaddition Reactions Observed in d-Metal(II) Malonates with N,N'-Containing Linkers** Vologzhanina A.V., et al.

MS31-P12 C **Dynamic, Breathing, Water-stable, Mixed-Ligand Zn(II) Metal-Organic Frameworks with Differing Water and Vapour Sorption […]** Oliver C.L.

MS31-P14 C **Thermo- / Mechano- Mechanically Responsive Cocrystals During Single-Crystal-to-Single-Crystal Phase Transitions** Liu G., et al.

MS31-P16 C **Structure / Reactivity Relationships from Detailed Reaction Mechanisms** Roodt A., et al.

MS32-P02 C **Efficient Recognition of Steroids by Planar Aromatic Molecules: A Novel Biomolecular Recognition Motif and its Potential Applications** Topic F., Friscic T.

MS32-P04 C **Towards the Linear $[S_2X]^+$ Systems: Metal Complexes and Halogen Bonding** Valkonen A., et al.

MS32-P06 C **Identification of Non-Covalent Interactions by Hirshfeld Surface and Energy Frameworks in Chalcone-Flavanone Isomers** Checinska L., et al.

MS32-P08 C **Intermolecular Chalcogen···Halogen Interaction in Organic Molecular Crystals** Kazmierczak M., Katrusiak A.

MS32-P10 C **Structural Landscape of Cu(II) Coordination Compounds with Isomers and Derivatives of Cyclic Triimidazole** Fonari M., et al.

MS32-P12 C **Examination of the Intermolecular Aurophilic Interactions in the Crystals of the $(ArCOC{=}C)(PEt_3)Au$ and $[(ArCOC{=}C)_2Au$ […]** Pawledzio S., et al.

MS32-P14 C **Hypervalent Chalcogen-Chalcogen Heteropentalenes and their Charge Transfer Adducts** Levendis D., et al.

MS32-P16 C **Interplay Between Occurrence Frequencies of Charged and Neutral Base Pairs in Small Molecule Crystals** Cabaj M., Dominiak P.

MS33-P02 C **Polarized Fluorescence Harvested from Fullerenes Loaded in Non-Centrosymmetric Ni-MOF** Vasylevskyi S., et al.

MS33-P04 C **Synthesis and Characterization of New Lanthanide MOFs Using a Semi-Flexible Bis-Imide Ligand** González Chávez F.

MS33-P06 C **Controlled Release of Natural Essential Oils from Microporous Metal-Organic Framework** Mazzeo P.P., et al.

Poster Session II (cont.)

MS33-P08 C **About the Polymorphism of Two Anti-Inflammatory Drugs within Thin Films** Kaltenegger M., et al.

MS33-P10 C **Mechanochemistry and Electron Crystallography: a Winning Combination for the Discovery of New Metal-Organic Materials** Lanza A., et al.

MS33-P12 C **Serial-MOF: Developing Serial Crystallography Methods for MOF Nano-crystals** De Zitter E., et al.

MS33-P14 C **Constructing Extended Bismuth(III) Structures Using Tridentate Organic Linkers** Senior L., Linden T.

MS33-P16 C **Giant Supramolecules as Molecular Containers** Virovets A., et al.

MS34-P02 C **Use of Crystal Structure Prediction to Design Template Crystallization Experiments of Nitrobenzoic Acid Derivatives** Berzinš A., Actinš A.

MS34-P04 C **DFT Studies of Structural, Electronic and Magnetic Properties of InP and $In_{0.75}X_{0.25}P$ (where X = Cr, Mn & Fe)** Kaur K., Sharma S.

MS34-P06 C **A Combined Theoretical and Experimental Investigation into the High Throughput Screening of Cocrystal Coformers** Sugden I., et al.

MS34-P08 D **Understanding of Cholesterol Transport in NPC Family Protein: A Computational Study** Yoon H., et al.

MS35-P02 D **Phase Transitions Associated with Conformational Changes of Ligand and Anion Reorientation Trigger Normal and Reverse Spin [...]** Kusz J., et al.

MS35-P04 D **Structural Studies of the Host-Guest Complexes of Carboxylated Pillar[n]arenes** Butkiewicz H., et al.

MS35-P06 D **Novel Coordination Compounds for Biological Applications** Garcia-Granda S., et al.

MS35-P08 D **Two Composite Mn(II)-squarate-dpe Supramolecular Networks Showing Interesting Water Hysteresis Phenomenon in Water [...]** Wang C.C.

MS35-P10 D **Hydrothermal Synthesis, Crystal Structure and Luminescent Properties of a New Praseodymium Coordination Polymer of [...]** Benmerad B., et al.

MS35-P12 D **New Titanium Calix[n]arene-based Scaffolds as Anti-tumour Agents** Elsegood M.

MS35-P14 D **Crystal Structure and Self-Assembly of Pillar[n]pyridiniums** Danylyuk O., et al.

MS35-P16 D **A Lamellar Structure Exhibiting Nano-Morphological Reversibility, Disassembly-and-Self-Assembly Crystallization into Novel [...]** Hung L.I., Chen P.

MS35-P18 D **Crystal Structures of Cholesterol Based Photo-Switchable Mesogenic Dimers. Strongly Bent Molecules Versus an [...]** Pruszkowska K., Zep A.

MS35-P20 D **Correlation Between Structural Studies and Third Order NLO Properties of Three New Semi-Organic Compounds** Benali-Cherif R., et al.

MS35-P22 D **Medium Chain Length (mcl)-PHA-based Nanocomposites for Biomedical Applications: System Evaluation Through XRD** Malagurski I., et al.

MS35-P24 D **Supramolecular Assemblies of Copper(II) Complexes: Supramolecular Synthon Transferability and Magnetic Properties** Penic N.

MS35-P26 D **Organic Cocrystals with Mechanically Interlocked Architectures: Unprecedentedly Stiff and Hard with Elastic Flexibility** Dey S., et al.

MS35-P28 D **Evaluation of Trends in a Series of Halogenated Isophthalamides** Gallagher J.F., Osman I.A.

MS35-P30 D **Halogenation Dictates Architectures and Properties of Amyloid Peptides** Terraneo G., et al.

MS35-P32 D **Hierarchical Design of Lipid-Polymer Composite Nanofibers: the Interplay of Multiscale Structures and Biofunctions** Sadeghpour A., et al.

MS35-P34 D **Controlling the Salt-Cocrystal Continuum and pKa rule: The Multi-Drug Ionic-Cocrystals of Lamatrigine and Valproic Acid** Lusi M., Kavanagh O.

MS35-P36 D **Multicomponent Crystal Formation of Baclofen with Acids and Bases** Malapile R., et al.

MS35-P38 D **The Photodimerization of Schiff Bases: Benzophenone Azine Crystals and their Weak C-H...pi Interactions** Smith M., Lemmerer A.

MS36-P02 D **Dynamical Disorder in the Solid State: Insights from Dielectric Relaxation Spectroscopies** Correia N., et al.

MS37-P02 D **Towards Understanding Phase Transitions of Confined Pharmaceuticals** Nartowski K., et al.

MS37-P04 D **The Drug Target Monoacylglycerol Lipase: Structure and Dynamics, Conservation and Divergence** Oberer M., et al.

MS38-P02 D **Pushing Data Quality for Laboratory Pair Distribution Function Experiments** Zobel M., et al.

MS38-P04 D **Measuring Accurate Single Crystal Diffraction Data Using a Pilatus3 CdTe Detector** Krause L., et al.

MS39-P02 D **A Novel X-Ray Diffraction Technique for in-situ Observations of Cathode/Anode Reaction in Electrolytes** Kubicek S.

MS39-P04 D **Silica Nanoparticle Agglomeration Studies Under Physiological Conditions Using Dynamical SAXS Methods** Iranpour N., et al.

MS39-P06 D **Recent Developments Towards High-Flux Time-Resolved and THz-SAXS-Experiments at the EMBL P12 BioSAXS Beamline** Schroer M.A., et al.

MS40-P02 D **Structural and Optical Properties of CuS Nanoparticles** Souici A., Chibani S.

MS40-P04 D **A Laboratory Rheo-SAXS Setup - Relating Nanostructure to Macroscopic Properties in one go** Jones A.O.F., et al.

