



**XX Congress**  
of the  
**International Union of Crystallography**  
**Congress and General Assembly**



**Program Book**

# XX Congress of the International Union of Crystallography

## Congress and General Assembly

### CONTENTS

	pag		pag
Welcome	III	Social Events	XIII
Patronage and Sponsors	IV	Congress Tours	XIV
Committees	V	Special Scientific Events	XV
Plan of the Congress Centre and Exhibition Area	VI	Computer Fayre	XV
Exhibitors	VII	Workshops	XV
General Information	VIII	Open Commission Meetings	XV
Venue	VIII	Round Table on Data Mining	XV
Language	VIII	Microsymposium on "Art and Crystallography"	XV
Registration	VIII	Seminar	XVI
Congress Bag Checklist	IX	Poster Prizes	XVI
Badges	IX	Opening day: Tuesday, 23 August	XVII
Internet Point	IX	Events	XVII
Commercial Exhibition	IX	Timetable	XVII
Exhibition on "Art and Crystallography"	IX	Closing Ceremony	XVIII
Coffee Points, Lunches	IX	Scientific Information	XVIII
Climate, Clothing	X	Instructions for the presenting authors	XVIII
Currency, Banks	X	Notes on the Detailed Scientific Program	XIX
Local Transportation	X		
Personal Sightseeing and Excursions	X	Detailed Scientific Programme	
Tourist Offices	X	Wednesday, August 24	B1
Smoking	XI	Thursday, August 25	B15
Electricity Supply	XI	Friday, August 26	B29
Time	XI	Saturday, August 27	B43
Medical Service and Pharmacies	XI	Sunday, August 28	B57
Post Office and Courier Services	XI	Monday, August 29	B71
Communications	XI	Tuesday, August 30	B85
Parking	XI	List of the Presenting Authors	B98
General Help Desk and Notices at the Congress	XII		
Insurance	XII		
Safety and Security	XII		

## WELCOME

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On behalf of the entire organizing committee, we welcome the participants of the XX IUCr Congress to Florence. We have done our best to put together a program of the highest possible quality and we are grateful to all the members of the international Scientific Program Committee who have shared with us the burden and responsibility for selecting excellent speakers and topics. The congress offers a detailed overview of crystallography, one of the most multidisciplinary sciences, that links together frontier areas of research. Florence, the cradle of the Renaissance, is naturally intertwined with science. Therefore, we have devoted special attention to highlight this aspect.

Furthermore, we have followed the mandate of the IUCr and made significant efforts in raising funds to allow the participation of the highest possible number of young researchers. Their presence is important for the diffusion of crystallography and its many associated areas of research. As a result, we hope that new and fruitful collaborations will be established. We encourage the older and distinguished delegates to interact scientifically and socially with the younger generations and share their enthusiasm.

A congress of this scale is obviously attractive for commercial sponsors and exhibitors, whose participation is synergetic and vital for the success of the event. The continuous assistance of the IUCr officials and the Associazione Italiana di Cristallografia as well as the support of our own Institutions (Consiglio Nazionale delle Ricerche and Università degli Studi di Firenze) has been extremely valuable during the many years of preparation. Now, we trust that all the participants will fully exploit this experience, from the scientific, cultural, social and tourist points of view. Hopefully, also the weather conditions will favour a pleasant immersion in the Italian atmosphere.

*Buon divertimento,*

**Carlo Mealli and Paola Paoli**

# XX Congress of the International Union of Crystallography

Congress and General Assembly

## UNDER THE PATRONAGE OF



Consiglio Nazionale delle Ricerche



Università degli Studi di Firenze



Associazione Italiana  
di Cristallografia



REGIONE  
TOSCANA



Comune di Firenze

## SPONSORS

The Organizing Committee of the XX IUCr Congress acknowledges with gratitude the support  
of the following Organizations and Companies:

- International Union of Crystallography
- Consiglio Nazionale Ricerche
- Università degli Studi di Firenze
- Regione Toscana
- Comune di Firenze
- Agenzia per il Turismo di Firenze
- Azienda Regionale Diritto Studio Universitario
- Associazione Italiana Cristallografia
- Società Chimica Italiana
- British Crystallographic Association
- Organization for the Prohibition of Chemical Weapons
- European Commission
- Ente Cassa Risparmio Firenze

Bruker AXS

CCDC

Crystal Impact

Marresearch

Merck & Co Inc - USA

Molecular Dimensions Ltd

Oxford Cryosystems

PANalytical

Protein Crystallography

RCSB PDB

Rigaku MSC

Unisantis SA

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## FORTEZZA DA BASSO



### LOWER FLOOR

Botticelli Hall  
Brunelleschi Hall  
Cimabue Hall  
Donatello Hall  
Giotto Hall  
Leonardo Hall

### GROUND FLOOR

Bank  
Coffee points  
Exhibition area  
Internet point  
Lunch area  
Newsstand  
Poster area  
Registration area  
Slide center

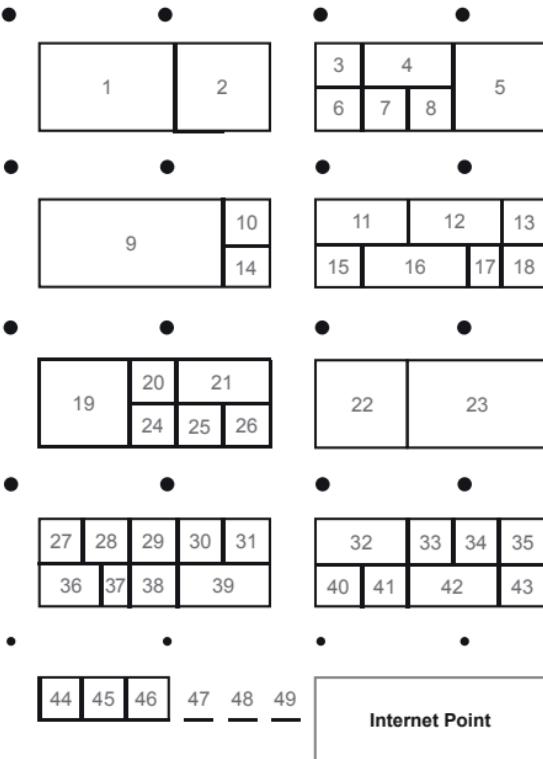
### PAVILION

Michelangelo Hall  
  
PAVILION

Benteghi Angelico Hall  
Ghirlandaio Hall  
Escher Hall

## EXHIBITION AREA (Pavilion A)

to Poster Session Area



## EXHIBITORS

ACCEL Instruments GmbH	31	Bid for the XXII IUCr Congress - Madrid 2011	47
Accelrys	30	Jena Bioscience GmbH	40
Area Detector Systems Corporation	32	Marresearch	19
Australian X-ray Capillary Optics Pty Ltd (AXCO)	14	Matrix Technologies	20
Axygen BioSciences	18	MicroCal, LLC	28
Beevers Miniature Models	37	Molecular Dimensions Ltd	2
BRUKER AXS GmbH - INCOATEC GmbH -	9	Nanomegas	10
BRUKER AXS BV		Nextal Biotechnologies Inc.	35
Cambridge Crystallographic Data Centre	4	Osmic Inc.	38
CCP4	11	Oxford Cryosystems	39
Corning Incorporated	7	Oxford Diffraction Ltd	5
Crystal Impact	41	OXFORD UNIVERSITY PRESS	49
Douglas Instruments Ltd	15	PANalytical	1
ECM23 - Leuven - Belgium - 2006	44	Protein Wave Corporation	2
ECM24 - Marrakech - Morocco 2007	45	ReactArray	25
Emerald BioSystems	27	Rigaku Inc.	23
European Molecular Biology Laboratory Hamburg	6	Robodesign Inc.	22
Fluidigm Corporation	16	Rubarth Apparate GmbH	2
GE Inspection Technologies (SEIFERT Analytical X-ray)	24	Springer	26
Genomic Solutions Ltd	8	Stoe & Cie GmbH	3
Greiner Bio-One GmbH	34	Thermo Electron Corporation	21
HECUS X-ray Systems GmbH	48	TriTek Corp.	2
HUBER Diffraktionstechnik GmbH & Co. KG	29	Unisantis SA	36
International Centre for Diffraction Data	13	wwPDB.org - the Worldwide Protein Data Bank (a collaboration between PDB, MSD and PDBj)	12
International Union of Crystallography	42	Xenocs S.A.	43
IUCr Newsletter and Regional Affiliates	33	Zeitschrift für Kristallographie	17
XXI IUCr Congress - Osaka, Japan 2008	46		

# XX Congress of the International Union of Crystallography

Congress and General Assembly

## GENERAL INFORMATION

### Venue

The site of the XX IUCr Congress and General Assembly is the Fortezza da Basso, Viale Strozzi 1, Florence, Italy (switch board 055 49721). The Congress Centre is within walking distance from the main railway station (Santa Maria Novella) and the downtown area of Florence (see map in the internal cover at the end of this booklet).

### Allocation of spaces:

Posted signs indicate the main meeting points and the conference halls, indicated by the name of famous artists: **Michelangelo, Botticelli, Cimabue, Donatello, Giotto, Leonardo, Brunelleschi, Ghirlandaio and Escher.**

Here, the main destinations of the various halls:

**Master Hall:** Michelangelo (Opening Ceremony, selected Keynote Lectures and Microsymposia, including the special event on "Art and Crystallography"). The hall is in Pavilion B (see map page VI).

**Halls for Keynote Lectures:** Michelangelo, Botticelli and Cimabue

**Halls for Microsymposia:** Michelangelo, Botticelli, Cimabue, Donatello, Giotto, Leonardo and Brunelleschi

**Halls for Open Commission Meetings:** Giotto, Leonardo, Brunelleschi and Beato Angelico

**Halls for Workshops:** Botticelli, Cimabue, Donatello, Giotto and Brunelleschi

**Hall for the Computer Fayre:** Ghirlandaio

**Hall for the special exhibition on "Art and Crystallography":** Escher

**Hall for the IUCr general Assembly:** Cimabue

### Language

The official language of the congress is English.

### Registration

The Registration Desk is situated inside Pavilion A, just after the main entrance. The opening hours are 8.00-18.00, August 23-30. The congress material will be delivered to pre-registered participants upon their arrival. On-site registration is possible and the fee can be paid in cash (euro currency), credit card or Traveller Checks. Certificates of Attendance are provided on request.

The participants are subdivided in the following categories: Full Participant, Student and Accompanying Person.

Registration fee for the full participant and student includes unlimited attendance of the Congress and Exhibition areas, congress bag with documentation, refreshments and lunches during the seven working days (from Wednesday 24 to Tuesday 30), admission to the opening ceremony and welcoming cocktail, concert and social banquet (with a booking charge of €20.00).

The registration fee of the accompanying persons includes access to the congress area, bag (scientific material excluded), daily lunches (from Wednesday 24 to Tuesday 30, August), access to the opening ceremony and welcoming cocktail, concert and social banquet (with a booking charge of €20.00). Additionally, two half-day tours are included.

## Congress Bag Checklist

This program booklet - Book of Abstracts - CD-rom - notepad - pen - map of Florence - Concert program - Banquet tickets (if reserved prior) - Tour tickets (if reserved prior) - vendors brochures, etc.

## Badges

At the registration time, each registered participant receives a colour-coded name badge: white for full participant and student, grey for exhibitor, pink for accompanying person. The badge must be clearly exhibited in order to access the congress area during all the scientific and social events. Failure to present the badge will exclude participation in any congress activity.

## Internet Point

A free of charge internet point (14 work stations) is accessible. A limited usage is requested in order to allow as many participants as possible to take advantage of the service. Additionally, two internet links and a designated area, equipped with a wireless hot point, allow the participants to use their own laptops for internet connection. All these facilities are situated at the Internet Point area in Pavilion A.

## Commercial Exhibition

A commercial exhibition of the companies, which produce crystallographic apparatuses, software, editorial material and other scientific facilities, takes place from Tuesday 23

to Saturday 27 in Pavilion A (see map page VI). The opening hours are 8.30 - 18.30 (9.00 - 18.30 on Tuesday 23).

## Exhibition on “Art and Crystallography”

An exhibition on “Art and Crystallography” takes place in the Escher Hall. The items on display consist of illustrations, sculptures and other media on the subject of art and crystallography. The exhibition is open from Tuesday 23 (15.00-19.00) to Saturday 27 (9.00-19.00 all the other days). The best two pieces of art will receive awards (with original etchings) during the Microsymposium on Art and Crystallography held on Friday 26.

## Coffee Points

Coffee, tea, milk, water and fruit juices are distributed at various Coffee Points in the Congress area. The facility is available all days between 9.30 to 11.30 and 13.00 to 17.30. Additionally, refreshment bars are located in the congress area and offer a wide selection of beverages and snacks for purchase (opening hours: 8.30-18.30).

## Lunches

Standing buffet lunch is daily served to all registered participants in a section of Pavilion A from Wednesday 24 to Tuesday 30 (from 12.35 - 14.45). On request, the badge must be shown to enter the lunch area. The participants are kindly requested to consume the food and beverages only in the reserved area of Pavilion A.

# XX Congress of the International Union of Crystallography

## Congress and General Assembly

### Climate

The weather is typical of the Italian summer, the average temperature being around 28°C. All the rooms in the Congress Centre are provided with air conditioning.

### Clothing

Comfortable and informal for all occasions.

### Currency, Banks

The official currency in Italy is Euro. Exchanges facilities are available in banks and authorized exchange offices, which are numerous in the downtown Florence area. Usual banking hours are: Monday through Friday 8.30-13.20 and 14.30-15.30. Banks are closed on Saturday and Sunday. Automatic cash dispensers are located outside the major banks and provide 24-hour service in different languages. A bank office is open inside the Congress area (opening hours: 8.30-13.00 and 14.30-16.00 from Tuesday 23 to Tuesday 30). All major credit cards are generally accepted, although not all ATM and Debit cards may be functional.

### Local Transportation

The historical area of Florence is quite compact and all major sites are within walking distance from the city centre. Many of the local bus routes stop at the Santa Maria Novella (S.M.N.) railway station, some 250 meters from the Congress venue. The city transportation (ATAF, [www.ataf.net](http://www.ataf.net), tel. 800 424500) covers the metropolitan area in between the hours of 6.00-24.00. Bus tickets must be purchased before boarding at bars, tobacconists, newsstands, etc. There is an ATAF central office just outside S.M.N. station, where free

bus route map can be obtained. The cost of a standard 60 min. ticket is €1.00 but also other types of tickets may be purchased. Please remember to stamp the bus ticket upon boarding at machines located in the front and rear of the bus. A taxi stand is available in front of the S.M.N. station. Radio-taxi is available at the tel. number 055 4242. Bicycles may be rented at economical cost.