MS40-P06 D **Study of Structural Polymorphism in Molecular Composites: Application to Energy Storage** Ouaaka E., et al.

MS40-P08 D **Morphology Characterization of Anatase TiO_2 Nanocrystals by Advanced Rietveld Refinement of Powder X-Ray Diffraction Data [...]** Yu J.

MS40-P10 D **The Dynamic Structure of $Au_{38}(SR)_{24}$ Nanoclusters Supported on CeO_2 under CO Oxidation** Pollitt S., et al.

MS40-P12 D **Nanocrystalline CdS and (Cd,Mn)S Particles: Structure and Morphology** Cherepanova S., Evtushok B.

MS41-P02 D **Multiferroic $Bi_2Fe_4O_9$: Tuning of Crystallization Pathways and Kinetics** Kirsch A., Gesing T.

MS41-P04 D **Two New Polymorphs of $CuCl_2$·2DMF Obtained via High-Temperature Crystallization** Goreshnik E.

MS41-P06 D **Dynamic Theory of Protein Crystallization** Hasek J., et al.

MS42-P02 E **Extracting Coherent Information About Phase Transformations in a Functional Material Studied by X-Ray Powder Diffraction** Gertenbach J., et al.

MS42-P04 E **SNBL's BM31 at ESRF Beyond 2020 - Combined XRD-PDF-XAS** van Beek W., et al.

MS42-P06 E **Testing a Home-Made Sample Holder with Flow-Through Capillary to Study in-situ Re-Solvation Process** Rohlicek J., et al.

MS42-P08 E **Latest Developments in Non-Ambient XRD Attachments from Anton Paar** Puhr B., et al.

MS42-P10 E **In-situ Wide-Angle X-Ray Scattering on Liquid Crystalline Elastomers for Orthopedic Applications** Dadivanyan N., et al.

MS42-P12 E **Operational Non-Uniformities of Lithium Distribution in Li-Ion Batteries Probed by Diffraction Techniques** Senyshyn A.

MS42-P14 E **Diffusion Mechanisms of Gas Adsorption by Porous Frameworks from Sub-Second Synchrotron Powder X-Ray Diffraction** Dovgaliuk I., et al.

MS43-P02 E **Instrumental Effects in Laboratory Pair Distribution Function (PDF) Analysis** Gateshki M., et al.

MS43-P04 E **Mapping Non-Crystalline Nanostructure With Low-dose Scanning Electron Pair Distribution Function Analysis** Laulainen J.E.I., et al.

MS44-P02 E **Hydraulic, Structural and Photocatalytic Behavior of Cementitious Phases Incorporating Nanocomposite Mixed Zn-Al-Ti Oxydes** Amor F.

MS44-P04 E **Effects of X-Ray Irradiation and Thermal Annealing on the Co Dopant Location in Co-Doped TiO_2 Nanocrystals** Soo Y.L., et al.

MS44-P06 E **Automated Serial Rotation Electron Diffraction Combined with Cluster Analysis as a Tool for Structure Determination** Smeets S., et al.

MS44-P08 E **Utilising MaXrd in the Study of Inclusion Compounds** Ramsnes S., et al.

MS44-P10 E **Indexing Grazing Incidence X-ray Diffraction Patterns of Thin Films** Salzmann I., et al.

MS45-P02 E **StructureFinder** Kratzert D.

MS46-P02 E **A Non-Ambient Single Crystal X-ray Diffraction Beamline at Taiwan Photon Source** Lee J-J., et al.

MS46-P04 E **The High Energy X-Ray Diffraction Beamline at the PETRA III Synchrotron Light Source at DESY** Noohinejad L., et al.

MS46-P06 E **Development of Microspectrophotometer for the Macromolecular Crystallography Beamline at the Photon Factory, Japan** Hikita M., et al.

MS46-P08 E **New Tricks for an Old Dog: The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY** Wharmby M., et al.

MS46-P10 E **Exploring New Data Collection Protocols with the Eiger2 Detector and SmarGon on the Variable and Microfocus Beamline I04 at [...]** Flaig R.

MS46-P12 E **FXE Status. Femtosecond X-Ray Experiments for Chemical Dynamics Research at the European Xfel** Rodriguez Fernandez A., et al.

MS46-P14 E **A New Single Crystal Diffractometer at BM20/ESRF** Hennig C., et al.

MS46-P16 E **Long-Wavelength Protein Crystallography at Diamond Light Source** Mykhaylyk V., et al.

MS48-P02 E **The HyPix-Arc 150°** White F., et al.

MS48-P04 E **CrysAlisPro 40: 64-bit, Synergy, HyPix-Arc 150°, AutoChem4.0, Ewald 3D** Meyer M.

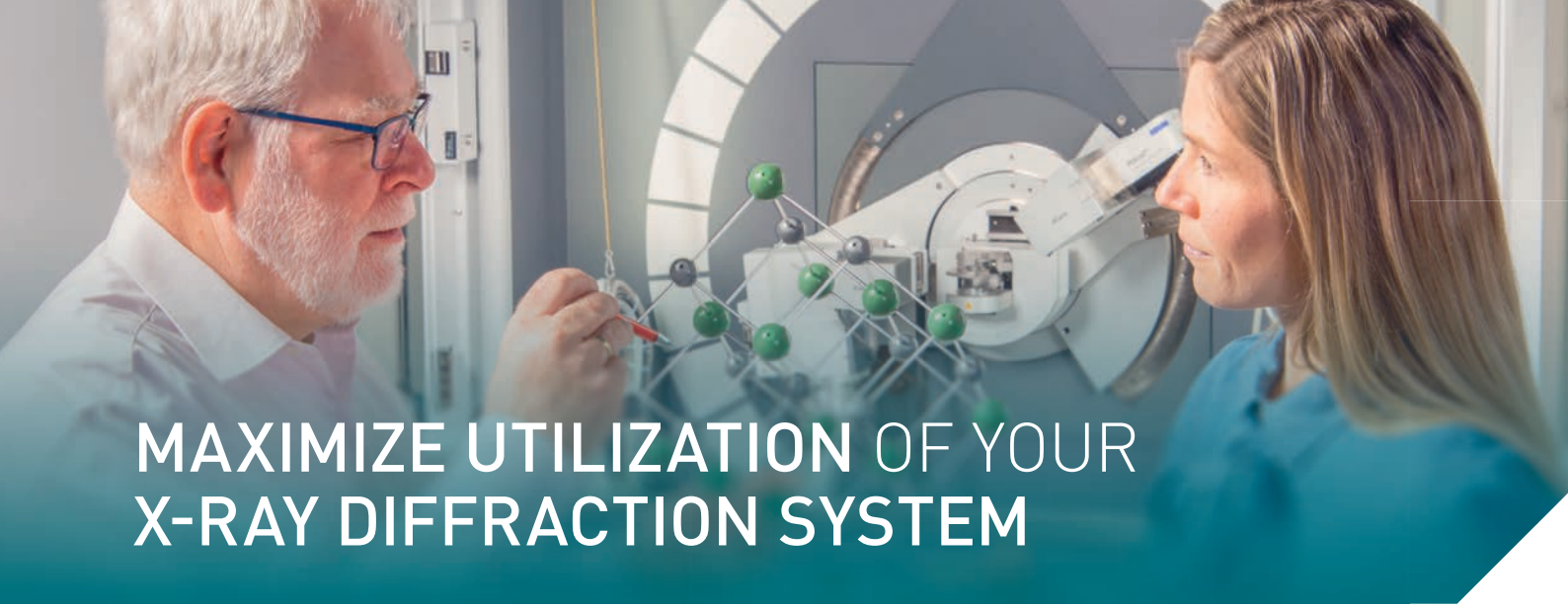
MS48-P06 E **A Life with Crystallography...** Đakovic M.

MS48-P08 E **Olex2: Teaching New Software Old AND New Tricks** Puschmann H., Dolomanov O.

MS48-P10 E **Mathematical Justifications for Crystal Systems, Bravais Lattices and a New Continuous Classification** Kurlin V.

MS48-P12 E **Overcoming Ambiguous Tautomer Assignment in 1,2,4-triazole Crystal Structures** Schwalbe C.

MS48-P14 E **Teaching Old Tricks: Rotation Conventions in Crystallography and cryoEM** Urzhumtsev A., Urzhumtseva L.



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Crystallographic Software Fayre

ECM32 in Vienna offers again a **Software Fayre**, where authors of academic and/or open-source software can present their newest developments. The Software Fayre will be held **from Mon 19.08.2019 to Thu 22.08.2019 during the lunch breaks**.

During the **Tutorial Sessions**, authors will demonstrate the features of their software on one or more practical examples.

Organizers: **Claudia Millan Nebot, Martin Lutz**

Location: Seminarraum 6 (SR6)

Tutorial Sessions by Day

Mon 19.08.2019	12:15-12:45	*"ALEPH" - Extract Libraries for Fragment Based MR* (**Ana Medina**)
	12:45-13:15	*"HKLF5Tools"* (**Sergej Ivlev**)
	13:15-13:45	*"EoSFit"* (**Ross J. Angel, Javier Gonzales-Platas, Matteo Alvaro**)
Tue 20.08.2019	12:15-12:45	*"AUSPEX"* (**Andrea Thorn**)
	12:45-13:15	*"ccCluster"* (**Gianluca Santoni**)
	13:15-13:45	*"py_convrot" Interactive Tool for Different Rotation Descriptions* (**Alexandre Ourjoumtsev**)
Wed 21.08.2019	12:15-12:45	*"Structure Finder"* (**Daniel Kratzert**)
	12:45-13:15	*"Phase and Model Preparation for MR"* (**Massimo Sammito**)
	13:15-13:45	*"NGL-HKL-Viewer"* (**Robert Oeffner**)
Thu 22.08.2019	12:15-12:45	*"Crystallographic Electron Microscopy in Python"* (**Joonatan Laulainen**)
	12:45-13:15	*"MoleCoolQt and ShelXle"* (**Christian Hübschle**)
	13:15-13:45	*"TopCryst" Knowledge About the Topology of Crystal Structures* (**Evgeny Alexandrov**)

Company Sponsored Workshops and Events

Sunday-Workshops (18.08.2019)

Bruker AXS GmbH	***IDEAL Workshop***	13:00–16:00	HS6
Thermo Fisher Scientific	***How to Engage Cryo-EM Single Particle Analysis***	16:00–17:00	HS3

The Sunday-Workshops take place at the ECM32 venue before and in parallel to the registration on Sunday afternoon.

Luncheon Events (Lunch Breaks on Mon, Tue, Wed)

Dectris AG	***DECTRIS Lunchtime Seminar***	Mon 19.08.	12:00–13:00	Kl. FS
Bruker AXS GmbH	***BRUKER Luncheon***	Tue 20.08.	12:30–13:00	Kl. FS
Rigaku Europe SE	***Rigaku Lunch and Learn***	Wed 21.08.	12:15–13:30	Kl. FS

As seating in the luncheon theatre (Kleiner Festsaal, Kl. FS) is limited, you can receive an invitation at the booth of the respective company. Participation is based on “first come - first served” principle.

Evening Events

CCDC	***CSD 1-Million Evening Reception***	Tue 20.08.	20:15	Kl. FS

Collect your reception ticket and drinks voucher at the CCDC booth.

Business Meetings (ECA/SIGs/GIGs)

ECA Business Meetings

ECA Executive Committee I	**Sun 18.08.**	12:00–15:00	SR1
ECA Council Meeting I	**Mon 19.08.**	12:00–14:00	HS5
ECA Executive Committee II	**Tue 20.08.**	12:00–14:00	HS5
ECA Council Meeting II	**Wed 21.08.**	12:00–14:00	HS5
ECA Council Meeting III (only on demand)	**Thu 22.08.**	12:00–14:00	HS5
ECM33 Programme Meeting	**Tue 20.08.**	12:00–14:00	SR3

Meetings of the SIGs and GIGs

SIG-1	**Mon 19.08.**	12:00–14:00	SR3
SIG-2	**Tue 20.08.**	12:00–14:00	SR5
SIG-3	**Tue 20.08.**	12:00–14:00	SR4
SIG-4	**Mon 19.08.**	12:00–14:00	SR4
SIG-5	**Thu 22.08.**	12:00–14:00	SR5
SIG-6	**Wed 21.08.**	12:00–14:00	SR5
SIG-7	**Thu 22.08.**	12:00–14:00	SR3
SIG-8	*no meeting scheduled*		
SIG-9	**Thu 22.08.**	12:00–14:00	SR1
SIG-11	**Wed 21.08.**	12:00–14:00	SR3
SIG-12	**Mon 19.08.**	12:00–14:00	SR5
SIG-13	**Wed 21.08.**	12:00–14:00	SR4
SIG-14	**Thu 22.08.**	12:00–14:00	SR4
GIG-1	**Tue 20.08.**	12:00–14:00	SR1
GIG-2	**Tue 20.08.**	12:00–14:00	SR2
GIG-3	**Wed 21.08.**	12:00–14:00	SR2

Satellite Workshops – Overview

The official **ECM32 Satellite Workshops** take place **between Tue 13.08.** and **Sun 18.08.2019** in the week ahead of the ECM32. The majority of the satellites are held at the TU Wien (at the building of the Department of Electrical Engineering).

26th WIEN2K workshop (P. Blaha, K.H. Schwarz), Tue 13. - Sat 17.08.2019

X-ray Spectrometry (C. Streli, P. Wobrauschek), Thu 15. - Fri 16.08.2019 (at the TU Wien Atominstitut)

Data Science Skills in Publishing – IUCr Committee on Data (J. Helliwell, B. McMahon), Sun 18.08.2019

CCP4 Structure Solution Workshop (E. Krissinel, C. Ballard), Sat 17.08.2019

MaThCryst Satellite Meeting (M. Nespolo, B. Souvignier, B. Stöger), Fri 16. - Sun 18.08.2019

Neutron Scattering and Imaging (J. Schefer, M. Meven), Wed 14. - Sat 17.08.2019

5th CrysAC Workshop – IUCr Commission on Crystallography in Art and Cultural Heritage (G. Artioli), Sat 17.08.2019

2019 IUCr and ECA High Pressure Workshop (R. Miletich), Tue 13.08. - Sat 17.08.2019

Young Crystallographers Satellite Meeting (P. Hans, F. Topic), Sun 18.08.2019

Olex2 Workshop (H. Puschmann, M. Bodensteiner), Sun 18.08.2019

Total Scattering Analysis with DISCUS (R.B. Neder, T.E. Proffen), Tue 13. - Sat 17.08.2019

European Crystallographic Computing Forum – SIG-9 (M. Lutz), Wed 14. - Sat 17.08.2019 (at Melk, Lower Austria)

Fixed Target Serial Crystallography (A. Pearson, J. Wierman, P. Mehrabi, E.C. Schulz), Sat 17.08.2019

Low Resolution Structure Determination with Phenix (P. Adams, D. Liebschner), Sun 18.08.2019

Crystal Engineering Using Cambridge Structural Database (I. Sovago), Sun 18.08.2019

Social Programme

Social Programme for Participants – Overview

Opening Ceremony, Welcome Reception, Closing Ceremony

Science Slam

Conference Concert

Young Crystallographer‘s Mixer

ECM32 Conference Dinner

Viennese Waltz Dancing Course

Conference Excursion and Other Tours

Social Programme for Participants – Overview

Registration for tours and events is possible through the webpage and during the conference at the registration desk.

Scientific Tours

Guided tour at MedAustron in Wiener Neustadt – Mon 19.08., 13:45–18:00, 20 € *
Guided tour at the „Atominstitut“ – 2 tours: Tue 20.08. or Thu 22.08., 10:15, 5 € *
Guided tour at Natural History Museum (NHM) – Wed 21.08., 08:30 or 10:30 or 12:30, 20 € *

Touristic Tours

City-tour I „St. Stephan‘s Cathedral“ – Wed 21.08., 14:00–16:00, 30 € *
City-tour II „Jewish Vienna“ – Wed 21.08., 14:00–16:00, 30 € *
City-tour III „Viennese Coffee Houses“ – Thu 22.08., 14:00–16:00, 30 € *
Half-day trip „Historical Vienna - Schönbrunn & Viennese Strudel Show“ – Tue 20.08., 13:30–16:30, 60 € *

ECM32 Events

Welcome Reception – Sun 18.08., 19:30–22:00, free
Viennese Waltz Dancing Course – 2 courses: Mon 19.08., Tue 20.08., 12:45–13:45, free *
Science Slam – Mon 19.08., 18:00–19:30, free
Conference Concert at Votivkirche – Mon 19.08., 20:00–21:15, 10 € *
Young Crystallographer‘s Mixer – Tue 20.08., 20:00–22:00, 30 € *
Conference Dinner at Schönbrunn – Wed 21.08., 19:30, 100 € *
One-day trip „Romantic Danube River Wachau“ – Fri 23.08., 08:30–19:00, 60 € *

** registration required*

Opening Ceremony, Welcome Reception, Closing Ceremony

Opening Ceremony

The **Opening Ceremony** will take place in the **Auditorium Maximum (Audimax)** at the ECM32 venue on Sun 18.08.2019 starting at 18:00.