### Personal Sightseeing and Excursions

The surroundings of Florence in the hills deserve a visit and they can be easily reached by bus (e.g., Fiesole, the ancient town constructed by the Etruscans, the church of San Miniato al Monte, Forte Belvedere, the Medici Villa la Petraia, etc.). An open double-decker sightseeing bus offers at the cost of €20.00 a complete tour of the city most important tourist attractions (for details see [www.ataf.net](http://www.ataf.net)). For more information on tourist sites contact the desk of Agenzia per il Turismo di Firenze (APT) in the exhibition area (opening hours: 10.00-17.00, 23-25 August). Also, frequent trains (Train Italia, [www.trenitalia.it](http://www.trenitalia.it), tel. 892021) and buses (e.g. SITA, [www.sita-on-line.it](http://www.sita-on-line.it), 800373760, or LAZZI) depart from S.M.N. area to reach famous towns in Tuscany such as Pisa, Lucca, Siena, San Gimignano, Volterra. Booking services for a variety of excursions are provided also by Newtours at the Social Events and Tours Desk in the Pavilion A.

### Tourist Offices

Tourist offices are located throughout the city. An information point is located at near the cathedral (Via Cavour 1R, opening hours: 8.30-18.30 from Monday to Saturday, tel. 055 290832) and provides guides and information about

# XX Congress of the International Union of Crystallography

Congress and General Assembly



the region of Tuscany. The main Florence tourist office (tel. 055 212245) is across from the S.M.N station and is open from 8.30 to 19.00, Monday through Saturday. A toll free telephone help service (Florence SOS Turista) is available for tourists in English, French, Spanish and German languages (055 2760382).

## **Smoking**

Italian law states that smoking is not permitted inside all public buildings, including offices, restaurants, pubs, bars, on public transports, etc. This also applies to the buildings of the Congress Centre. Smoking outside is permitted.

## **Electricity Supply**

Electricity is supplied with voltage of 220 V and 50-cycle AC. Italians outlets take only round-prong plugs. Appliances designed to operate on 110/120V need a voltage converter and a plug adapter.

## **Time**

The time in Florence is the Central European Time (Summer Time GMT+1).

## **Medical Service and Pharmacies**

The number for the medical emergency and ambulance service is 118. The tourist Medical Service, opened 24 hours, is located in via Lorenzo il Magnifico 59 (tel. 055 475411) and a number of languages are spoken. In the core of the downtown area, the main hospital is Santa Maria Nuova (055 27581). Pharmacies are open from 9.00 to 13.00 and from 16.00 to 20.00, Monday through Friday. On holidays,

each pharmacy displays a list of the nearest open stores. The pharmacy inside the S.M.N. station is open 24 hours. In the congress area, a first aid centre is available for the entire congress (hours: 8.30 - 18.30). Please contact first the Registration Desk in case of need.

## **Post Office and Courier Services**

A Post Office is located next to S.M.N. station and it is open from 8.15 to 19.00, Monday to Friday. Stamps may be purchased at Post Offices and Tobacconists (Tabacchi). For sending UPS and FedEx documents and parcels, Internet Train stores may be used.

## **Communications**

For public telephones it is highly recommended to purchase Telecom Phone Cards. Other international phone cards can be purchased and used from public telephones by dialling the indicated toll free number.

A number of internet point shops and bookstores offer internet access.

## **Parking**

The majority of hotels have private parking facilities. An underground paying parking lot is located next to the S.M.N. station. Since in August many Florentines are vacationing, it shall not be too difficult to find parking spots on the streets near the Congress Centre. In this respect, be aware that 1) the entire downtown area (Forteza da Basso is at the border of this zone) is restricted to private traffic. Only hotel residents and traffic in a specific direction to S.M.N. station are permitted downtown. 2) parking in the outside traffic-

## XX Congress of the International Union of Crystallography

### Congress and General Assembly

limited area (only within the blue outlined spaces) is not free during working hours. The tickets for the hourly charge can be paid by inserting coins in the automatic dispensers.

Registered congress participants can take advantage of the following parking lots at discounted rate: "Parcheggio Parterre" (Piazza della Libertà and via Madonna della Tosse, 9), "Parcheggio Beccaria" (Piazza C. Beccaria), "Parcheggio Sant'Ambrogio" (Piazza L. Ghiberti). For more information please ask at the Hotel Accommodation-Information Desk

### Safety and Security

As in most tourist cities around the world, visitors are advised to take all the necessary precautions. Although Florence is generally safe, caution should be exercised when visiting a crowded place and on public transports where pick pocketing is not unusual. There is a special police unit for assisting foreigners, located in Via Pietrapiana 50R (tel. 055 203911), where thefts should be reported.

### General Help Desk and Notices at the Congress

Assistance and general information is available at the Registration Desk. A "Messages and Daily Notices" board is located close to the Registration Desk. On the board, a limited area is reserved for personal communications. Please do not forget to date your messages, as they will be removed after two days of posting.

### Insurance

The XX IUCr Congress, Newtours and Firenze Fiera cannot be held responsible for any personal injury, loss, damage, accident to private property or additional expenses incurred as a result of delays or changes in air, rail, sea, road or other services, weather, war or any other cause. Congress participants are advised to have their own insurance.

## SOCIAL EVENTS

The following social program is organized for registered participants, students and accompanying persons.

A **Welcome Cocktail** party is scheduled to take place immediately after the Opening Ceremony on Tuesday 23 August, in the main courtyard in front of the Pavilion A, preceded by a colourful parade of the historical characters from the Republic of Florence.

A chamber music **Concert**, with compositions from A. Webern, E. Bosso, H. Dutilleux and R. Schumann will be performed by the "Quartetto di Torino" and the pianist Tiziano Mealli. The event will take place at the "Teatro Verdi", Via Ghibellina 99, Firenze, starting at 21.15 of Saturday 27.

The program of the concert is inserted in the participant bags. People, who made an advanced booking, can withdraw the invitation ticket at the Social Events and Tours Desk not later than Friday August 26. Additional tickets will be distributed until the evening of the Concert depending on the availability of the seats (~1500). The "Teatro Verdi" can be easily reached on foot from any place downtown. However, the ATAF bus n. 14 has a stop next to the theatre ("Teatro Verdi" bus stop).

The **Social Banquet** takes place on Monday 29 in the "Meridiana" courtyard of Palazzo Pitti at 20.00. The place can be easily reached on foot or by the ATAF bus D ("Pitti" bus stop). The deadline for paying the booking fee of €20.00 is Friday 26 at 18.00. By this time, also non-registered persons

can purchase tickets at the cost of €75.00, each. The maximum number of allowed participants is 1500.

The IUCr hosts a **Cheese and Wine party** to celebrate the arrival of the IUCr's latest journal, *Acta Cryst. F*, and the upcoming launch of International Tables Online. Congress participants are invited to attend at Exhibition Stand n. 42, on Friday 26 from 18.30 to 19.30.

Marresearch invites Congress participants to sign up for its **Traditional party**, organized in the magnificent Villa di Maiano in the hills of Florence (Friday 25, at 19.00). Bus transport to the location and back will be available. Since there is a limited number of available places, it is recommended to register at the Hotel Accommodation-Information Desk by Thursday August 24 at 18.00.

Two **free tours** are offered to the registered accompanying persons. Advanced booking is requested.

- 1) City Centre, Wednesday, August 24 (9.15-12.00)
- 2) Gallery of the Accademia and SS. Annunziata Square, Friday, August 26 (12.45-15.00)

# XX Congress of the International Union of Crystallography

## Congress and General Assembly

### CONGRESS TOURS

Special tours are organised for delegates and accompanying persons. A professional English-speaking guide will accompany all tours. The purchased tickets for the reserved tours are distributed together with the other congress material, otherwise new tickets may be purchased, according to the availability of the moment, at the Social Events and Tours Desk. The short list of possible tours is reported below. The full description and the additional information may be obtained at the Social Events and Tours Desk.

#### CITY CENTRE

**Wednesday, August 24 - 09.15-12.00 / half day.**

€30,00 per person (*free of charge for accompanying person*)

#### UFFIZI GALLERY

**Wednesday, August 24 or Saturday, August 27 - 16.30-18.45 / half day.** €35,00

#### PISA AND LUCCA

**Thursday, August 25 / full day, by bus.** €95,00

#### THE MEDICI FAMILY

**Thursday, August 25 - 09.15-12.00 / half day.** €38,00

#### SANTA CROCE, THE MONASTERY AND DISTRICT

**Friday, August 26 - 09.15 - 12.00 / half day.** €35,00

#### GALLERY OF THE ACCADEMIA AND SS. ANNUNZIATA SQUARE

**Friday, August 26 - 12.45 - 15.00 / half day.** €35,00

(*free of charge for accompanying person*)

#### CHIANTI AREA

**Saturday, August 27 - 09.00-17.00 / full day, by bus.**  
€95,00

#### MEDICI VILLAS

**Sunday, August 28th - 09.00 - 17.00 / full day, by bus.**  
€95,00

#### FLORENTINE HILLS

**Sunday, August 28 - 09.15 - 12.00 / half day, by bus.**  
€40,00

#### THE PITTI PALACE

**Sunday, August 28 - 16.30 - 18.45 / half day.** €35,00

#### SIENA AND SAN GIMIGNANO

**Monday, August 29 - 09.00 - 18.00 / full day, by bus.**  
€95,00

#### THE GREAT WINES OF TUSCANY

**Wednesday, August 31 - 08.30-19.00 / full day,**  
by bus. €115,00

## SPECIAL SCIENTIFIC EVENTS

### Computer Fayre

A fair of both non-commercial crystallographic software developers and software users takes place, from Thursday 25 until Tuesday 30 August 2005, in the Ghirlandaio Hall. The daily opening hours and the different events are on display at the Hall's entrance. Eight PCs and a laser printer, all connected in a local network, are available to the participants. The room is also equipped with an audio system and video projector. Since the size of the Hall is limited (max. 30 people), a first arrived – first served procedure is followed. However, repeat demonstration may be arranged depending on the requests.

### Workshops

Six different workshops are scheduled on Tuesday 23 in the different halls of Pavilion A, before the official opening of the congress.

A registration fee, other than that required for participating in the XX IUCr Congress is required.

For late participants this may be paid on site at the congress Registration Desk, provided that there is still availability. The scientific contents program of each workshop are available in the respective halls.

The events are the following:

- Workshop n.1: **Membrane Proteins: From Gene to Crystal.** (10.00-12.30) Donatello Hall.
- Workshop n.2: **Putting the Pedal to the Metal: High Throughput Protocols for Crystallization.** (14.00-16.30) Donatello Hall.
- Workshop n.3: **Introduction to Small-Angle Scat-**

tering (9.00-17.00) Brunelleschi Hall.

- Workshop n.4: **Structural Analysis of Aperiodic Crystals** (9.30-16.30) Giotto Hall.
- Workshop n.5: **Small Molecule Crystallization** (9.00-17.00) Botticelli Hall.
- Workshop n. 6: **A Protein Crystallographic Toolbox: CCP4 Software Suite** (8.30-17.00) Cimabue Hall

### Open Commission Meetings

Various Open Commission Meetings (OCM) are held daily between 12.35-14.35, (except for August 23,28,29 and 30). The detailed programs and the halls hosting the different OCM are given on a daily basis in the Scientific Program of this booklet (sections Other Activities, in between Microsymposia and Posters).

### Round Table on Data Mining

A round table on data mining from PDB takes place on Saturday, August 27 (12.35-14.35) in the Cimabue hall. The participants are H. Berman, K. Henrick, H. Nakamura and P. Bourne. The discussion will be extended to the audience.

### Microsymposium on “Art and Crystallography”

The MS30 on Art and Crystallography, chaired by C. Acidini and E. Meyer, has been structured as an evening plenum session held in the Michelangelo Hall on Friday 26 August, at 21.00. The intrinsic beauty of crystals and molecules together with their symmetric properties have been a source of inspiration for numerous artists. The invited speakers are re-

## XX Congress of the International Union of Crystallography

### Congress and General Assembly

nowned authorities who have made important links between Science and Art. Opening remarks on the Florentine Art will be made by the Supervisor of the "Opificio delle Pietre Dure di Firenze", Dr. Cristina Acidini. Doris Schattschneider, Martin Kemp and George Tsoucaris will illustrate direct relations between Art and Crystallography. Edgar Meyer will close the session with his own presentation and remarks. During the MS, prizes for the best pieces of work presented in the exhibition on "Art and Crystallography" will be awarded.

#### Seminar

A seminar with title "The Crystallographic Game" will be given by Jan Boeyens on Friday August 26, at 10.00 in the Giotto Hall. This session overlaps with six other Morning Microsymposia.

#### Poster Prizes

The Cambridge Crystallographic Data Centre (CCDC) awards three prizes for the best poster contributions in chemical crystallography. Each prize consists of a commemorative item and a monetary sum. Candidates should not be older than 35 on the date of January 1, 2005.

The IUCr awards a prize to the best posters presented from students belonging to each of the three IUCr areas (ACA, AsCA and ECA). The prizes consist of either a complimentary online access to all IUCr journals for one year, a volume of the International Tables or another IUCr publication.

**Molecular Dimensions Ltd** awards a monetary prize for one poster within the subject of protein Crystal Growth.

The **Oxford Cryosystems** prize is awarded to a poster concerning low temperature crystallography.

The **RCSB PDB** prize is awarded to best poster presentation from students.

More details are available from the stands of the companies or Institutions (in the Exhibition Area) who sponsor the awards.

Authors are kindly requested to collect from the different sponsor stickers, which must affix on their posters to indicate that they are in the competition. For each category, an independent panel of judges will evaluate the posters. The prizes will be awarded on Tuesday, 30 August, during the Closing Ceremony of the congress.

## **OPENING DAY: TUESDAY, 23 AUGUST**

### **Events**

Pre-congress workshops take place in the Halls of Pavilion A.  
The details on page VIII

Opening of the Commercial Exhibition in Pavilion A (till Saturday 27).

Opening of the Exhibition on "Art and Crystallography" in the Escher Hall

Opening Ceremony and the Welcome Cocktail.  
These events are opened to all the registered participants,  
accompanying persons and exhibitors.

The Opening Ceremony and the Ewald Prize Lecture will take place in the Michelangelo Hall of the Congress Centre.  
Welcome Cocktail will take place outdoors in the courtyard of the Congress Centre next to Pavilion A.