Welcome Reception

The Opening Ceremony on Sunday will be followed by a **Welcome Reception** from ~19:30 to 22:00 in the **Arcaded Courtyard**, the main exhibition area of ECM32. Admission is free for all registered participants and you are cordially invited to join us!

Closing Ceremony

The official **Closing Ceremony** of ECM32 is supposed to take place in the **Auditorium Maximum (Audimax)** on Thu 22.08.2019 between 19:00 and 20:00.

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Science Slam

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After the successful original first event at Basel, we will have the **Science Slam** again in Vienna! This unique event allows ECM participants to present crystallographic science even to a non-professional audience.

> While the presented content is scientific, the clear focus is entertainment. The given presentations will teach the audience about modern crystallography in an understandable and funny way.

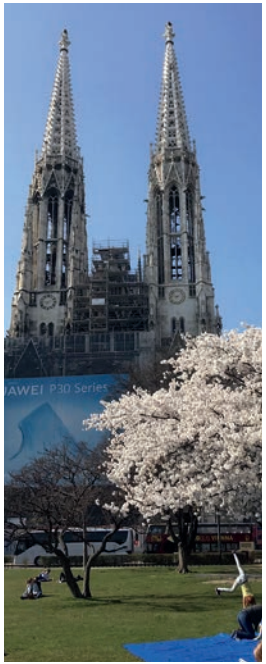
The best presentation will receive an award and price, donated due to generous sponsoring of Stoe & Cie GmbH.

The second ECM Science Slam

Mon 19.08.2019, 18:00-19:30, Auditorium Maximum (Audimax)

STOE SINCE 1887

Conference Concert



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ECM32 Conference Concert at the Votivkirche

The TU Wien Orchestra will give a classical concert on the occasion of the ECM32 in the Votivkirche next to the conference venue performing:

Wolfgang Amadeus Mozart, Symphony no. 40 in G minor (KV550, „Great G minor symphony“)

Franz Schubert, Symphony no. 5 in B major (D485)

Mon 19.08.2019, 20:00–21:15

Votivkirche
1090 Wien, Rooseveltplatz

(5–7 minutes walk from the ECM32 conference site. Guides will show you the pathway to the Votivkirche. A map how to find the church is also provided at the end of the booklet)

Concert tickets 10 € (limited to max. 800 participants) can be obtained at the registration desk.

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Young Crystallographer‘s Mixer

The Mixer is open to delegates who qualify for membership of the Young Crystallographers Group.
This includes not only students but postdoctoral fellows and other younger scientists up to an age limit of 35 years.

Refreshments, a light informal dinner and DJ entertainment will be provided.

Tue 20.08.2019, 20:00–22:00

6th Floor Rooftop Terrace, TU Wien, Gußhausstraße 25–29

It takes about 20-25 minutes time with public transportation including walking distances to the event site.
A map guiding you to the TU is provided in the back of the booklet.

Tickets for the Mixer (30 €, limited to 70 participants) can be obtained at the ECM32 registration desk.

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ECM32 Conference Dinner

The **ECM32 Conference Dinner** will take place in the **orangery** of the famous **Schönbrunn Palace**, the main summer residence of the Habsburg Emperors.

Schloß Schönbrunn Meetings & Events

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Wed 21.08.2019, 19:30–22:30

„Orangerie, Schloß Schönbrunn“
1130 Wien, Schönbrunner Schloßstraße

50–55 minutes by public transportation from the ECM32 site, including walking distances. You are supposed to find the way on your own. Guides will help you to find the pathway from the subway station „Schönbrunn“ to the main entrance at the palace. Be in time, if you want to enjoy the access from the park and the apero! Note that after 20:00 access for individuals is only possible through the side entrance at the Schönbrunner Schloßstraße. A map how to find the orangery is provided at the end of the booklet.

Remaining **tickets for the conference dinner** (100 €, limited to 500 participants) can be purchased at the registration desk.

© SKB bildgewaltig, Hannes Grundschober

© SKB bildgewaltig, Hannes Grundschober

Viennese Waltz Dancing Course

© Vienna Convention Bureau, Peter Rigaud

Due to generous sponsoring of ELDICO Scientific we are able to offer free one-hour dancing courses at lunch breaks, where you can **learn to dance the Viennese Waltz** guided by professional teachers from the „Tanzschule Watzek“ at Vienna.

Our dance teacher Danny is not only a professional dance teacher, but as a chemist he also publishes crystallographic structures...

Mon 19.08.2019, 12:45–13:45
Tue 20.08.2019, 12:45–13:45

ECM32 site – Garderobe Senatssaal
(first floor, anteroom next to Senatssaal and Großer Festsaal)

The admission to the dancing courses is free. Due to limitations in space (maximum 15 couples per course) we ask for booking at the registration desk (first come, first served).

Suitable shoes would be beneficial for enjoying the music in three quarter time...

Conference Excursion and Other Tours

Conference Excursion to the Romantic Danube River Valley „Wachau“

The official **Conference Excursion** is scheduled for the last day of ECM32 bringing the participants to the famous romantic Danube valley „Wachau“, located about 80 km west of Vienna. The tour with buses and a boat trip includes:

Visit to Baroque monastery in Melk
Lunch break at Melk
Boat trip on the Danube river from Melk to Spitz/Krems
City tour in the medieval town centre of Krems

Fri 23.08.2019, 08:30–19:00

Meeting point: 08:30 on the south side of the university building (ECM32 venue) – buses will leave from there (Rathausplatz / Grillparzerstraße).

A picnic lunch bag will be provided for the lunch break in Melk.
Buses are supposed to return to Vienna by 19:00.

Remaining tickets for the excursion (60 €, limited to 350 participants) can be obtained at the registration desk.

© Uoaei1 (commons.wikimedia.org)

© Manfred Wildner
„Fivefold Cube“ (Olafur Eliasson, 2000, 2015)

Touristic Tours during the ECM32 conference

City-tour I „St. Stephan‘s Cathedral“
Wed 21.08., 14:00–16:00, 30 €

Tour programme: Discover St. Stephan‘s Cathedral, the landmark of Vienna and the main motif of the ECM32 logo. A guided tour will show you the treasures of this largest church in Austria including a visit of the catacombs.

City-tour II „Jewish Vienna“
Wed 21.08., 14:00–16:00, 30 €

Tour programme: Starting at the Jewish Museum this tour gives you an insight into the history of Jewish Vienna, including a walk through the city centre and a visit of the Holocaust Memorial on the Judenplatz.

City-tour III „Viennese Coffee Houses“
Thu 22.08., 14:00–16:00, 30 €

Tour programme: Following the Motto „From Sacher Cake to Gugelhupf“ you will learn about the secrets of the Viennese coffee house culture, visiting the most famous places such as Café Sacher, Demel, and Bräunerhof.

Half-day trip „Historical Vienna – Schönbrunn Palace & Viennese Strudel Show“
Tue 20.08., 13:30–16:30, 60 €

Tour programme: Guided tour through Schönbrunn Palace, then participating in a „Viennese Strudel Show“ where you will see how the famous „Apfelstrudel“ is made, and a tour along the Ringstraße on the way back to the ECM32 site.

Information on remaining tour tickets and the individual meeting points can be obtained at the registration desk.

Scientific Tours during the ECM32 conference

Guided tour at MedAustron in Wiener Neustadt

Mon 19.08., 13:45-18:00, 20 € (max. 45 participants)

Tour programme: Visit of MedAustron, one of the most advanced centres in ion-beam therapy and research. Buses will depart at 14:00 next to the ECM32 site and bring you to Wiener Neustadt (45 km south of Vienna) and return to Vienna by 18:00.

Meeting point: South side of the university building (Rathausplatz / Grillparzerstraße, place of bus departure) at 13:45.

Guided tour at Natural History Museum (NHM)

Wed 21.08., 08:30 or 10:30 or 12:30, 20 € (max. 45 participants per tour)

Tour programme: You will be guided by Vera M.F. Hammer, mineralogist and crystallographer, to the famous collections of the NHM, including the mineral collection, the famous meteorite collection, and the prehistoric „Austrian Venus".

Meeting point: In the Aula in front of the ECM32 registration desk. You will be guided to the NHM (20-25 minutes walking distance).

Guided tour at the „Atominstitut" (ATI) of the TU Wien

Tue 20.08. or Thu 22.08., 10:15, 5 € (max. 20 participants per tour)

Tour programme: Visit the TRIGA Mark II research reactor of the TU Wien.

Meeting point: In the Aula in front of the ECM32 registration desk. You will be guided to the ATI (35–40 minutes by tram and subway).

Information on remaining tour places can be obtained at the registration desk.

General Information

International Kálmán Prize

Best Young Scientist Lecture Award & Poster Prizes

Oral Presentations and Posters – Instructions

Information – ECM32 Meeting

Child Care Facility

Information – Vienna and Austria

International Kálmán Prize

The ECA is pleased to announce the first Alajos Kálmán Prize. The Prize is awarded to an individual researcher in recognition of outstanding scientific contributions in the field of structural sciences within the last 5-10 years. The award lecture will be held on Wednesday 21. August 2019.

The International Kálmán Prize preserves the memory of the late Alajos Kálmán, an eminent scientist in the field of chemical crystallography. The Prize is established by the Hungarian Chemical Society, is endorsed by ECA, and awarded in the ECM years. The prize consists of a medal and a financial award. The awardee delivers a Prize Lecture at the ECM. The selection of the awardee is conducted by ECA SIG13, although the recognised field is wider, including all structural sciences.

Kálmán Prize Award Ceremony and Award Lecture
Wed 21.08.2019, 16:00-16:30, Großer Festsaal (gr FS)

Best Young Scientist Lecture Award and Poster Prizes

It is our pleasure to announce the following 15 scientific prizes and awards:

Boehringer Ingelheim Best Young Scientist Lecture Award

IUCr Journals Poster Prizes, three prizes in the three categories: Structural Biology, Structural Chemistry, and Applied Crystallography.

STOE Poster Prize, for a student's work presented in the field of functional materials.

Prof. Philip Coppens SIG2 Quantum Crystallography Poster Award, sponsored by Rigaku in the field of quantum crystallography.

Boehringer Ingelheim Poster Prize Awards, two poster prizes for outstanding work in the field of structural biology.

NanoMEGAS Poster Prizes, two poster prizes to young scientists for their work in the field of electron crystallography.

PDBe Poster Prizes, two poster prizes for young scientists work in structural biology.

Austrian Academy of Sciences (OeAW) Poster Prizes, two poster prizes for young scientists in any field of crystallographic research.

Judith Flippen-Anderson Journal on Structural Dynamics Poster Prize, sponsored by the ACA for excellent research on structural determination and dynamics of systems.

We are grateful to the sponsors donating the respective awards and prizes.
They will be presented and awarded at the Closing Ceremony on Thu 22.08.2019.

Oral Presentations and Poster Presentations – Instructions

Oral Presentation / Uploading your presentation

At ECM32 there will be no central facility for uploading presentations. Therefore, **all presentations will be uploaded directly in the respective lecture hall.**

Speakers are kindly requested to bring their **presentation preferred on an USB stick** directly to the respective lecture room **not later than 15 minutes prior to the beginning of the session**. An assistant will upload the presentation in the on-site system. Please make sure your presentation is in a commonly used and widely compatible file format. When producing a PowerPoint file we recommend embedding all used fonts in order to guarantee a smooth presentation avoiding any surprises. If you want to use your own laptop we kindly remind you not to forget adapters in case.

Poster Presentation / Mounting and Removing Posters

At ECM there will be two poster session: **Session I – odd poster numbers, on Mon+Tue, Session II – even poster numbers, on Wed+Thu**. The posters are allocated to one of the **five poster areas A, B, C, D and E**).

Posters need to be in the standard format A0 portrait (84.1 cm x 118.9 cm). Mounting material is available during the poster mounting times as indicated below in the respective poster areas, or on request at the registration desk. Please, do not use any other materials for mounting than the provided ones.

Poster Session I:	Mounting: Sun 18.08. between 15:00 and 18:00, or Mon 19.08. between 08:30 and 14:00 Removing: Tue 20.08. between 17:00 and 19:00 *
Poster Session II:	Mounting: Wed 21.08. between 08:30 and 14:00 Removing: Thu 22.08. between 17:00 and 19:00 *

** Note: Posters, which are not removed by 19:00 will be disposed by our ECM32 staff*

Abstracts

Abstracts will be compiled on a USB stick which you receive on registration. The abstract booklet will also be published on online supplement to Acta Crystallographica Section A.

Badges

Admission to the conference venue is possible with a valid name badge only. **Badges must be used throughout the entire congress and at the official social events.** Do not forget your badge even for excursion or the conference dinner. In case of loss you can obtain a replacement at the registration desk at a fee of 30 €. Return of badges is highly appreciated (in the box located at the registration desk).

Coffee and Lunch Breaks

Food, hot and cold beverages will be served during coffee and lunch breaks free of charge. **Lunch** is available for all participants **on four places in the exhibition area** (three under the arcades, one inside the tent) on **Mon, Tue, Wed, and Thu between 12:00 and 14:00. Coffee** is served in the same places from **09:30–10:00** in the morning and from **16:00–17:00** in the afternoon. Special dietary requirements have been communicated to the congress caterer. Please inform the waiters and adapted meals will be provided. Do not forget to wear your badge during lunch and coffee breaks. For ECA business meetings lunch boxes will be provided. Exclusively for exhibitors with valid badges lunch is provided already between 11:30 and 12:00 at in area B of the exhibition. Beverages will be provided for exhibitors between 09:00 and 16:00 in HS16.

Child Care

See page 95.

Cloakroom

A room (HS16) is available as a wardrobe and for storage of luggage. It will be open on Sun from 15:00 to 22:00, on Mon, Tue, Wed and Thu from 08:30 to 19:00. Notice that the room will be attended during these times, but storage is on your own risk with respect to loss and damages.

Exhibition Opening Hours

The commercial exhibition in the Arcaded Courtyard and in the tent is open for all ECM32 participants as follows:

Sun 18.08. 16:00–21:00
Mon 19.08., Tue 20.08., Wed 21.08., Thu 22.08. 09:30–17:00

The exhibition area will be dismantled starting on Thu 22.08. 17:00 immediately after the exhibition is closed.

Health Care on ECM32 site

We have on-duty medical service at the ECM32. In case you need assistance for urgent medical issues or any injuries please contact either the registration desk, a member of the ECM32 staff, or call +43 664 60277 17630.

Information / Message boards

Take notice of the two information boards next to the registration desk for general important announcements, last minute changes, and the possibility for you to place messages. News are also posted on our conference social media accounts: https://www.instagram.com/social_ecm, and https://twitter.com/EcmSocial.

Insurance

The ECM32 cannot accept liability for personal injuries sustained, or for loss or damage of personal belongings either during or as a result of the meeting. Please check the validity of your personal insurance.

Language

The official meeting language is English.

Meeting Point

We have set up an „ECM32 meeting point“ just next to the registration desk in the Aula.

Photographer

The entire conference will be documented by a team of professional photographers. You can find images being displayed on screen and/or board in the corners of the tent (exhibition area D).

Presentations (Orals and Posters)

See instructions on page 91.

Registration Desk

All participants can collect their conference material (name badge, programme book, USB stick with abstracts, tickets) on arrival at the registration desk located in the Aula, directly when entering the main entrance of the university building. Attendees who decide late to participate in ECM32 can also register on-site, book tickets for individual social events, and receive any information related to the conference. Opening hours of the registration are:

Sun 18.08. 15:00–19:30
Mon 19.08., Tue 20.08., Wed 21.08., Thu 22.08. 08:00–18:00

Smoking at the ECM32

Smoking is not allowed on the entire area of the main building of the University of Vienna. Thank you for your understanding.