### **Timetable**

- |              |   |
|--------------|---|
| 8.00 - 18.00 | Registration of the participants                  |
| 9.00 - 18.30 | Commercial Exhibition                             |
| 12.30-13.30  | Lunch (only for registered workshop participants) |
| 15.00-18.00  | Exhibition on "Art and Crystallography"           |

### **18.00 Opening Ceremony**

Introductory talks from the chairpersons, the President of IUCr and other scientific and local authorities

**18.30 Award of the Ewald Prize and conference of the recipient Professor Philip Coppens**

Musical Interlude

**19.30 IUCr Award for exceptional service to crystallography**

**19.45 Parade of the historical characters of the Republic of Florence**

**20.00 Welcome Cocktail Party**

# XX Congress of the International Union of Crystallography

Congress and General Assembly

## CLOSING CEREMONY

The closing Ceremony takes place in the Michelangelo Hall immediately after the last keynote lecture on Wednesday, 30 August (at about 18.30). Departing messages will be delivered by the organizers, the president of the IUCr and other authorities.

During the ceremony the poster prizes will be awarded to the winners.

An *arrivederci a presto* in Osaka, Japan will complete the congress.

## SCIENTIFIC INFORMATION

### Instructions for the Presenting Authors

#### ORAL PRESENTATION

All the meeting rooms are equipped with PowerPoint-based projectors. The audiovisual presentations are supervised by the in-house group TecnoConference who has a central assistance Slide Center (opening hours 8:30-18:30) in the ground floor of Pavilion A. Here, the file(s) for presentation, supplied on Windows formatted CD-Roms, pen drives, floppy disks or zip disks, must be delivered by the speakers at least 6 hours before the afternoon session or, in the case of morning sessions, the day before (not later than 17.00). Any concern regarding the presentation should be directed towards the

TecnoConference operators, sufficiently in advance. This applies in particular for those using non-standard configurations (i.e., not processable with standard Windows XP operative system and Office XP applications). The usage of PowerPoint 2003 with standard true type characters is highly recommended. To this purpose, before saving the file, select in the menu Tools/Options/Save the box "Font options for current document only"/"Embed TrueType fonts"/"Embed characters in use only". During the PPT presentation, the usage of a well visible mouse-controlled pointer is preferred to a laser pointer (press CTRL/A during to keep the cursor on the screen even when inactive.) Usage of personal laptop computers for presentation is not allowed to prevent any loss of time. For practical and security

reasons, internet facilities are not available to the speakers during their presentation. Although all care will be taken in handling the presentation files, the organizers cannot take responsibility for loss or damage

## POSTER PRESENTATION

Poster sessions are held between 13.45 and 14.45 daily from Wednesday 24 to Tuesday 30, August. Please check in this booklet or in the web-site for the date when your poster must be displayed and the assigned board number. On the presentation day, authors are kindly requested to set up their poster with the supplied sticky gum in between 8.00 and 8.30 and to remove it not later than 18.30 of the same day. Authors submitting posters submitted for the Topic and Subtopic 28.2 (Art, Cultural Heritage and Crystallography - Crystallography and Art) are kindly requested to move their contributions to the Escher Hall at the end of their poster session. These posters will remain on display until Saturday, 27 August.

## Notes on the Detailed Scientific Program

The titles of all the scientific contributions are grouped on a daily basis and in the following order: Keynotes, Microsymposia, Other Scientific Activities (e.g. Open Commission Meetings, Round Table, Seminars, General Assembly, etc.) and Posters.

Each session of the seven parallel Microsymposia (Morning or Afternoon) is presented in two consecutive pages (left and right). The first column at the left side reports the

starting and ending time of each oral presentation.

Specific Code Numbers identify the category of the scientific contributions, matching those used in the Book of Abstracts (BoA). Additionally, the page number of the corresponding abstracts is given after the Code.

Specifically the following formats are used throughout this booklet:

**KN.nn.dd** (Czz), where **nn** is the number of the Keynote Lecture, **dd** is the number of the day in August and **zz** is the page number in the BoA.

**MSnn.xx.yy** (Czz), where **nn** is the number of the Microsymposium, **xx** is the number of the day in August 2005, **yy** is the order of the talk within the MS and **zz** is the page number in the BoA.

**CCnn.xx.yy** (Czz), where **nn** is the number of the Open Commission Meeting, **xx** is the number of the day in August 2005, **yy** is the order of the talk within the OCM and **zz** is the page number in the BoA.

**P.xx.yy.oo** (Czz.nn), where: **xx** and **yy** are the Topic and Subtopic numbers, respectively, **oo** is the serial number, **zz** is the page number in the BoA and **nn** is the poster board number assigned to the presentation.



# **XX Congress**

of the

# **International Union of Crystallography**

**Scientific Program**



**WEDNESDAY, AUGUST 24 2005 – KEYNOTE LECTURES**

**MORNING SESSION 8.30-9.30**

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Michelangelo (**KN 1**)

**KN01.24(CI)** | Roald Hoffmann:  
A Theoretician's View of Crystallography

*Chair: Joel Bernstein*

**AFTERNOON SESSION 17.30-18.30**

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Botticelli (**KN 2**)

**KN02.24(CI)** | Martino Bolognesi:  
Structure and Recognition in the BARS/CtBP-dependent Transcription Regulation

*Chair: Dusan Turk*

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Michelangelo (**KN 3**)

**KN03.24(CI)** | Chikashi Toyoshima:  
Ion Pumping by  $\text{Ca}^{2+}$ -ATPase of Sarcoplasmic Reticulum

*Chair: Giuseppe Inesi*

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Cimabue (**KN 4**)

**KN04.24(CI)** | Walter Reimers:  
Neutrons and X-rays for Microstructure and Strain/Stress Analysis in Materials

*Chair: Anatoly Balagurov*

# WEDNESDAY, AUGUST 24 2005 – MORNING - MICROSYMPOSIA

TIME	Michelangelo ( <i>MS 1</i> )	Botticelli ( <i>MS 2</i> )	Cimabue ( <i>MS 3</i> )
10.00-10.05 Opening Remarks	<b>WHEN BAD CRYSTALS TURN GOOD: TRANSFORMING POORLY DIFFRACTING CRYSTALS</b> <i>Chairs:</i> Naomi Chayen, Janet Newman	<b>CHAMELEON PROTEINS</b> <i>Chairs:</i> L. Regan, P. Curmi	<b>CHIRAL AND NON-CENTROSYMMETRIC STRUCTURES</b> <i>Chairs:</i> S. P. Halasyamani, R. Kuroda
10.05-10.35	<b>MS01.24.1(C9)</b>   A. Hassell: Optimizing Your Crystals--Is it Really Worth the Time?	<b>MS02.24.1(C10)</b>   A. Gronenborn: The Amazing Versatility of Proteins - Structural Polymorphism and Evolution	<b>MS03.24.1(C11)</b>   P. Metrangolo: Spontaneous Resolutions in Halogen Bonded Fluorinated Networks
10.35-11.05	<b>MS01.24.2(C9)</b>   V. Stojanoff: Improvement of Crystal Quality by Time Controlled Annealing	<b>MS02.24.2(C10)</b>   F. Chiti: The Mechanisms of Conversion of Proteins into Amyloid Fibrils	<b>MS03.24.2(C11)</b>   M. K. Strumpel: Invariom Modeling for Improving Absolute Structure Determination
11.05-11.35	<b>MS01.24.3(C9)</b>   M. G. Gruetter: Designed Ankyrin Repeat Proteins as Tools for the Crystallization of Proteins	<b>MS02.24.3(C10)</b>   S. Tilley: The Molecular Hole Punch: Structural Changes in the Bacterial Toxin Pneumolysin during Pore Formation	<b>MS03.24.3(C11)</b>   W. Kaminsky: Optical Topographies of Chiral Structures
11.35-12.05	<b>MS01.24.4(C9)</b>   C. Schall: Effect of Crystal Size and Cooling Method on Cryoprotection and Data Quality	<b>MS02.24.4(C10)</b>   J. Whisstock: Obeying Anfinsen: a Serpin that Folds to the Most Stable State	<b>MS03.24.4(C11)</b>   A. Persoons: Nonlinear Optical Properties of Chiral Polymers and Systems
12.05-12.35	<b>MS01.24.5(C9)</b>   B. Rupp: Data Mining and Machine Learning for Improved Crystallization Success - Expectations and Reality	Chair Remarks and Discussion	<b>MS03.24.5(C11)</b>   J. Bernstein: Some Reminiscences of Non-centrosymmetric Structures

# WEDNESDAY, AUGUST 24 2005 - MORNING - MICROSYMPOSIA

Giotto ( <i>MS 4</i> )	Leonardo da Vinci ( <i>MS 5</i> )	Brunelleschi ( <i>MS 6</i> )	Donatello ( <i>MS 7</i> )
<b>POLYMORPHISM</b> <i>Chairs: E. Vlieg, R. D. Rogers</i>	<b>STRUCTURAL PHASE TRANSITIONS</b> <i>Chairs: J. M. Perez-Mato, U. Bismayer</i>	<b>CRYSTALLOGRAPHY AND FORENSIC SCIENCE</b> <i>Chairs: D. Rendle, I. Nakai</i>	<b>CRYSTAL CHEMISTRY OF INORGANIC AND MINERAL COMPOUNDS</b> <i>Chairs: W. Depmeier, H. Effenberger</i>
<b>MS04.24.1(C12)</b>   <u>K. Sato</u> : Modifying Nucleation Kinetics of Polymorphic Crystals in Bulk and Emulsion States	<b>MS05.24.1(C13)</b>   <u>C. J. Howard</u> : Structural Transitions in Perovskites: Successes of a Group Theoretical Approach	<b>MS06.24.1(C14)</b>   <u>W. Kugler</u> : Application of X-ray Diffraction in the Forensic Science Laboratory of Stuttgart; Germany	<b>MS07.24.1(C15)</b>   <u>A. Vegas</u> : The Zintl-Klemm Concept Applied to Cations in Oxides. An Alternative Interpretation of the Structures of Silicates
<b>MS04.24.2(C12)</b>   <u>S. M. Reutzel-Edens</u> : Controlling Crystal Polymorphism: from Stability Prediction to Crystallization Process Design	<b>MS05.24.2(C13)</b>   <u>D. Pandey</u> : Phase Transitions in Relaxor Ferroelectric Based Solid Solutions	<b>MS06.24.2(C14)</b>   <u>R. W. Fitzpatrick</u> : Soil Mineralogy and other Properties in Forensic Investigations	<b>MS07.24.2(C15)</b>   <u>S. Krivovichev</u> : Uranyl Selenates: from Finite Clusters to Nanotubules
<b>MS04.24.3(C12)</b>   <u>F. J. J. Leusen</u> : Crystal Structure Prediction: Theory, Applications and Challenges	<b>MS05.24.3(C13)</b>   <u>M. Braden</u> : The Phase Diagram of $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$ : Crystal Structure and Physical Properties	<b>MS06.24.3(C14)</b>   <u>W. Heijnen</u> : Applications of XRD in Forensic Casework	<b>MS07.24.3(C15)</b>   <u>C. A. Geiger</u> : Molecule-Mineral Inner-Surface Interactions in Nanoporous Silicates
<b>MS04.24.4(C12)</b>   <u>M. Zaworotko</u> : Polymorphism in Co-Crystals and Pharmaceutical Co-Crystals	<b>MS05.24.4(C14)</b>   <u>T. K. Chatterji</u> : Volume Collapse at the Jahn-Teller Transition in $\text{LaMnO}_3$	<b>MS06.24.4(C15)</b>   <u>Y. Terada</u> : X-ray Chemical Analysis for Forensic Applications Using Synchrotron Radiation	<b>MS07.24.4(C16)</b>   <u>C. Ferraris</u> : TEM and XPS Evidences of O/F Ordering in $\text{NbO}_2\text{F}$
<b>MS04.24.5(C13)</b>   <u>C. Pulham</u> : An Exploration of Polymorphism in Molecular Crystals Using High Pressure	<b>MS05.24.5(C14)</b>   <u>S. Leoni</u> : Nucleation and Growth Mechanisms in Solid-Solid Phase Transitions	Chair Remarks and Discussion	<b>MS07.24.5(C16)</b>   <u>N. Zubkova</u> : Crystal Structures and Topology of New and Rare Arsenates

# WEDNESDAY, AUGUST 24 2005 - AFTERNOON - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 8</b> )	Brunelleschi ( <b>MS 9</b> )	Botticelli ( <b>MS 10</b> )
14.45-14.50 Opening Remarks	<b>MEMBRANE PROTEIN STRUCTURE AND FUNCTION</b> <i>Chairs: J. M. Gulbis, M. R. Garavito</i>	<b>COMBINED XAS AND XRD TECHNIQUES IN PHYSICS CHEMISTRY AND MATERIALS SCIENCE</b> <i>Chairs: S. Mobilio, J. Garcia-Ruiz</i>	<b>INTEGRATED CRYSTALLOGRAPHIC, SPECTROSCOPIC, AND COMPUTATIONAL APPROACHES</b> <i>Chairs: A. Roodt, S. Alvarez</i>
14.50-15.20	<b>MS08.24.1(C16)</b>   <u>X.-D. Li</u> : Does the Crystal Structure of Ammonium Transporter Tell us its Function?	<b>MS09.24.1(C18)</b>   <u>A. San Miguel</u> : XAS and XRD: Complementary Tools to Explore Matter under Extreme Pressure	<b>MS10.24.1(C19)</b>   <u>P. Coppens</u> : Time-Resolved Photo-crystallography of Short-Lived Molecular Excited States
15.20-15.50	<b>MS08.24.2(C16)</b>   <u>L. Vandeputte-Rutten</u> : Two OMPs: autotranslocation and LPS-deacylation	<b>MS09.24.2(C18)</b>   <u>D. Haskel</u> : Element- and Site-Specific Study of the Atomic Origin of Magnetic Hardness in Modern Magnets	<b>MS10.24.2(C19)</b>   <u>K. Schwarz</u> : Crystal Structure Prediction with WIEN2k
16.50-16.20	<b>MS08.24.3(C17)</b>   <u>H. Aoyama</u> : X-ray Structures of Phospholipids in Bovine Heart Cytochrome <i>c</i> Oxidase	<b>MS09.24.3(C18)</b>   <u>J.-D. Grunwaldt</u> : X-rays to Elucidate the Structure of Catalysts: Probing the Local and the Crystalline Structure by XAS and XRD	<b>MS10.24.3(C19)</b>   <u>P. Comba</u> : Correlation of Structures and Reactivity of Bispidine Coordination Compounds
16.20-16.50	<b>MS08.24.5(C17)</b>   <u>C. Olesen</u> : Dephosphorylation of the Calcium pump Coupled to Conterion Occlusion.	<b>MS09.24.4(C18)</b>   <u>M. G. Proietti</u> : Structural Properties of Semiconductor Nanostructures via X-ray Anomalous Diffraction (DAFS) and Absorption (EXAFS)	<b>MS10.24.4(C19)</b>   <u>S. Troyanov</u> : Structure of Halofullerenes Using Experimental and Theoretical Approaches
16.50-17.20	<b>MS08.24.4(C17)</b>   <u>J. Li</u> : Structure of Rhodopsin as a G Protein-Coupled Receptor	<b>MS09.24.5(C18)</b>   <u>S. Quartieri</u> : Multi-Disciplinary Approaches to the Study of Minor and Trace Element Incorporation in Geo- and Technological Materials	<b>MS10.24.5(C20)</b>   <u>P. Gilli</u> : The Nature of the HB. 3. Towards a Comprehensive HB Theory