Wi-Fi

Free Wi-Fi internet access is available throughout the entire venue. A voucher for individual Wi-Fi access will be handed out on registration.


IT HAS ARRIVED!
Come to IUCr Booth D16 to browse a copy of the much-anticipated
International Tables Volume H: Powder diffraction
edited by Christopher J. Gilmore, James A. Kaduk and Henk Schenk
it.iucr.org/H/

Child Care Facility

Following up the past conferences, ECM32 is a **family-friendly meeting** thus providing a free **child-care facility** for children of participants registered in advance.

In cooperation with professional nursery-school teachers from *Kinder in Wien (KiWi)*, ECM32 offers a childcare service on Mon, Tue, Wed, and Thu (either half or full days). On Fri there is no service available, as your kids can accompany you to the conference excursion free of charge (registration required!).

KiWi Childcare – Mon 19.08. to Thu 22.08.2019
Opening hours: 08:00–17:00

Location: Marietta-Blau Saal

The ECM32 childcare service includes professional day care (half day/full day) in the morning (08:00–12:00), during lunch breaks (12:00–14:00), and in the afternoon (14:00–17:00).

The service includes free meals, and two guided tours to the Technical Museum (Monday afternoon) and to the Schönbrunn Zoological Garden (Thursday afternoon) in addition to activities at the conference site. We are grateful to the TU Wien for sponsoring the bags for our junior ECM32 participants!

KINDER IN WIEN TU WIEN

Information – Vienna and Austria

Calling to and from Austria

The international country code for Austria is +43, the local city code for Vienna is 1. National calls: 0 + city code + telephone number. International calls: 00 + country code + city code + telephone number.

Currency / ATM

The currency used in Austria is the Euro (€). You may exchange foreign currencies at one of the bank institutes next to the university building: Volksbank (1010 Wien, Schottenring 1, Mon–Fri 08:00–12:30); UniCredit Bank Austria (1010 Wien, Schottengasse 11, 24h service foyer); Oberbank (1010 Wien, Schottengasse 2, Mon–Fri 09:00–12:30). There are also cash machines/ATMs (in Austria called „bankomat“) available at these places. In addition, there is one ATM available inside the university building in the corridor on the ground level leading to the Audimax lecture hall.

Electricity

The electric current in Austria is 230 V AC (at 50 Hz). You can use your equipment, if the outlet voltage in your country ranges between 220 and 240 V, otherwise you have to use an adapter (100–240 V 50/60Hz). You have to use 2-pin type C or type F plugs for Austrian sockets.

Emergency Calls

Fire brigade: 122, Police: 133, Ambulance: 144, European emergency call: 112

Health Service / Hospital

If you need medical care the next hospital is the „Allgemeine Krankenhaus (AKH) Wien“ (www.akhwien.at), 1090 Wien, Währinger Gürtel 18-20.

Parking

Parking is very restricted in Vienna, in particular in the area of the city centre. You have to use pre-paid tickets („Kurzparkscheine“), which exist in four colours (red = ½ hour, 1.05 €; blue = 1 h, 2.10 €; green = 1½ h, 3.15 €, and yellow = 2 h, 4.20 €). These tickets can be purchased at any newspaper kiosk („Trafik“). The next one from ECM32 venue is directly located at Schottentor, next to the tram station of lines 43, 44, D, and 71. Parking with these tickets is limited to at most 2 hours. You can also use equivalent electronic tickets by using an app when registering your car on www.handyparken.at. If you want to park for longer you have to use one of the car parks. The next one is the „WIPARK Votivpark-Garage“ in the Universitätsstrasse (24 hours open, 4.30 € per hour, 43 € per day).

Post Office

It takes about 10–15 minutes to the next post office, which is located in the Alserstraße: „Postfiliale und Bawag PSK, 1080 Wien, Alserstraße 31, Mon–Fri 08:00–18:00. Take tram no 43 or 44 for 2 stations from Schottentor.

Public Transportation

This is the most economical way to travel in Vienna. You can purchase tickets online (www.wienerlinien.at) or use one of the vending machines at Schottentor. You can find them downstairs on the way to the subway station of the U2 (violet line), just before entering the escalator down to the platforms. Do not forget to validate your ticket on one of the blue validation machines. The public transportation organisation (Wiener Linien) also provides special tourist tickets called Vienna Card, which combine public transport with reduced fees to the most popular touristic sites in Vienna.

Supermarkets

The next supermarkets within 5-6 minutes walking distance from the ECM32 site are: BILLA (1090 Wien, Universitätsstraße 6-8, Mon–Fri 07:40–20:00), and SPAR Gourmet (1010 Wien, Schottengasse 7, Mon-Fri 07:30–20:00).

Taxi

The closest taxi stands are located in the Schottengasse (next to the Schottentor) or on Rooseveltplatz (opposite of the hotel „Regina“). You can also call a taxi (+43 1 40 100 or +43 1 31 300). Uber is available in Vienna as well. For ordering a taxi to the airport we recommend to use one of the airport taxi shuttle services at a fixed prize (30–35 €), e.g. www.airportdriver.at

Weather in Vienna and Eastern Austria

In summer there is significant continental influence. The average temperature is 18 °C in the morning, 27 °C during the day. It can be hot and humid, with maximum temperatures up to 33 °C, and minimum temperatures down to 12 °C in case of cold and rainy periods.

High-end data collection system

excillum MetalJet D2+ 250 W (dual port)

DECTRIS EIGER R 4M

marLiN$_2$ liquid nitrogen refill system

mardtb goniostat

marXperts

Also available as upgrade for existing systems!

Author and Sponsor Index

Author and Sponsor Index

Index of Presenting Authors[1]

[1] The listing includes all contributions submitted before 16.07.2019

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International Union of Crystallography
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Kinder in Wien (KiWi)
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NanoMEGAS SPRL
www.nanomegas.com

NHM, Naturhistorisches Museum Wien
www.nhm-wien.ac.at

ÖAW, Austrian Academy of Sciences
www.oeaw.ac.at/en

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www.swissci.com

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www.tuwien.ac.at/en

Thermo Fisher Scientific
www.thermofisher.com

Trabitsch Catering
www.trabitsch.at

University of Vienna
www.univie.ac.at

Vienna Convention Bureau
www.vienna.convention.at

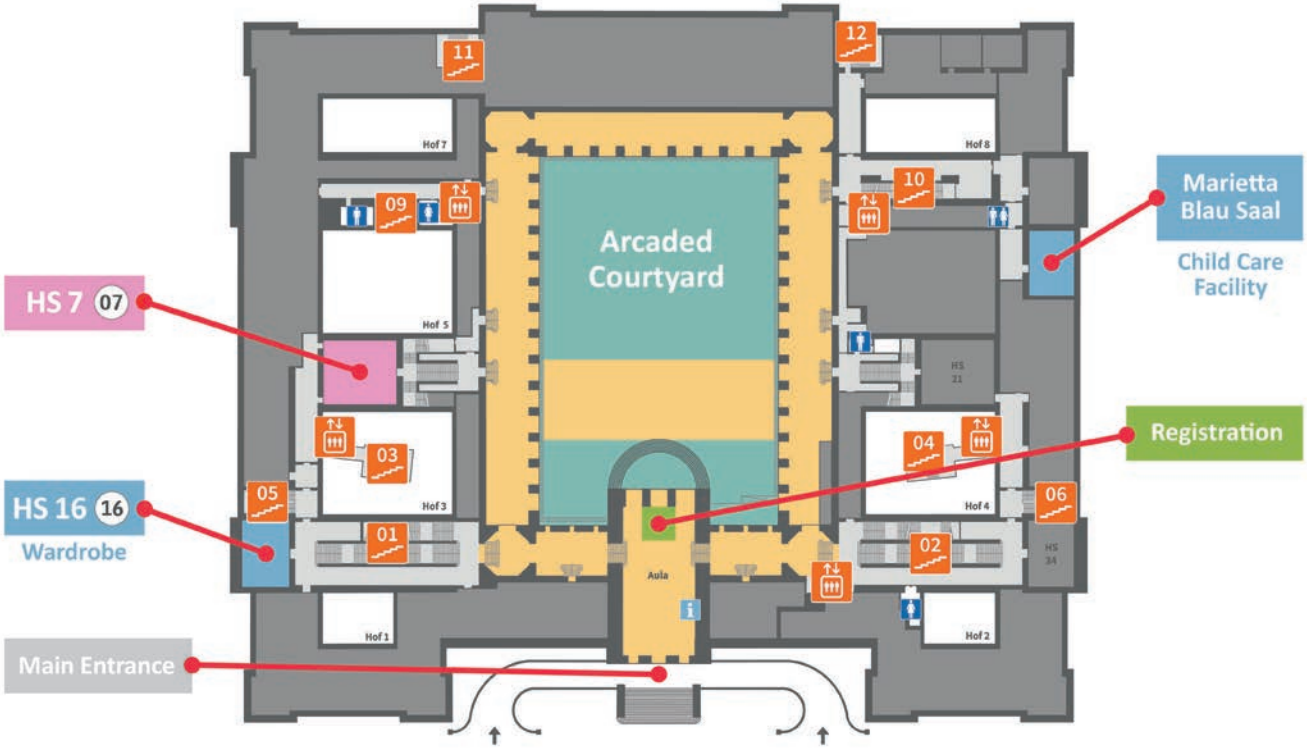
Tanzschule Watzek
www.watzek.at/tanzschule

Wyatt Technolgy Europe GmbH
www.wyatt.com

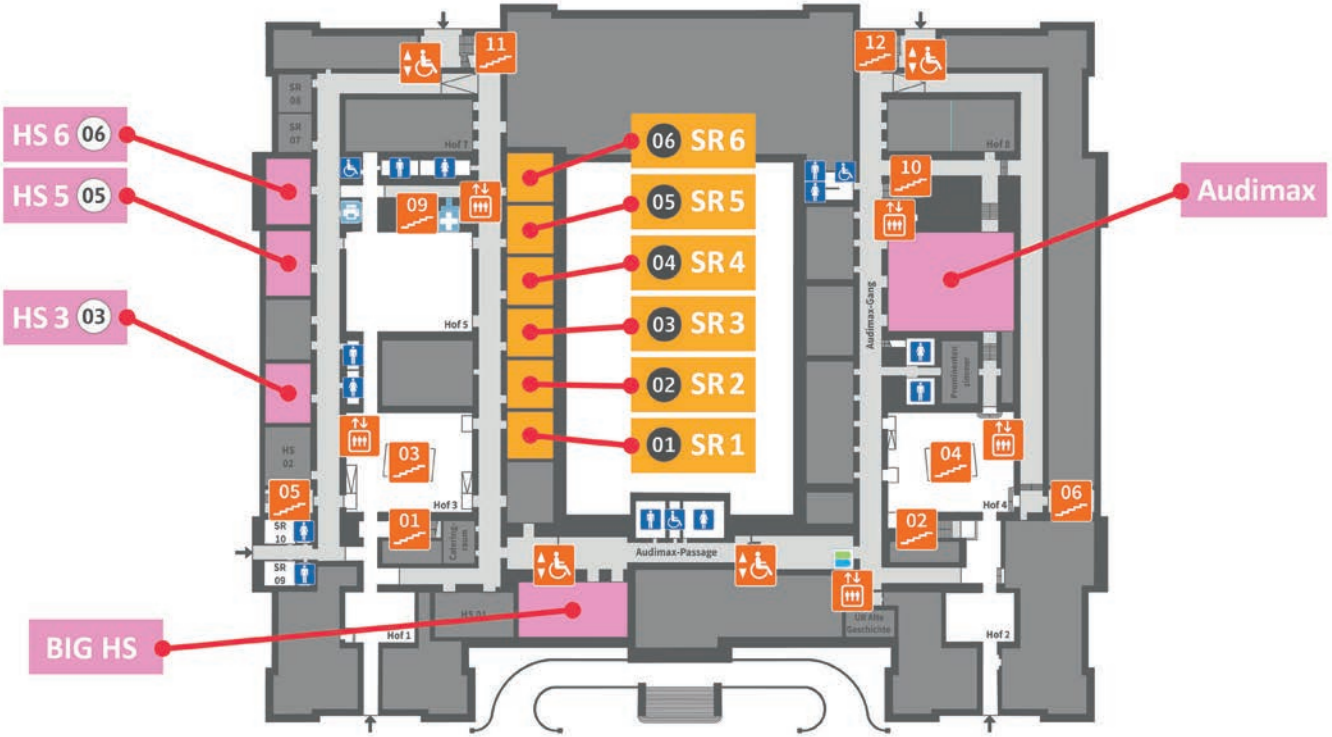
Xtal Concepts GmbH
www.xtal-concepts.com

Maps and Floorplan

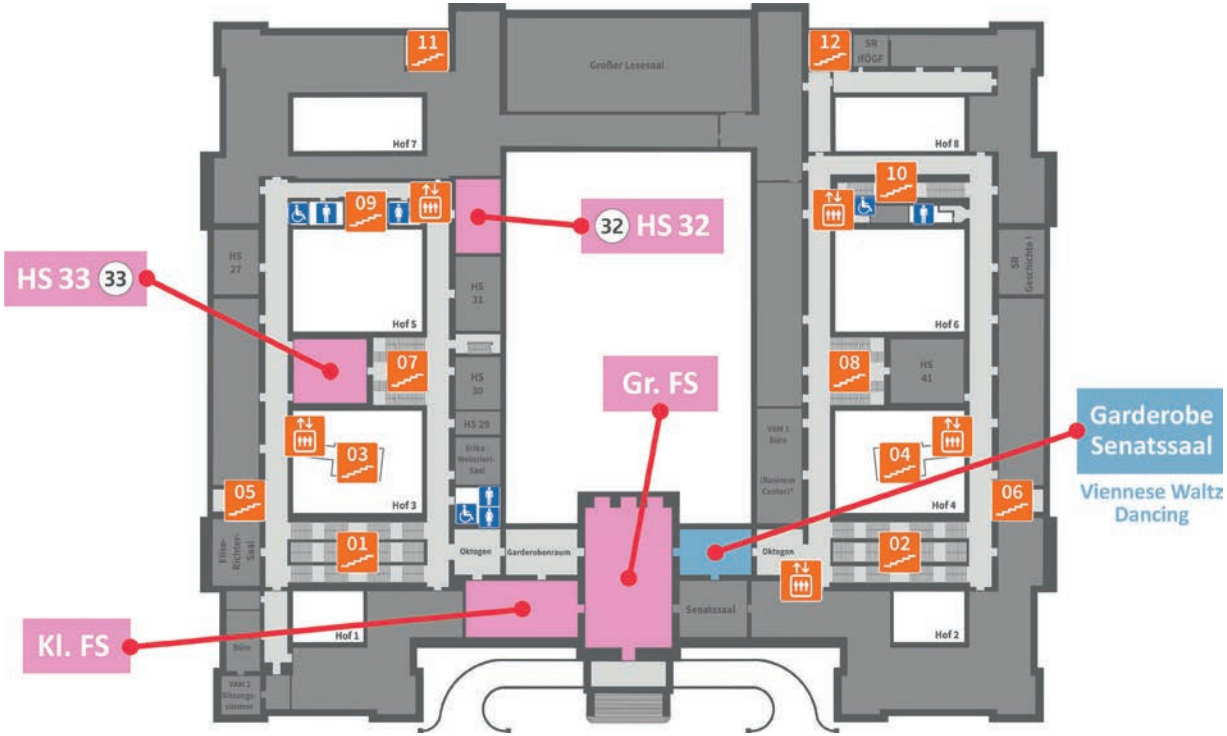
Floorplan of the Ground Floor (Hochparterre, HP)



Floorplan of the Semi Basement (Tiefparterre, TP)