# WEDNESDAY, AUGUST 24 2005 – AFTERNOON - MICROSYMPOSIA

Giotto ( <i>MS 11</i> )	Leonardo da Vinci ( <i>MS 12</i> )	Cimabue ( <i>MS 13</i> )	Donatello ( <i>MS 14</i> )
INSTRUMENTATION AT NEXT GENERATION X-RAY SOURCES <i>Chairs:</i> T. Tschentscher, J. Arthur	DISORDER DIFFUSE SCATTERING <i>Chairs:</i> R. Neder, T. Proffen	ADVANCES IN COMPUTATIONAL METHODS FOR POWDER DIFFRACTION <i>Chairs:</i> B. H. Toby, L. M. D. Cranswick	MODULARITY AND MODULATION IN INORGANIC AND MINERAL STRUCTURES <i>Chairs:</i> E. Makovicky, S. Merlini
<b>MS11.24.1(C20)</b>   <u>M. Yabashi</u> : Roles of X-ray Optics in the Next Generation X-ray Source	<b>MS12.24.1(C21)</b>   <u>T. R. Welberry</u> : Diffuse Scattering and Monte Carlo Studies of Relaxor Ferroelectrics	<b>MS13.24.1(C22)</b>   <u>A. Wills</u> : Application of Symmetry to Magnetism and its Consequences for Crystallography	<b>MS14.24.1(C23)</b>   <u>L. Cario</u> : Layered Compounds: from Modular Description to Rational Design
<b>MS11.24.2(C20)</b>   <u>K. Gaffney</u> : Ultrafast X-ray Studies of Structural Dynamics	<b>MS12.24.2(C21)</b>   <u>K. Harata</u> : Order and Disorder in Lysozyme Crystals Caused by the Phase Transition	<b>MS13.24.2(C22)</b>   <u>J. Rodríguez-Carvajal</u> : CrysFML: a Library to Develop Crystallographic Programs in Fortran 95. Powder Diffraction Examples	<b>MS14.24.2(C23)</b>   <u>G. Ferraris</u> : Recurrent Modules in Modular Structures
<b>MS11.24.3(C20)</b>   <u>S. Marchesini</u> : Imaging of Single Molecules	<b>MS12.24.3(C21)</b>   <u>L. Kaiser-Bischoff</u> : X-ray and Neutron Diffuse Scattering by Cation and Anion Deficient Zirconia	<b>MS13.24.3(C22)</b>   <u>S. J. L. Billinge</u> : Peter Piper Picked a Problem Trickier than most. Can Computer Science Solve the Problem Peter Piper Picked?	<b>MS14.24.3(C24)</b>   <u>J. Hybler</u> : Refinement of Partially Disordered OD Structures
<b>MS11.24.4(C20)</b>   <u>B. Lengeler</u> : Parabolic Refractive X-ray Lenses	<b>MS12.24.4(C22)</b>   <u>B. Campbell</u> : Diffuse Scattering Study of 2D Superstructure in a T' Electron-doped Cuprate Superconductor	<b>MS13.24.4(C23)</b>   <u>G. Vaughan</u> : Single Crystal Quality Structures from Polycrystalline Samples	<b>MS14.24.4(C24)</b>   <u>L. Bindi</u> : Incommensurately Modulated Structure in Natural Melilites
<b>MS11.24.5(C21)</b>   <u>C. Broennimann</u> : Solid State Detectors for Present and Future X-ray Sources	<b>MS12.24.5(C22)</b>   <u>T. Weber</u> : Cooperative Evolution: a New Algorithm for Refining Disordered Structures	<b>MS13.24.5(C23)</b>   <u>S. Chong</u> : 'Pushing the Boundaries' of Differential Evolution in SDPD	<b>MS14.24.5(C24)</b>   <u>D. O. Charkin</u> : Modular Approach Applied to Tailoring of Bismuth-Containing Layered Perovskites

## **WEDNESDAY, AUGUST 24 2005 – OTHER ACTIVITIES**

### **OPEN COMMISSION MEETINGS**

Giotto (12.35-14.35)

#### **OCM01 COMMISSION ON JOURNALS (I)**

*Chair: John Helliwell*

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#### **OCM01.24.1(CI25) | J. R. Helliwell:**

Overview of IUCr Journals

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#### **OCM01.24.2(CI25) | D. Schwarzenbach:**

Acta Crystallographica Section A: Foundations of Crystallography

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#### **OCM01.24.3(CI25) | C. P. Brock:**

Acta Crystallographica Section B: Structural Science

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#### **OCM01.24.4(CI25) | G. Ferguson:**

Acta Crystallographica Section C: Crystal Structure Communications

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#### **OCM01.24.5(CI25) | E. N. Baker:**

Acta Crystallographica Section D: Biological Crystallography:2002-2004

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#### **OCM01.24.6(CI26) | W. Clegg:**

Structure Reports Online (Acta E): Rapid Growth 2001-2004

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#### **OCM01.24.7(CI26) | H. Einspahr:**

Acta Crystallographica Section F, Launch Year Report

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#### **OCM01.24.8(CI26) | G. Kostorz:**

Journal of Applied Crystallography

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#### **OCM01.24.9(CI26) | D. Mills:**

Journal of Synchrotron Radiation: Current Status and Issues

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### **IUCr GENERAL ASSEMBLY**

Cimabue (19.00-22.00)

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

## 02 METHODS FOR STRUCTURE DETERMINATION

### 4. Anomalous Dispersion/MAD/MIR Phasing

**P.02.04.1(C153.1)** | Y. Kitago: Structure Determination of a Novel Protein by Sulphur SAD Using Novel Crystal Mounting Method

**P.02.04.2(C153.2)** | D. Siliqi: IL MILIONE: a Compleat Package for a Global Phasing, from Powders to Proteins

**P.02.04.3(C153.3)** | H. Fan: OASIS-2004 and Difficult SAD Phasing

**P.02.04.4(C153.4)** | H. Miyatake: A Novel Method to Prepare Iodine Derivatives for In-house Phasing

**P.02.04.5(C154.5)** | D. Yao: SAD Phasing at Bijvoet Ratio Below 0.6%

**P.02.04.6(C154.6)** | B. Schierbeek: SAD Phasing Using a Home Source, What is the Limit?

**P.02.04.7(C154.7)** | G. Pompidor: A new Lanthanide Complex for Solving Protein Structures Using Anomalous Scattering

**P.02.04.8(C154.8)** | R. Kahn: Comparative Study of the Binding of Different Gd Complexes in Protein Crystals

**P.02.04.9(C155.9)** | C. Yang: In-house S-SAD and Se-SAD Phasing with Cr-Kalpha Radiation

### 7. EXAFS and XANES

**P.02.07.1(C155.10)** | L.O. Fabregas: Local Structure of the Metal-oxygen Bonds in ZrO<sub>2</sub>-CeO<sub>2</sub> Nanopowders

### 10. Structure Prediction: Computational Methods

**P.02.10.1(C155.11)** | F. Baysen: Investigating the Molecular Formation Properties of 4-(2-Oxobenzothiazolin-3-Yl) Butanoic Acid Using Pm3, Am1, MnD Methods

**P.02.10.2(C155.12)** | L.A. Mossakowska: Crystal Structure Prediction of Nitrobenzene Derivatives.

**P.02.10.3(C156.13)** | L. Viitanen: Structural Modeling of Sterol Carrier Protein-2 from Plants

**P.02.10.4(C156.14)** | L. Vella-Zarb: Powder Diffraction and Crystal Structure Prediction: A Two-Way Relationship?

**P.02.10.5(C156.15)** | S.A. Barnett: Can a Computational Search Predict Complications in Single Crystal Growth?

**P.02.10.6(C156.16)** | A. Kahraman: Binding Pocket Shape Analysis for Protein Function Prediction

## 03 COMPUTERS IN ANALYSIS, MOLECULAR MODELLING AND MOLECULAR DESIGN

### 2. Atomic Displacement Analyses and Variable Temperature Analyses

**P.03.02.1(C165.17)** | D.M.S. Martins: Combined Experimental and Theoretical Studies of Solid State Proton Migration.

### 5. Materials Design

**P.03.05.1(C166.18)** | I. Yarovsky: Effect of Nanoscale Surface Modification on Interfacial Adhesion: a Theoretical Modelling Study

**P.03.05.2(C166.19)** | T. Timofeeva: Modeling of Crystal

Structures of Materials: Which Goals Can Be Achieved?

**P.03.05.3(C166.20)** | L. Lykke: A Global Search for the Optimal Bandstructure for Thermoelectric Applications

### 6. Structure Simulations: Inorganic Crystals

**P.03.06.1(C166.21)** | T. Petrova: Computer Modeling of Local Structure and Properties of Oxide Solid Solutions with NaCl Type Structure.

**P.03.06.2(C167.22)** | R. Dovesi: The Vibrational Properties of Katoite Ca<sub>3</sub>Al<sub>2</sub>[(OH)<sub>4</sub>]<sub>3</sub>: a Periodic Ab-initio Study

## 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

### 2. Enzymes and Enzyme Catalysis

**P.04.02.82(C199.23)** | M. Goto: Crystal Structures of Serine Racemase from *S. pombe*

**P.04.02.83(C199.24)** | T. Umeda: Crystal Structures of Formaldehyde Dehydrogenase Complexed with Inhibitors

**P.04.02.84(C199.25)** | M.J. Lemieux: Molecular Basis for Tay-Sachs Revealed by the Crystal Structure of Human  $\beta$ -HexosaminidaseA

**P.04.02.85(C199.26)** | R. Omi: Structural Basis for the Induced Fit, Substrate Recognition, and Mechanism of Threonine Synthase

**P.04.02.86(C200.27)** | Y. Kusakari: Structure and Mutational Analysis of *Trypanosoma brucei* Prostaglandin F<sub>2</sub><sub>a</sub> Synthase

**P.04.02.87(C200.28)** | K. Tokuoka: Crystal Structure of

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

Prostaglandin F<sub>2α</sub> Synthase from *Leshmania major*

**P.04.02.88(C200.29)** | K. Kanbayashi: Structural Evidence of pH-induced Changes of the Reduction Potential of Mavicyanin from Zucchini

**P.04.02.89(C200.30)** | T. Ogawa: Crystal Structure of Rice Rubisco Complexed with NADPH

**P.04.02.90(C201.31)** | Y. Kakuta: Crystal Structure of Sulfotransferase from Mycobacterium Tuberculosis H37Rv

**P.04.02.91(C201.32)** | A. Henriksen: Structure of a Class 4 aldo/keto Reductase

**P.04.02.92(C201.33)** | K. McAuley: Crystal Structure and Catalytic Regulation of an S-Formylglutathione Hydrolase

**P.04.02.93(C201.34)** | H. Yamaguchi: Crystal Structure of m-hydroxybenzoate Hydroxylase from *Comamonas testosteroni*

**P.04.02.94(C202.35)** | P. Arjunan: The *E. coli* PDHc E1 Component Complex with a Reaction Intermediate Analogue

**P.04.02.95(C202.36)** | T. Matsuura: Crystal Structure of Chitin Binding Domain of Chitinase A1

**P.04.02.96(C202.37)** | A. Toms: Characterization of TenA from *Bacillus subtilis*: A Thiaminase II

**P.04.02.97(C202.38)** | A. H. Teh: Crystal Structure of Inhibitor-Bound Mouse Cytidine Deaminase at 1.5 Å

**P.04.02.98(C202.39)** | J. Berglund: *Arabidopsis thaliana* Acyl-CoA Oxidase 1 in Complex with AcetoAcetyl-CoA

**P.04.02.99(C203.40)** | D. Bordo: Structural Studies on Sulfurtransferase/Phosphatase Enzymes

**P.04.02.100(C203.41)** | A. Kadziola: Regulation of *Sulfolobus solfataricus* Uracil Phosphoribosyl-transferase

**P.04.02.101(C203.42)** | T. Yadani: Crystal Structure of Glutathione-dependent Dehydroascorbate Reductase from Spinach Chloroplast

**P.04.02.102(C203.43)** | T. Holyoak: Snapshots Along the PEPCK Catalytic Pathway

**P.04.02.103(C204.44)** | P. Dessanti: Crystal Structures of *Bacillus cereus* AdoP Complexed with Substrates

**P.04.02.104(C204.45)** | C. Naoe: Crystallographic Study of the Archaeal DNA Repair Enzymes: EXOIII and APE

**P.04.02.105(C204.46)** | M. Morar: Study of Substrate-Complexed Formylglycinamide Ribonucleotide Amidotransferase

**P.04.02.106(C204.47)** | J. Barbosa: Structural Studies of Infestin 4, a Factor XIIa Inhibitor

**P.04.02.107(C205.48)** | Y. Zhang: Structural Studies on 3-hydroxyanthranilate-3,4-dioxygenase

**P.04.02.108(C205.49)** | R. Anand: Structure of *S. typhimurium* Formylglycinamide Ribonucleotide Amidotransferase

**P.04.02.109(C205.50)** | J. Lundqvist: Towards the Structure of the BchI Hexameric Complex of Magnesium Chelatase.

**P.04.02.110(C205.51)** | Y. Takahashi: Crystal Structure of Glutaredoxin of CxxC1 Type from Poplar

**P.04.02.112(C206.52)** | J. Yin: Crystal Structure of HAV 3C Protease Complexed with a β-lactone Inhibitor: a New Crystal Form of HAV 3C and Its Application for Studying Enzyme-inhibitor Interaction

**P.04.02.113(C206.53)** | G. De Simone: Crystal Structure of a Protein Disulfide Oxidoreductase from *Aquifex aeolicus*

**P.04.02.114(C206.54)** | A. Pesaresi: *Pseudomonas aeruginosa* PA3859: From Structure to Function

**P.04.02.115(C207.55)** | L. Lehtiö: Crystal Structure of a Glycyl Radical Enzyme from *Archaeoglobus fulgidus*

**P.04.02.116(C207.56)** | C. Levy: Crystal Structure of Dihydropteroate Synthase from *Streptococcus pneumoniae*

**P.04.02.117(C207.57)** | M. Kim: Crystal Structure of NH<sub>3</sub>-dependent NAD<sup>+</sup> Synthetase from *Helicobacter pylori*