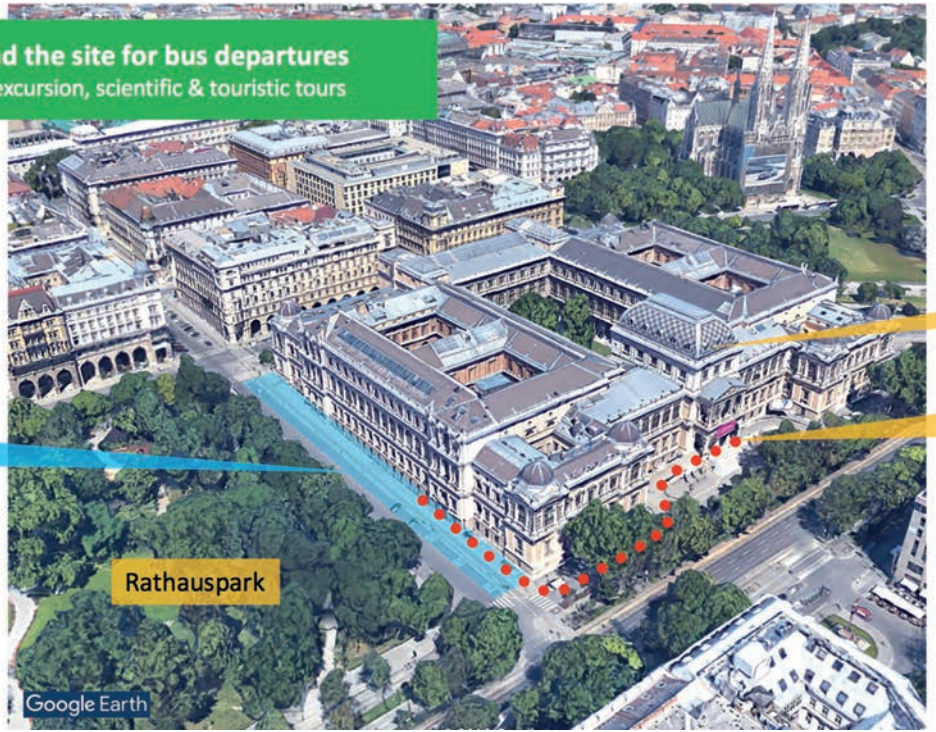


Floorplan of the First Floor (1.Stock / 1.Obergeschoß, 1.OG)



How to find the site for bus departures

conference excursion, scientific & touristic tours



ECM 32
VIENNA AUSTRIA 2019

University

main entrance

bus departures

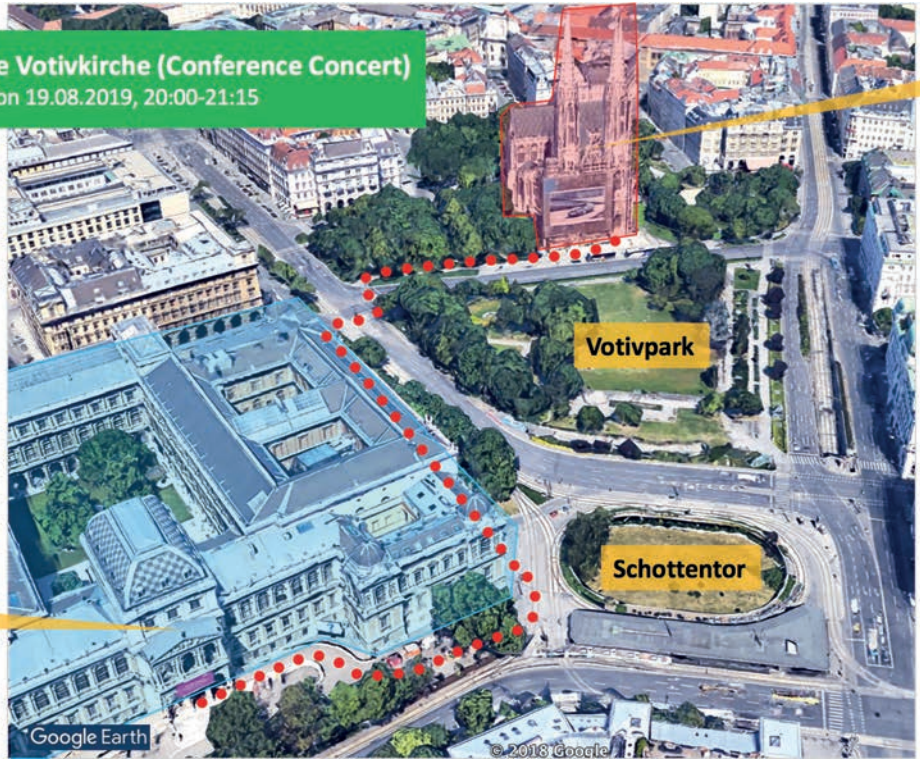
buses depart from the south side of the university

Pathway from the main entrance to the bus departure area (1-2 minutes walk)

How to find the Votivkirche (Conference Concert)

Mon 19.08.2019, 20:00-21:15

Estimated walking time: 5-7 minutes

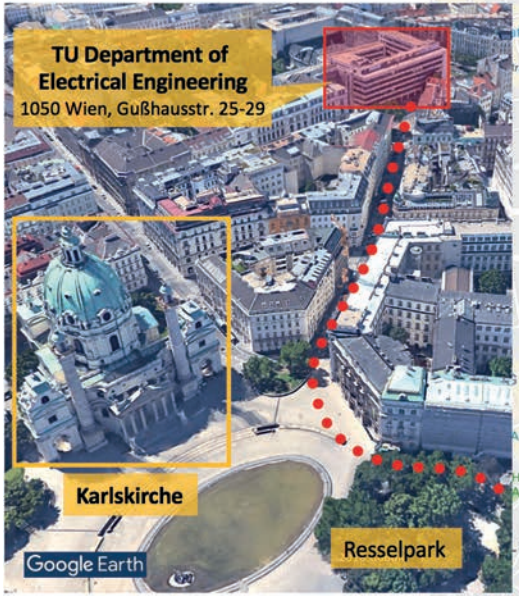


Pathway from the main entrance of the university to the "Votivkirche"

ECM 32
VIENNA AUSTRIA 2019

How to find the Young Crystallographer Mixer

Technical University, Tue 20.08.2019, 20:00-22:00



Enter the tram no. 1, 71 or D, or the subway U2 at Schottentor next to the university

Get off the tram at the station "Oper", the U2 at its final destination "Karlsplatz"

Walk across the Karlsplatz and through the Ressel-park, passing by the "Karlskirche"

Walk along the "Karlsgasse", which directly leads you the event site!

Total transfer time: 20-25 minutes

How to find the "Orangerie" at Schönbrunn – I

Conference Dinner, Wed 21.08.2019, 19:30-22:30

Enter the tram no. 1, 71 or D at Schottentor next to the university

Change at Dr.-Karl-Renner-Ring to subway line U3 (heading for Ottakring)

Change at Westbahnhof to subway line U6 (heading for Siebenhirten/ Alterlaa)

Change at at Längenfeldgasse to U4 (heading for Hütteldorf) and get off at Schönbrunn

ECM 32
VIENNA AUSTRIA 2019

University

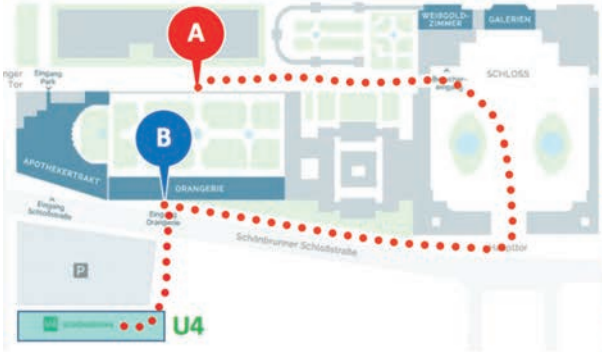
Note: due to constructions in July & August the green line (U4) is closed between Längenfeldgasse and Karlsplatz!

Estimated transfer time: 50-55 minutes

How to find the "Orangerie" at Schönbrunn – II

Conference Dinner, Wed 21.08.2019, 19:30-22:30

Pathway from the subway station "Schönbrunn" (green line, U4) to the entrances of the "Orangerie"



Walk 10-12 minutes through the main entrance of Schönbrunn, passing by the famous palace, and enter the garden of the "Orangerie" (A) through the park (Schloßpark Schönbrunn). At 20:00 the park entrance will be closed. After 20:00 please use the side entrance (B) from the road side only.

Notes

Notes