**P.04.02.118(C207.58)** | V. A. Money: Structural Insights into a Glycoside Hydrolase Family 26 Lichenase

**P.04.02.119(C207.59)** | H. Tamura: Crystal Structure of Methylthioribose-1-phosphate Isomerase from *Bacillus subtilis*

**P.04.02.120(C208.60)** | I. Krastanova: Structural and Functional Studies of Carbohydrate Esterase Family 7 Enzymes

**P.04.02.121(C208.61)** | S. W. Au: Differential Maturation of SUMO Precursors by SUMO-specific Protease, SENP1

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

P.04.02.122(C208.62) | K. Schirwitz: High Resolution Structures of Formate Dehydrogenase Mutants from *Candida boidinii*

## 20. NMR Applications to Macromolecule

P.04.20.1(C254.63) | S. Mangani: Integration of XAS and NMR Techniques for the Structure Determination of Metallo-proteins. Examples from the Study of Copper Transport Proteins

P.04.20.2(C255.64) | M. Hackert: Unraveling the Structures of Antizyme and its Complexes

## 21. Time Resolved Studies

P.04.21.1(C255.65) | S. Larsen: Structural Studies of a Novel Phosphotriesterase Capable of Degrading Soman

P.04.21.2(C255.66) | V. Srager: Studies of Heme Proteins by Time-resolved Crystallography: Allosteric Action and Structural Relaxation

## 22. Structural Genomics

P.04.22.1(C255.67) | A. Fedorov: Crystal Structure of Conserved Hypothetical Protein YBEY from *Escherichia Coli*

P.04.22.2(C256.68) | H. Yang: Crystal Structure of *Pfu* 838710: the First Model of a Pfam CYTH Domain

P.04.22.3(C256.69) | S. Pletney: Structural Studies of Hyperthermophilic Enzymes from *Pyrococcus horikoshii*

P.04.22.4(C256.70) | C. Rife: Crystal Structures of pmbA and CsrA: Both Reveal New Folds

P.04.22.5(C256.71) | A. Teplyakov: Structure of the Bacterial YhcH Protein, a Putative Copper Aminosugar Epimerase

P.04.22.6(C256.72) | J. Wang: Crystallographic Studies of Several Essential Proteins Concerning the Nucleotide Metabolism in *Bacillus subtilis*

P.04.22.7(C257.73) | A. Criswell: ACTOR Gets an AGENT: Automation for Multiple Instruments

P.04.22.8(C257.74) | R. Zhang: Crystal Structures of Sortase B from *Staphylococcus aureus* and *Bacillus anthracis* Reveal Catalytic Amino Acid Triad in the Active Site

P.04.22.9(C257.75) | M. Elsliger: The Joint Center for Structural Genomics: A Multi-tiered Approach to Structural Genomics.

P.04.22.10(C257.76) | L. Shuvalova: When Structures of Unknown Proteins are Determined, What is next?

P.04.22.11(C258.77) | Y. Liang: A High-efficiency, Low-cost Platform for Structural Genomics Studies at Peking University

P.04.22.12(C258.78) | A. Ebihara: Progress in the Whole Cell Project of a Model Organism, *Thermus thermophilus* HB8

P.04.22.13(C258.79) | G. Zanotti: Structural Proteomics of Proteins Coded by the *cag* PAI of *Helicobacter pylori*

P.04.22.14(C258.80) | J. Brunzelle: Trying To Deduce Function From Structural Variability And Conservation

P.04.22.15(C258.81) | H. Itou: Comprehensive Structure-

based Functional Analysis on Transcription Factors

P.04.22.16(C259.82) | X.-D. Su: TIMomics: Genome-wide Search for Evolutionary Relationships Among TIM (triose-phosphate isomerase) Fold Proteins via Structural Genomics Approaches

P.04.22.17(C259.83) | E. N. Baker: Functional Discoveries from Crystal Structures of Proteins from *M. tuberculosis*

P.04.22.18(C259.84) | A. Joachimiak: Establishing High-throughput Protein Structure Determination Pipeline for Structural Genomics

## 05 CRYSTALLOGRAPHY OF BIOLOGICAL SMALL MOLECULES

### 1. Peptides

P.05.01.1(C273.85) | L. Tomcova: Crystallization of Cytochromes from *Thiocapsa roseopersicina*

P.05.01.2(C273.86) | V. Ferretti: New Class of Proteasome 20S Inhibitors: a Crystallographic and Molecular Modelling Study

P.05.01.3(C273.87) | S. Ramakumar: Glycine Zipper Motif in the Association of Helices in a Designed Peptide

P.05.01.4(C273.88) | M. L. Glowka: Crystal Structures Puzzle of the DSDH Gramicidin Channel

P.05.01.5(C273.89) | Y. In: Conformation Comparison of  $\mu$ -Selective Endomorphin-2 with Its C-Terminal Free Acid

P.05.01.6(C274.90) | A. Guerri: New Monocyclic and Acyclic hNK-2 Antagonists Retaining the  $\alpha$ -turn Feature

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

## 2. CNS Agents

**P.05.02.1(C274.91)** | J. R. Deschamps: Absolute Configuration of the  $\kappa$ -Agonist Salvinicin A

## 4. Steroids

**P.05.04.1(C274.92)** | Y.-J. Park: Crystal Structures of Cholesterol Derivatives

## 6. Other Biosynthetic and Exotic Molecules

**P.05.06.1(C276.93)** | M. Markiewicz: Xanthone Derivatives: Conformational Study and Development of Force Field

## 7. Hydrogen Bonding and Included Water Structure

**P.05.07.1(C276.94)** | S. Harte: Diffraction and Computational Studies of Hydrogen Bonded Base Paired Systems

**P.05.07.2(C276.95)** | E. Boldyreva: Polymorphism of Crystalline Amino Acids. The Role of Non-covalent Interactions

**P.05.07.3(C277.96)** | G. Le Bas: Neutron Diffraction Structure of the Complex  $\alpha$ -Cyclodextrin Ibuprofen at 15K

## 06 CRYSTALLOGRAPHY OF ORGANIC COMPOUNDS

### 1. Sugars

**P.06.01.1(C279.97)** | R. Gonnable: Concomitant Polymorphs Exhibiting Differences in the Halogen Bonding Contacts

**P.06.01.2(C279.98)** | M. D. Estrada: Hydrogen Bonding study by X-ray Diffraction of Sugars and Aminoacids

**P.06.01.3(C279.99)** | E. Alvarez: X-Ray Structure of a Mixed Spiroketal-Xylylene Macroyclic Receptor

**P.06.01.4(C279.100)** | P. Ochsenebein: Trisaccharide Crystal Structures from X-ray Powder Diffraction and Solution NMR

## 2. Lipids

**P.06.02.1(C279.101)** | L. P. Cavalcanti: Lipid Model Membranes for Drug Interaction Study

**P.06.02.2(C280.102)** | H. Schenk: Crystal Structure of Chocolate from Powder Diffraction Data

## 3. Alkaloids

**P.06.03.1(C280.103)** | J. K. Maurin: X-ray Analysis as the Important Tool in Controlling Stereoselective Synthesis of Drugs

**P.06.03.2(C280.104)** | K. Turgunov: Structures of Cocrystals of Peganole with 6-Brompeganole

## 4. Fused Ring Systems

**P.06.04.1(C280.105)** | J. Brüning: Crystal Structures of Fluorescent Bisazomethine Pigments

**P.06.04.2(C281.106)** | K. Haller: Structure of 19-Hydroxyneohopane

**P.06.04.3(C281.107)** | J. Wojciechowski: X-ray Investigations of Bicyclic  $\alpha$ -methylene- $\delta$ -valerolactones

**P.06.04.4(C281.108)** | M. Krishnaiah: Conformation of Dioxaphosphorin Ring – Structures of 6-Substituted

Benzo and Dibenzo [d,f] [1,3,2] Dioxaphosphorin 6-oxide (I) and Sulphide (II).

**P.06.04.5(C281.109)** | G. Pavlović: N-isopropylamidino-substituted Derivatives of Benzo[b]thiophene-2-carboxanilides and Benzo[b]thieno[2,3- c]quinolones: DNA Binding by Intercalation

**P.06.04.6(C282.110)** | K. Shinashi: Photooxygenation of Rubrene (5,6,11,12-tetraphenylnaphthacene)

**P.06.04.7(C282.111)** | A. Florence: Deuterium Isotope Effect on the Crystal Structures of Pyrene: a Lab XRPD Study

## 5. Fullerenes and Carbon Cages

**P.06.05.1(C282.112)** | K. Bouchouit: Single Crystal and the Third Order non-linear of the Adeninium Dimitrate

**P.06.05.2(C282.113)** | L. Marques: In-situ Diffraction Study of C<sub>60</sub> Polymerization under High-pressure High-temperature

## 6. Supramolecular Assemblies

**P.06.06.1(C282.114)** | N. Báthori: *Ortho*-halogeno Piedforts

**P.06.06.2(C283.115)** | M. Botoshansky: Crystal Structure of Some Representatives of Fluorenonocrownophanes

**P.06.06.3(C283.116)** | D. Bescrovny: Crystal Structure of Isosteviol and its Derivatives

**P.06.06.4(C283.117)** | G. Ramon: Inclusion Compounds from a Decomposing Host: a Cautionary Tale

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

**P.06.06.5(C283.118)** | L. Randaccio: Design and Crystallographic Characterization of Multi-Porphyrins Complexes

**P.06.06.6(C284.119)** | B. Bialonska: Strychnine and Brucine Self-Assemblies: Structures and Properties

**P.06.06.7(C284.120)** | D. Chopra: Polymorphism in an Anti-implantation Agent: A Subtle Interplay of Weak Intermolecular Interactions

**P.06.06.8(C284.121)** | A. Kalman: Morphotropism: A Link Between the Similarity and Polymorphism of Organic Crystals

**P.06.06.9(C284.122)** | B. Tashkhodjaev: The Crystal Structural Variety of Tricyclic Quinazoline Salts

**P.06.06.10(C284.123)** | T. Borowiak: Macrocyclic Amines and Their Adducts with Acids

**P.06.06.11(C285.124)** | C. Tedesco: Calix[4]dihydroquinone as Building Blocks in Supramolecular Chemistry

**P.06.06.12(C285.125)** | O. V. Shishkin: Molecular and Crystal Structure of Crown Ethers Containing Biphenyl Fragment

**P.06.06.13(C285.126)** | K. Ejsmont: Experimental and Theoretical Evaluation of N-H...O Hydrogen Bonds in Alkylamine Oxalate Crystals

**P.06.06.14(C285.127)** | J. Chisholm: Extended Hydrogen Bond Patterns in Small Molecule Crystal Structures: a CSD study

**P.06.06.15(C286.128)** | A. C. Bényei: New Class of

Compounds: Quinoidal Tetrazines

**P.06.06.16(C286.129)** | A. J. Edwards: Rings, Restraints and Resolving the Superbowl in CRYSTALS

**P.06.06.17(C286.130)** | T. Gelbrich: Familial Relationships in Molecular Crystal Structures

**P.06.06.18(C286.131)** | R. K. R. Jetti: Supramolecular Synthesis of Caffeine Solvates and Cocrystals

**P.06.06.19(C287.132)** | A. N. Sobolev: Exploiting Phenyl Embraces and δ-stacking in the Assembly of Supramolecular Arrays of Tetraphenylphosphonium and p-sulfonatocalix[n]arene (n=4,6,8)

## 10. No sub theme

**P.06.10.1(C290.133)** | C. M. Sayil: Crystal Structure and Properties of a Tetrakis(tert-butylthio) Butatriene Compound

**P.06.10.2(C290.134)** | N. G. Deniz: Crystal Structure of a Tetrakis(4-chlorophenylthio) Butatriene Compound

**P.06.10.3(C290.135)** | H. B. Napolitano: Structural Insights of a Potential Inhibition against Leishmania Major

**P.06.10.4(C290.136)** | C. Schauerte: Crystal Structures of *trans*- and *cis*-octenes

**P.06.10.5(C291.137)** | N. Marchini: Influence of the p-substituent for the Diastereomeric Resolution of Carboxylic Acids

**P.06.10.6(C291.138)** | A. A. Pimenta Jr.: Structure by 2D NMR and X-ray crystallography of a Triterpene from *M. imbricate*

**P.06.10.7(C291.139)** | J. Duskova: The Structure Characterization of Molecules with ESR Spin Labels of Pyrrole and Piperidine Type

**P.06.10.8(C291.140)** | J. Montejo Bernardo: Crystallization of the Azithromycin 11,12-hydrogenborate. Can we Have the Control?

**P.06.10.9(C292.141)** | T. R. Welberry: Modelling Disorder in 3,3'-dimethoxybenzil, C<sub>16</sub>H<sub>14</sub>O<sub>4</sub>.

**P.06.10.10(C292.142)** | M. Rafilovich: Serendipitous Rediscovery of Three Polymorphs of Benzidine

**P.06.10.11(C292.143)** | A. Ozek: Structures of Some Hydroxynaphthaldehyde Schiff Bases

**P.06.10.12(C292.144)** | A. F. Jensen: Two Polymorphs - Which One is Stable at Ambient Conditions?

**P.06.10.13(C293.146)** | A. Uchida: Epimerization of α-amino nitriles to single stereoisomers in the solid state

**P.06.10.14(C293.147)** | M. Dincer: Two oxime derivatives including succinimid and morpholin groups

**P.06.10.15(C293.148)** | A. Erdönmez: 3-Methoxy-5-(4-methylphenyldiazenyl) Salicylaldehyde and 3-methoxy-5-(2-methylphenyldiazenyl) Salicylaldehyde

**P.06.10.16(C293.149)** | K. V. A. Gowda: Crystal Structure of 2-cyclohexyl-5-formyl-6-(4-bromophenyl)imidazo[2,1-b] [1,3,4] Thiadiazole

**P.06.10.17(C293.150)** | O. Au-Alvarez: Structure of 2-[4-(Dimethylamino)phenyl]-4,5-diphenyl-1H-imidazole Isopropanol Solvate

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

**P.06.10.18(C294.151)** | I. Svoboda: Substituents at Oxygen Influence N,O-Distances in Thiohydroxamates

**P.06.10.19(C294.152)** | J. A. Beukes: X-ray Induced Radiation Damage in Taurine – a Combined X-ray and Raman Study

**P.06.10.20(C294.153)** | F. Ozkok: Crystal Structure of 2-Nitro-3,4,4-trichloro-1-mono(dodecyl thio)-1-mono([(4-fluorophenyl)piperazine]-1,3-butadiene Compound

## 07 CRYSTALLOGRAPHY OF ORGANOMETALLIC, COORDINATION AND MAIN GROUP COMPOUNDS

### 7. Bio-inorganic Structures

**P.07.07.3(C311.154)** | J. Lennon: Palladium(II) and Platinum(II) Complexes with Tridentate Iminophosphine Ligands and their Phosphine Derivatives; Synthesis and Structural Studies

## 08 STRUCTURE/PROPERTY RELATIONSHIP

### 7. Analysis of Atomic Displacement Parameters

**P.08.07.1(C328.155)** | T. Areé: Atomic Displacement Parameters and Specific Heat of *p*-Dichlorobenzene Polymorphs between 10 and 230 K

**P.08.07.2(C328.156)** | T. Luthi Nyffeler: Anisotropic Displacement Parameters for Normal Mode Analysis: Which Refinement is Needed?

### 8. Intermolecular Interactions

**P.08.08.1(C328.157)** | V. D. Danchuk: Intermolecular Interaction and Molecular Dynamics in Carboxylic Acid Crystals

**P.08.08.2(C328.158)** | A. Zakrassov: Synthesis, Crystal Structures and Dielectric Properties of the Novel Linear High k Molecular Materials

**P.08.08.3(C329.159)** | M. Podsiadlo: Cl–Cl Interactions in Dichloromethane

**P.08.08.4(C329.160)** | W. H. Ojala: Molecular Packing Preferences of “Bridge-Flipped” Isomeric Molecules

**P.08.08.5(C329.161)** | A. P. Kuzin: A Conserved Core in the SufE Sulfur-acceptor Protein Mediates Interdomain Interactions in Variety of Redox Protein Complexes

**P.08.08.6(C329.162)** | P. W. Codding: Halogen-substituted Drugs and their Intermolecular Interactions

**P.08.08.7(C330.163)** | W.-C. Wang: Increasing Thermostability of N-carbamoyl-D-amino Acid Amidohydrolase by Introducing Additional Intermolecular Disulfide Bridges

**P.08.08.8(C330.164)** | C. Besnard: How Close Can Halogen Atoms Get in a Crystal - Triphenylmethylbromide

**P.08.08.9(C330.165)** | C. Esterhuysen: 4-membered Metallothiophosphinate Rings - Flat or Puckered?

**P.08.08.10(C330.166)** | S. Chatziefthimiou: Keto Forms in Schiff Bases of Salicylaldehydes: Structural and Theoretical Aspects

**P.08.08.11(C330.167)** | K. Ogawa: Role of Self-Association in Proton Tautomerism of Salicylideneanilines

**P.08.08.12(C331.168)** | H. Koizumi: The First Observation

of All Six Elastic Constants in Tetragonal Hen Egg-white Lysozyme Crystals

**P.08.08.13(C331.169)** | I. Wolska: 5,5'-Disubstituted-3,3'-Methanediyl-*bis*-Indoles as Potential Antitumorals

**P.08.08.14(C331.170)** | I. Sainz-Diaz: Intermolecular Interactions in 1,1'-Binaphthyl, Polymorphs and Symmetry Breaking

**P.08.08.15(C331.171)** | B. Civalleri: Experimental and Theoretical Study of Weak Interactions in Simple Molecular Solids

**P.08.08.16(C332.172)** | V. B. Medakovic: Orientations of Axially Coordinated Ligands in Model Systems of Cytochromes

**P.08.08.17(C332.173)** | M. K. Milcic: CH/π Interactions between Chelate and Phenyl Rings in Acetylacetone Complexes

### 13. Hydrogen Bonding Studies

**P.08.13.1(C338.174)** | G. Gilli: The Nature of the HB. 1. HB Empirical Rules from Crystal Structure Correlations

**P.08.13.2(C338.175)** | L. Pretto: The Nature of the HB. 2. Predicting HB Strength by the pKa Slide Rule

**P.08.13.3(C339.176)** | C. K. Spanswick: Proton Migration In Hydrogen Bonded Donor-Acceptor Complexes

**P.08.13.4(C339.177)** | M. Adam: Multi-temperature Neutron & X-ray Studies of Hydrogen Bonded Molecular Complexes

**P.08.13.5(C339.178)** | E. Bartoszak-Adamska: Proton

# WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION

Sponges of 1,2-Bis(di-*R*-aminomethyl)benzene Type

**P.08.13.6(C339.179)** | Y. Cai: Ordering of Hydrogen Bonds in High-Pressure Low-Temperature Ices

**P.08.13.7(C340.180)** | D. Semmingsen: The Crystal Structure of Tetraformylethane

**P.08.13.8(C340.181)** | C. C. Wilson: Computing the Solid-state: Novel Plane-wave DFT Approaches to Hydrogen Bonding

**P.08.13.9(C340.182)** | C. Bazzicalupi: Conformational Database Study on the Intramolecular NH<sup>+</sup>-δ Interaction

## 09 CRYSTAL ENGINEERING

### 1. General Applications and Strategy

**P.09.01.1(C353.183)** | P. Gavan: Investigating Weak Interactions in Pharmaceutical Co-crystal Systems

**P.09.01.2(C353.184)** | C. B. Aakerøy: Design and Synthesis of Co-crystals: From Molecular Sense to Supramolecular Sensibility

**P.09.01.3(C353.185)** | M. Rademeyer: Crystal Engineering of Arylammonium Perhalometallates

**P.09.01.4(C353.186)** | S.-J. Fu: Towards Electrochemical Artificial Muscles: A Supramolecular Machine Based on One-Dimensional Copper-containing Organophosphonate System

### 2. Organic Compounds

**P.09.02.1(C353.187)** | S. F. Alshahateet: Molecularly Designed Functional Materials; Can We Really Control

their Supramolecularity?

**P.09.02.2(C354.188)** | M. A. Hyacinth: Interactions of Supramolecular Synths Formed by Secondary Propargylic Alcohols

**P.09.02.3(C354.189)** | K. N. Lehane: Stereochemistry in Crystal Engineering

**P.09.02.4(C354.190)** | G. M. Rosair: Ringing the Changes with Tetrazole: Hydrogen Bonding Studies

**P.09.02.5(C354.191)** | A. Criado: Structure of *N,N*-dimethylaminopyridinium *L*-malate

**P.09.02.6(C354.192)** | E. Marfo-Owusu: Complexes of Non-chiral Surfactant Molecules with Chiral and Racemic Compounds

**P.09.02.7(C355.193)** | A. Višnjevac: Spontaneous Resolution of *N*-sulfonylpurimidine Compounds Induced by Chemical Modification

### 3. Inorganic Compounds

**P.09.03.7(C356.194)** | L. Brammer: Highly Fluorinated Silver Carboxylate Layered Structures

### 4. Organometallic Complexes

**P.09.04.7(C359.195)** | H. Stoeckli-Evans: Trisiloxane-Diols and Cyclosiloxanes with Bulky Substituents on the Si Atoms

### 7. No Sub-theme

**P.09.07.1(C365.196)** | E. Pidcock: Crystal Packing:

Molecular Shape and Intermolecular Interactions

## 10 INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES 6. Zeolites (Natural and Synthetic)

**P.10.06.8(C382.197)** | T. M. Gesing: Gallium Substitution in Alumosilicate Halide Soda-lites

**P.10.06.9(C382.198)** | C. H. Rüscher: Na/K and Na/Li Substituted Aluminosilicate Nitrate Cancrinites

## 12 SURFACES, INTERFACES, LIQUIDS AND THIN FILMS

### 4. X-ray Reflectivity: Instrumentation and Applications

**P.12.04.1(C410.199)** | A. Kryazhev: The X-ray Reflectometry and the Phase Contrast Methods for Crystal Analysis

### 7. Small Angle Scattering

**P.12.07.1(C411.200)** | P. Konarev: ATSAS 2.1 - A Program Suite for Small-angle Scattering Data Analysis

**P.12.07.2(C411.201)** | A. Sokolova: Probing Intermediate Filament Structure and Assembly with Small-angle X-ray Scattering

**P.12.07.3(C411.202)** | R. Lazzari: Grazing Incidence Small Angle X-Ray Scattering from Nanoparticles : Beyond Classical Analysis Approximations

**P.12.07.4(C412.203)** | M. Sztucki: USAXS: A Tool to Probe the Structure and Dynamics of Complex Fluids

**P.12.07.5(C412.204)** | U-S. Jeng: Anomalous SAXS and WAXS for the Structure of Pt/Ru Catalyst Nanoparticles

## **WEDNESDAY, AUGUST 24, 2005 – POSTER SESSION**

**P.12.07.6(C412.205)** | A. J. Allen: Interface Structure in Solid Oxide Fuel Cells by Anomalous/High-Energy SAXS/WAXS

**P.12.07.7(C412.206)** | I. L. Torriani: Structural SAXS Studies of the Human Amyloid Precursor Protein

### **8. Diffuse Scattering**

**P.12.08.1(C412.207)** | C. Steiner: Diffuse scattering of Pt-Rh in Grazing Incidence

### **10. Micelles**

**P.12.10.1(C413.208)** | S. Vass: Shape, Polydispersity and Aggregation Number of Alkyl Sulphate Micelles

### **13. No Sub-theme**

**P.12.13.1(C416.209)** | Y. Frenkel: Hydrophobic Drug Aggregates: Structure and Biology

**P.12.13.2(C416.210)** | A. E. Smith: A First Principles Study of Stacking Fault and Surface Energies in Magnesium

## **28 ART, CULTURAL HERITAGE AND CRYSTALLOGRAPHY**

### **2. Crystallography and Art**

**P.28.02.1(C493.211)** | E. Lemus-Fuentes: Stained Glass of Crystals

**P.28.02.2(C493.212)** | W. Depmeier: Crystallography and Art in Kiel, and elsewhere

**P.28.02.3(C493.213)** | C. Temperini: Knowledge and Art from Crystallography Images

**P.28.02.4(C494.214)** | N. Benali-Cherif: Symmetry in the Life of the Aurès Chaouia Tribes (Algeria)

**P.28.02.5(C494.215)** | H. Schenk: The Production History of Naples Yellow and the Discoloration of the Blue Pigment Smalt

**THURSDAY, AUGUST 25, 2005 – KEYNOTE LECTURES****MORNING SESSION 8.30-9.30**

Michelangelo (**KN 5**)

**KN05.25(C1)** | David Sayre:  
Single-particle Diffraction

*Chair:* John Spence

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Botticelli (**KN 6**)

**KN06.25(C1)** | Lynne Mc Cusker:  
Elucidating the Structures of Nanoporous  
Microcrystals

*Chair:* Reinhard Fischer

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Cimabue (**KN 7**)

**KN07.25(C2)** | Vaclav Petricek:  
Structure Analysis of Modulated Crystals: Trends and  
Tendencies

*Chair:* Ray L. Withers

**AFTERNOON SESSION 17.30-18.30**

Michelangelo (**KN 8**)

**KN08.25(C2)** | Raymond Stevens:  
High Throughput Technologies in Structural Biology

*Chair:* Mamannamana Vijayan

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Botticelli (**KN 9**)

**KN09.25(C2)** | Peter Stephens:  
Structure Solution of Pharmaceutical Compounds  
from Powder Diffraction Data

*Chair:* Kenneth Shankland

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Cimabue (**KN 10**)

**KN10.25(C2)** | Akiji Yamamoto:  
Quasicrystal Structure Analysis. The State of the Art

*Chair:* Marc De Boissieu

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# THURSDAY, AUGUST 25 2005 - MORNING - MICROSYMPOSIA

TIME	Michelangelo ( <i>MS 15</i> )	Donatello ( <i>MS 16</i> )	Botticelli ( <i>MS 17</i> )
10.00-10.05 Opening Remarks	<b>THE BIG QUESTION IN STRUCTURAL GENOMICS: GETTING FUNCTION FROM STRUCTURE</b> <i>Chairs: S.-H. Kim, E. N. Baker</i>	<b>HIGH RESOLUTION X-RAY INELASTIC SCATTERING</b> <i>Chairs: G. C. Ruocco, A. Baron</i>	<b>NON-COVALENT INTERACTIONS IN CRYSTALS OF SMALL MOLECULES AND MACRO-MOLECULES</b> <i>Chairs: G. R. Desiraju, M. Jaskolski</i>
10.05-10.35	<b>MS15.25.1(C25)</b>   <u>W. Shepard</u> : Crystal Structure of Rv0813c Reveals a New Family of Putative FABPs	<b>MS16.25.1(C26)</b>   <u>D. Fioretto</u> : Dynamics of Glassy Materials by High Resolution Inelastic X-ray Scattering	<b>MS17.25.1(C27)</b>   <u>F. Diederich</u> : Multipolar Interactions in Structural Chemistry and Biology
10.35-11.05	<b>MS15.25.2(C25)</b>   <u>O. Herzberg</u> : Chasing the Function of Hypothetical Proteins	<b>MS16.25.2(C26)</b>   <u>S. Hosokawa</u> : Collective Dynamics of Liquid Metals: from Simple to Extremely Non-Simple	<b>MS17.25.2(C27)</b>   <u>F. H. Allen</u> : Carbonyl...Carbonyl Interactions are Structurally Ubiquitous and Important
11.05-11.35	<b>MS15.25.3(C25)</b>   <u>J. Joseph</u> : Functional & Structural Proteomics of SARS: Defining a Rational Response to Emerging Diseases	<b>MS16.25.3(C26)</b>   <u>J. T. Sage</u> : Vibrational Dynamics of Iron in Proteins	<b>MS17.25.3(C27)</b>   <u>A. Schmidt</u> : Small Molecules and Macromolecules Make Contact: Messages from Protein structures to atomic resolution
11.35-12.05	<b>MS15.25.4(C25)</b>   <u>S. Kuramitsu</u> : Whole-Cell Project of <i>Thermus Thermophilus</i> HB8 toward Atomic-Resolution Biology	<b>MS16.25.4(C26)</b>   <u>G. Fiquet</u> : High-Resolution Inelastic X-ray Scattering of Materials of Geophysical Interest	<b>MS17.25.4(C28)</b>   <u>M. Egli</u> : Protein-Protein Interactions in the Cyanobacterial KaiABC Circadian Clock
12.05-12.35	<b>MS15.25.5(C26)</b>   <u>A. Edwards</u> : Structural Proteomics: A Rich Source of Purified Proteins for Functional Assays	<b>MS16.25.5(C27)</b>   <u>J. Wong</u> : Phonon Dispersions in fcc δ Pu-Ga by High Resolution Inelastic X-ray Scattering	<b>MS17.25.5(C28)</b>   <u>W. L. Duax</u> : Unusual Ion Coordination in Membrane Channels and CH Hydrogen Bonds in Enzyme Catalysis

# THURSDAY, AUGUST 25 2005 - MORNING - MICROSYMPOSIA

Giotto ( <b><i>MS 18</i></b> )	Leonardo da Vinci ( <b><i>MS 19</i></b> )	Cimabue ( <b><i>MS 20</i></b> )	Brunelleschi ( <b><i>MS 21</i></b> )
<b>POWDER DIFFRACTION ON MICRO- AND MESOPOROUS MATERIALS</b> <i>Chairs:</i> C. Baerlocher, S. Krivovichev	<b>NEWS FROM INCOMMENSURATE CRYSTALS</b> <i>Chairs:</i> S. Van Smaalen, S. Lidin	<b>ADVANCES IN COMPUTATIONAL METHODS FOR SMALL MOLECULE CRYSTALLOGRAPHY</b> <i>Chairs:</i> S. Parsons, L. Cascarano <b>(Dedicated to the late Prof. Nardelli)</b>	<b>BASIC TO INDUSTRIAL APPLICATIONS OF STRESS AND STRAIN ANALYSES WITH SYNCHROTRON AND NEUTRON RADIATIONS</b> <i>Chairs:</i> A. Lodini, L. Edwards
<b>MS18.25.1(C28)   K. G. Strohmaier:</b> Structure Determination of Zeolites: Making All the Pieces Fit	<b>MS19.25.1(C29)   D. Fredrickson:</b> Nowotny Chimney Ladders and Giant Cubic Structures: Electron Driven Interfaces	<b>MS20.25.1(C31)   C. Giacovazzo:</b> Phasing via Full Pattern Powder Decomposition by Monte Carlo and Patterson Methods	<b>MS21.25.1(C32)   M. Daymond:</b> Insights into Deformation Mechanisms from in-situ Diffraction Experiments
<b>MS18.25.2(C28)   J. Rocha:</b> Structural Characterisation and Properties of New Microporous Materials	<b>MS19.25.2(C30)   J. M. Perez-Mato:</b> Ordering as Occupational Modulations, and their Superspace Description	<b>MS20.25.2(C31)   G. Oszlanyi:</b> Ab-initio Structure Solution without the Use of Atomicity	<b>MS21.25.2(C32)   M. Fitzpatrick:</b> Strain Mapping Methods and Instruments: Recent Advances and Future Implications
<b>MS18.25.3(C29)   J.-L. Hodeau:</b> Direct Localization of Atoms in Nanoporous Powders by Resonant Contrast Diffraction	<b>MS19.25.3(C30)   R. Withers:</b> Flexible Local Crystal Chemistry and its (Modulated) Consequences	<b>MS20.25.3(C31)   K. Okada:</b> A DS5 (Direct-Searcher Automatic System Version 5) Program for Small Molecules Running on Windows PCs	<b>MS21.25.3(C32)   J.-M. Sprauel:</b> Contribution of Numerical Simulation to Stress Evaluation by Neutron or Synchrotron Diffraction
<b>MS18.25.4(C29)   B. Marler:</b> Structural Characterisation of Encapsulated Nanoparticles inside Mesoporous MCM-48 with XRD, TEM and EXAFS	<b>MS19.25.4(C30)   Y. Michiue:</b> Incommensurate Crystallographic Shear Structure of $\text{Ba}_x\text{Bi}_{2-2x}\text{Ti}_{4-x}\text{O}_{11-4x}$ ( $x=0.275$ )	<b>MS20.25.4(C31)   J. Evans:</b> Maximising the Information Obtainable from Diffraction Experiments	<b>MS21.25.4(C32)   M. Golshan:</b> Study of Elasto-Pastic Deformation in Mg Alloy using Synchrotron Radiation
<b>MS18.25.5(C29)   O. I. Lebedev:</b> Zeolite and MCM Nano- and Mesoporous Structures	<b>MS19.25.5(C30)   G. Borgstahl:</b> Solving Modulated Crystals of Profilin:Actin	<b>MS20.25.5(C31)   D. J. Watkin:</b> Small Molecule Crystallographic Computing – What is the Future?	<b>MS21.25.5(C33)   E. Zolotoyabko:</b> Depth-resolved Strain Measurements by Energy-variable X-ray Diffraction

**THURSDAY, AUGUST 25 2005 - AFTERNOON - MICROSYMPOSIA**

<b>TIME</b>	<b>Botticelli (MS 22)</b>	<b>Michelangelo (MS 23)</b>	<b>Giotto (MS 24)</b>
14.45-14.50 Opening Remarks	<b>SINGLE PARTICLE X-RAY DIFFRACTION IMAGING</b> <i>Chairs: J. Hajdu, H. Chapman</i>	<b>PUTTING THE PEDAL TO THE METAL: SPEEDING UP BIOLOGICAL STRUCTURE DETERMINATION</b> <i>Chairs: E. Y. Jones, P. R. Mittl</i>	<b>MOLECULAR CRYSTALS UNDER NON AMBIENT CONDITIONS</b> <i>Chairs: J.A.K. Howard, J. Cole</i>
14.50-15.20	<b>MS22.25.1(C33)   D. Shapiro:</b> Diffraction Imaging of the Yeast Cell: First Results	<b>MS23.25.1(C34)   M. A. Walsh:</b> Development of a High-throughput Structure Determination Pipeline at BM14	<b>MS24.25.1(C35)   C. Wilson:</b> Blowing Hot and Cold and its Effect on Some Crystals
15.20-15.50	<b>MS22.25.2(C33)   S. Eisebitt:</b> Imaging Magnetic Nanostructures by X-Ray Holography	<b>MS23.25.2(C34)   W.F. Anderson:</b> Automating Crystallographic Structure Determination Calculations	<b>MS24.25.2(C35)   B. Gillon:</b> Photo-induced Molecular Switching: Neutron Diffraction Studies
16.50-16.20	<b>MS22.25.3(C33)   S. Hau-Riege:</b> Prospects for X-ray Diffraction Imaging of Single Biological Molecules	<b>MS23.25.3(C34)   J. Rose:</b> HT Structure Determination at SER-CAT: Five Structures in 23 Hours	<b>MS24.25.3(C35)   Y. Ozawa:</b> Photo Excited State Crystallography of Iodo-Bridged Dicopper (I) Complex.
16.20-16.50	<b>MS22.25.4(C33)   Z. Jurek:</b> Imaging of Atom Clusters by Hard X-ray Free Electron Laser Pulses	<b>MS23.25.4(C35)   W. Minor:</b> The Integration of Data Reduction and Structure Solution - from Diffraction Images to an Initial Model in Minutes	<b>MS24.25.4(C36)   M. Y. Antipin:</b> Multitemperature X-Ray Diffraction Analysis in the Study of Phase Transitions, Molecular Dynamics and Crystal Disorder
16.50-17.20	<b>MS22.25.5(C34)   G. Huldt:</b> Three-Dimensional Data Merging of Randomly Oriented Continuous Diffraction Patterns	<b>MS23.25.5(C35)   K. S. Wilson:</b> Medium throughput Protein Crystallography: limiting Steps in the Pipeline	<b>MS24.25.5(C36)   K. Dziubek:</b> Melting-point Variation in Isomeric Dibromobenzenes

# THURSDAY, AUGUST 25 2005 – AFTERNOON - MICROSYMPOSIA

Cimabue ( <b>MS 25</b> )	Leonardo da Vinci ( <b>MS 26</b> )	Brunelleschi ( <b>MS 27</b> )	Donatello ( <b>MS 28</b> )
<b>STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA (ORGANICS)</b> <i>Chairs: A. Fitch, J. Faber</i>	<b>RECENT ADVANCES IN QUASICRYSTAL RESEARCH</b> <i>Chairs: K. Saitoh, R. Lifshitz</i>	<b>DETECTORS: DEVELOPMENTS AND REQUIREMENTS FOR X-RAY, SYNCHROTRON AND NEUTRON SOURCES</b> <i>Chairs: N. Yagi, C. Broennimann</i>	<b>STRUCTURE/PROPERTIES RELATIONSHIPS OF TECHNOLOGICALLY RELEVANT INORGANIC AND MINERAL COMPOUNDS</b> <i>Chairs: J. Rocha, A. Gualtieri</i>
<b>MS25.25.1(C36)</b>   <u>V. Favre-Nicolin</u> : Solving Organic Structures from Powder Diffraction: News from the FOX	<b>MS26.25.1(C37)</b>   <u>R. McGrath</u> : Fabricating Novel Symmetry Nanoscale Systems using Quasicrystal Surfaces	<b>MS27.25.1(C38)</b>   <u>B. Gebauer</u> : Development of Very-high Rate and Resolution Neutron Detectors in DETNI	<b>MS28.25.1(C40)</b>   <u>B. Grobety</u> : Chrysotile, a Naturally Occurring Nanotube Material
<b>MS25.25.2(C36)</b>   <u>V.V. Chernyshev</u> : Molecular Structures from Low-Resolution Powder Diffraction Data: Reliability and Validation of the Results	<b>MS26.25.2(C38)</b>   <u>Z. Papadopoulos</u> : Maximum or Minimum Density Principle Determines the Bulk Terminations of Quasicrystals?	<b>MS27.25.2(C39)</b>   <u>J. Hendrix</u> : A Direct-Conversion Se-Based 2D-Detector for Protein Crystallography	<b>MS28.25.2(C40)</b>   <u>F. Taulelle</u> : Solid State NMR Crystallography of Inorganic Materials
<b>MS25.25.3(C37)</b>   <u>C. Liang</u> : Close Contact Penalty Functions In Direct Space Methods and Energetic Considerations in Structure Refinement	<b>MS26.25.3(C38)</b>   <u>M. de Boissieu</u> : Diffuse Scattering and Phasons in the i-Zn-Mg-Sc Phase and its 1/1 Approximant	<b>MS27.25.3(C39)</b>   <u>G. S. Huelsen</u> : Protein Crystallography with the PILATUS 1M Detector	<b>MS28.25.3(C40)</b>   <u>C. Lamberti</u> : Combined XRPD and Spectroscopic Study of Molecules Hosted in Zeolitic Channels
<b>MS25.25.4(C37)</b>   <u>P. Fernandes</u> : Differential Thermal Expansion and Laboratory Capillary X-ray Powder Diffraction: Progress, Practicalities and Performance	<b>MS26.25.4(C38)</b>   <u>G. Krauss</u> : A High Pressure High Temperature Study of Co-rich d-Al-Co-Ni	<b>MS27.25.4(C39)</b>   <u>R. Durst</u> : A New High-Speed, Photon-Counting X-Ray Area Detector	<b>MS28.25.4(C40)</b>   <u>J. M. Delgado</u> : Diffraction Study of the Semiconducting Cu <sub>2</sub> (Se,Te) <sub>3</sub> -(Ga,In) <sub>2</sub> (Se,Te) <sub>3</sub> Systems
<b>MS25.25.5(C37)</b>   <u>K. Shankland</u> : Rapid Structure Solution using Global Optimisation and Distributed Computing	<b>MS26.25.5(C38)</b>   <u>Y. Matsushita</u> : Mesoscopic Archimedean Tilings in Polymeric Stars	<b>MS27.25.5(C39)</b>   <u>D. Laundy</u> : Dead-time in X-ray Photon Counting Detectors	<b>MS28.25.5(C41)</b>   <u>M. Moore</u> : The Growth and Morphology of Diamond Crystals

## **THURSDAY, AUGUST 25 2005 – OTHER ACTIVITIES**

### **OPEN COMMISSION MEETINGS**

Giotto (12.35-14.35)

#### **OCM02 COMMISSION ON JOURNALS (II)**

*Chair: John Helliwell*

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#### **OCM02.25.1(CI26) | P. Strickland:**

Getting the Best out of IUCr Journals (Practical Advice and Demonstrations)

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#### **COMPUTER FAYRE** Ghirlandaio

(10.30-12.00)      R. E. Dinnebier:

Powder3D - Freely Available Software, a Program for Multi-Pattern Data Reduction and Graphical Presentation

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#### (14.30-17.00)      S. Billinge:

DANSE Software Demonstration. (Distributed Data Analysis for Neutron Scattering Experiments)

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### **IUCr GENERAL ASSEMBLY**

Cimabue (19.00-22.00)

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

## 02 METHODS FOR STRUCTURE DETERMINATION

### 1. Difficult Structure

**P.02.01.1(C151.1)** | J. Nan: Ab-initio Structure Determination of SMU.440 Protein from Streptococcus mutans

**P.02.01.2(C151.2)** | A. Heine: X-ray Structure Determination of Hydroxyphenylpyruvate Reductase at 1.47Å Resolution

### 3. Maximum Entropy Methods

**P.02.03.1(C152.3)** | M. Tanaka: Electron Density of ScRh3Bx: Relation of the Electron Density to the Hardness

## 11. Ab initio Powder Diffraction Solutions: Molecular Compounds

**P.02.11.1(C157.4)** | B. Dacunha: Powder Struture Resolution of 1,7-dioxaspiro[4.4]nonane

**P.02.11.2(C157.5)** | E. Nishibori: The Structure Determination of Single-component Molecular-metal.

**P.02.11.3(C157.6)** | H.-S. Sheu: Ab-initio Structure Determination of C18H19N4S from Powder X-Ray Diffraction

**P.02.11.4(C157.7)** | A. Fitch: Structure Determination from Powder Data of Two Sub-peptides of Leu-enkephalin

**P.02.11.5(C157.8)** | W. Lasocha: Crystal Structures of 8-Styrylxanthine Analogs from Powder Diffractin Data

## 03 COMPUTERS IN ANALYSIS, MOLECULAR MODELLING AND MOLECULAR DESIGN

### 1. Programs for Refinement and Analysis

**P.03.01.1(C163.9)** | Y. Zhou: Lafire: a Software for Automatic Protein Structure Refinement

**P.03.01.2(C163.10)** | B. Hinrichsen: Powder3D: Towards Automatic Image Plate Analysis

**P.03.01.3(C163.11)** | J. Ondracek: HipHop. A Novel Refinement Method for Protein Structures

**P.03.01.4(C163.12)** | V. Piskarov: Deconvolution of X-ray Diffraction Profile by Using the Regularization Technique

**P.03.01.5(C163.13)** | S. Pantos: Faster Least-Squares Refinement of Larger Molecules Using the Program CRYSTALS

**P.03.01.6(C164.14)** | A. Guagliardi: Whole Powder Pattern Fitting Methods Focused on Nanocrystalline Materials

**P.03.01.7(C164.15)** | H. Puschmann: Automatic Element Assignment and Model Completion for Small Molecule Structures

**P.03.01.8(C164.16)** | M. Gutmann: SXD2001 - a Program for Treating Data from TOF Neutron Single-crystal Diffraction

**P.03.01.9(C164.17)** | T. Degen: Phase Mixture Detection by Fuzzy Clustering of X-ray Powder Diffraction Data

### 3. Graphics and Virtual Reality

**P.03.03.1(C165.18)** | J. Gonzalez-Platas: EdMol: a Graphical Molecular Editor

**P.03.03.2(C165.19)** | M. Kroeker: DRAWxtl 5.1 - A Multi-Platform Computer Program to Display Crystal Structures

### 12. No Sub-theme

**P.03.12.1(C169.20)** | I. Baburin: Sizes of Molecules in Organic Crystals: the Voronoi-Dirichlet Approach

**P.03.12.2(C169.21)** | F. White: The Rational Design of Molecules for Use as Friction Modifiers

**P.03.12.3(C169.22)** | R. Pai: Identifying NCS: a Pattern Recognition Approach

**P.03.12.4(C170.23)** | Y. Tsuchiya: Structural Classification and Analysis of Homo Oligomer Interfaces of Proteins

**P.03.12.5(C170.24)** | M. Zehnder: Monte-Carlo Simulations of Radiation Damage Produced in Protein Crystals

**P.03.12.6(C170.25)** | A. Pähler: Visualization of Structural Information with xPSSS

**P.03.12.7(C170.26)** | E. Germaneau: Monte-Carlo Simulation of the Incommensurate Structure of 4,4'-azoxyphenetole

**04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES**

### 5. Nucleic Acids

**P.04.05.1(C218.27)** | S. Yoshiteru: Preliminary X-ray Analysis of RNA Oligomers Containing CUG Repeats

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

<p><b>P.04.05.2(C218.28)</b>   <u>A. Adams</u>: Crystal Structures of Two Minor Groove Binders Complexed with d(CGCGAATTGCG)2</p>	<p><b>P.04.06.5(C221.39)</b>   <u>C. Creze</u>: Structural Study of the Nucleolin-G-quartet Complex</p>	<p><b>P.04.06.16(C223.50)</b>   <u>J. Murray-Rust</u>: Structure of XPF Endonuclease from <i>A. pernix</i></p>
<p><b>P.04.05.3(C218.29)</b>   <u>P. D. Pytel</u>: A New Highly Symmetric DNA G-4 Quadruplex/Drug Structure</p>	<p><b>P.04.06.6(C221.40)</b>   <u>H. Hashimoto</u>: Crystal Structure of DNA Polymerase from Bacteriophage M2</p>	<p><b>P.04.06.17(C224.51)</b>   <u>C.-H. Pai</u>: Structural Study of DNA Binding Protein pdcd5 from <i>Sulfolobus solfataricus</i></p>
<p><b>P.04.05.4(C219.30)</b>   <u>S. Miles</u>: Structural Studies on Acridine Derivatives Binding to Telomeric DNA</p>	<p><b>P.04.06.7(C221.41)</b>   <u>C.-Y. Chen</u>: The Role of Water in Protein-DNA Complexes from High Resolution X-ray Crystallography</p>	<p><b>P.04.06.18(C224.52)</b>   <u>J. A. Cuesta-Seijo</u>: Serendipitous SAD Phasing</p>
<p><b>P.04.05.5(C219.31)</b>   <u>J. Kondo</u>: Crystallographic Studies of <i>Homo sapiens</i> A-sites Complexed with Aminoglycosides</p>	<p><b>P.04.06.8(C221.42)</b>   <u>C.-D. Hsiao</u>: Crystal Structure of PriB – a Primosomal DNA Replication Protein of <i>E. coli</i></p>	<p><b>P.04.06.19(C224.53)</b>   <u>O. Barabas</u>: Altered Structure and Function of a Beta-retroviral dUTPase</p>
<p><b>P.04.05.6(C219.32)</b>   <u>M. Tsunoda</u>: X-Ray Analyses of DNA Dodecamers Containing 2'-Deoxy-5-formyluridine</p>	<p><b>P.04.06.9(C222.43)</b>   <u>R. Fedorov</u>: Structure of a Dimeric Single-stranded DNA Binding Protein from <i>Thermus aquaticus</i></p>	<h3>7. Protein - RNA Interactions</h3>
<p><b>P.04.05.7(C219.33)</b>   <u>K. Van Hecke</u>: A 1.1 Binding Mode for Netropsin in the Minor Groove of d(GGCCAATTGG)</p>	<p><b>P.04.06.10(C222.44)</b>   <u>M. Shirakawa</u>: Crystal Structure of SUMO1-conjugated Thymine DNA Glycosylase</p>	<p><b>P.04.07.1(C224.54)</b>   <u>M. Konno</u>: Y225F/A for Met-tRNA Synthetase Reveals Importance of Hydrophobic Circumstance</p>
<p><b>P.04.05.8(C220.34)</b>   <u>K. Robeyns</u>: Cyclohexene Oligonucleotides: Structure of the L-CeNA Sequence GTGTACAC</p>	<p><b>P.04.06.11(C222.45)</b>   <u>J. Timmins</u>: Crystal Structure of <i>Deinococcus radiodurans</i> RecO</p>	<p><b>P.04.07.2(C225.55)</b>   <u>M. Roe</u>: Insights into mRNA Recognition from a PIWI-siRNA Complex</p>
<h3>6. Protein - DNA Interactions</h3>	<p><b>P.04.06.12(C222.46)</b>   <u>D. Baba</u>: Crystal Structure of SUMO2-conjugated Thymine DNA Glycosylase</p>	<p><b>P.04.07.4(C225.56)</b>   <u>S. Bilokapic</u>: Structure and Function of Unusual Archaeal Serly-tRNA Synthetases</p>
<p><b>P.04.06.1(C220.35)</b>   <u>E. Hooley</u>: Detection of 8-hydroxy-2'deoxyadenosine and 8-hydroxy-2'deoxyguanosine by Avidin</p>	<p><b>P.04.06.13(C223.47)</b>   <u>T. Shimizu</u>: Crystal Structure of Leucine Zipper Protein Hy5 Complexed with DNA</p>	<p><b>P.04.07.5(C225.57)</b>   <u>B. Gomes Guimaraes</u>: Crystallographic and Functional Studies of Nip7 a Conserved Protein Involved in pre-rRNA Processing</p>
<p><b>P.04.06.2(C220.36)</b>   <u>S. Russi</u>: Unveiling the DNA Strand Transfer-mechanism of Relaxase TrwC</p>	<p><b>P.04.06.14(C223.48)</b>   <u>T. Imasaki</u>: Crystal Structures of Restriction Endonuclease EcoO109I DNA Bound to Divalent Metal</p>	<h3>8. Protein Design and Engineering</h3>
<p><b>P.04.06.3(C220.37)</b>   <u>Q. Zhao</u>: Crystal Structure and Function of Human Spindlin1</p>	<p><b>P.04.06.15(C223.49)</b>   <u>R. Huether</u>: Sense/Antisense Open Reading Frames and the Amino Acid Composition of Ribosomal Proteins</p>	<p><b>P.04.08.1(C226.59)</b>   <u>F. Meneghetti</u>: Crystal Structures of <i>ox</i> and <i>sq</i> S64C Flavodoxin (<i>D. vulgaris</i>) Monomer and Dimer</p>
<p><b>P.04.06.4(C220.38)</b>   <u>E. Struble</u>: The Structure of λ O Protein Fragment Provides Insights About Replisome Assembly</p>		<p><b>P.04.08.2(C226.60)</b>   <u>J. K. Dattagupta</u>: Role of a Scaffold in the Inhibitory Process of a Serine Protease Inhibitor</p>
<p><b>B22</b></p>		<p><b>P.04.08.3(C226.61)</b>   <u>C. Meramveliotaki</u>: Structure</p>

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

Determination of scPvuII by Crystallographic and SAXS Methods

**P.04.08.4(C226.62)** | M. Archer: Structure of NADH: Quinone Oxidoreductase from *Acidianus ambivalens*: Electron Entry Point of Aerobic Respiratory Chain

## 9. Protein Biosynthesis

**P.04.09.1(C226.63)** | K. Suzuki: X-Ray Structural Analysis of Carbonic Anhydrase from *Chlamydomonas reinhardtii*

**P.04.09.2(C227.64)** | T. Sekiguchi: Crystallographic Study of Fructokinase from *Sulfolobus tokodaii* Strain 7

**P.04.09.3(C227.65)** | M. Yao: Crystal Structure of Translation Initiation Factor IF2 $\beta$ -IF2 $\gamma$  Complex

**P.04.09.4(C227.66)** | S. Hansson: Fusidic Acid Resistance and Sensitivity in Ribosomal Elongation Factor G

**P.04.09.5(C227.67)** | L. Jenner: The *thrS* Messenger Path on the Ribosome

**P.04.09.6(C227.68)** | R. Berisio: Productive and Non-productive Binding of Polyketides to the Ribosome Large Subunit

**P.04.09.7(C228.69)** | M. Kanagawa: Crystal Structure of a Conserved Hypothetical Protein TT1657 from *Thermus thermophilus* HB8

**P.04.09.8(C228.70)** | A. Zagari: Structural Characterization of Archaeal Elongation Factors

**P.04.09.9(C228.71)** | T. Lin: Engineering the Substrate Specificity and Catalysis from Crystal Structures of the

beta-subunit of Acyl-CoA Carboxylase

## 05 CRYSTALLOGRAPHY OF BIOLOGICAL SMALL MOLECULES

### 5. Other Natural Products

**P.05.05.1(C274.72)** | E. Mironova Ekaterina: Structure and Tautomerism of Mercapto-1,2,4-triazole Derivatives in the Solid State

**P.05.05.2(C275.73)** | P. Chimsook: An Investigation of Interactions in Barakol Complexes

**P.05.05.3(C275.74)** | P. Lozano-Casal: Amino Acids at High Pressure

**P.05.05.4(C275.75)** | M. Rossi: Structural Studies on ST1481, Gimatecan, a 7-substituted Camptothecin with Anti-tumor Activity

**P.05.05.5(C275.76)** | F. R. Fronczeck: Hydrogen Bonding and Absolute Configuration in Manzamine Alkaloids

**P.05.05.6(C275.77)** | M. Shiono: The Structure of Protocyanin, a Complex Pigment from Blue Cornflower

**P.05.05.7(C276.78)** | U. J. Griesser: Crystal Structures of the Fungal Metabolite Oosporein

### 8. No Sub-theme

**P.05.08.1(C277.79)** | D. Firley: Electrostatic Properties of Two Precursors of Potent HIV-1 Integrase Inhibitors

**P.05.08.2(C277.80)** | J. M. Kalinowska-Tluscik: Crystal Structures of Potential Sweeteners. The Kier Glucophore Geometry

**P.05.08.3(C277.81)** | A. Orlow: Chloroquine Derivatives. Conformation and Intermolecular Interactions

**P.05.08.4(C278.82)** | J. L. Pinto Camargo: Synthesis and Structural Characterization of 3-(4-fluorophenyl)-2-( $\alpha$ -naphthyl)-1,3-thiazolidin-4-one.

**P.05.08.5(C278.83)** | K. Sasaki: Structural Analysis of the N-terminal Domain of PriA from *E. coli*

**P.05.08.6(C278.84)** | L. Benguedouar: Crystal Structure Determination of a Valinium Hybrid Compound

**P.05.08.7(C278.0)** | S. Chattopadhyay: SAXS Studies of Nucleation of Glycine from its Supersaturated Solution

## 06 CRYSTALLOGRAPHY OF ORGANIC COMPOUNDS

### 7. Inclusion Compounds and Complexes

**P.06.07.1(C287.85)** | N. Fridman: Chromotropism of Imidazole, 2,2'-(2,5-thiophenediy)bis[4,5-diphenyl]

**P.06.07.2(C287.86)** | K. C. Corin: Selective Encapsulation of Picolines

**P.06.07.3(C287.87)** | I. Zouev: Anisotropy in the Photodimerization of 9-Acetylanthracene in Inclusion Compound

**P.06.07.4(C287.88)** | L. Y. Izotova: Temperature Dependent Selectivity of Inclusion

**P.04.02.12(C183.89)** | Z. Tiljakov: Inclusion of Molecular Iodine into Channels of the Organic Zeolite Gossypol

**P.06.07.5(C288.90)** | D. Gallois-Montbrun: Different Building Modes of a-Cyclodextrin/Monoalkyl Amphiphiles Complexes

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

P.06.07.6(C288.91)   <u>A. Jacobs</u> : Inclusion Compounds of Isomeric Xanthenol Hosts with Aniline	P.07.04.1(C305.100)   <u>S.-X. Liu</u> : Structures of Three 36-azametallacrown-12 Complexes	P.07.04.12(C307.111)   <u>D. Vujovic</u> : 1-D and 2-D Uranium(VI) Coordination Polymers
P.06.07.7(C288.92)   <u>O. Celik</u> : Structural Features of Some Schiff Base Disulfide Compounds	P.07.04.2(C305.101)   <u>E. E. Castellano</u> : A Lower Rim Tert-butyl Calix[4]arene Derivative that Binds Ag(I)	P.07.04.13(C308.112)   <u>A. Hountas</u> : Inclusion Compounds of Plant Growth Regulators in Cyclodextrins
P.06.07.8(C288.93)   <u>J. Zukerman-Schpector</u> : Structural Studies of Human Cathepsin B Inhibitors: Telluroxetanes	P.07.04.3(C305.102)   <u>O. E. Piro</u> : Two Isomeric Calix[4]arene Complexes with Mercury(II)	P.07.04.14(C308.113)   <u>H. Akashi</u> : X-ray Structures and Characterizations of Iron Complexes of Thiocalixareninetrasulfonate
P.06.07.9(C289.94)   <u>G. D. Enright</u> : Structural Variety in Tris(5-acetyl-3-thienyl)methane (TATM) Inclusion Compounds	P.07.04.4(C305.103)   <u>J. G. Ferreira</u> : 2D Supramolecular Sheet Generated by $\pi$ Interactions for Cadmium(II) Compounds	P.07.04.15(C308.114)   <u>G. Diaz de Delgado</u> : New Metal Carboxylates prepared at Room Temperature and by Hydrothermal Methods
P.06.07.10(C289.95)   <u>L. Matijasic</u> : Molecular Recognition of Racemic Salts by Inclusion Complexation with the Chiral BINOL	P.07.04.5(C306.104)   <u>L. Russo</u> : Connectivity Variation in Coordination Compounds of Isophthalate and Transition Metals	P.07.04.16(C308.115)   <u>F. Brisse</u> : Silver Coordination Polymers with Flexible Ligands. Effect of the Size of the Ligand and the Solvent on the Network Formation
P.06.07.11(C289.96)   <u>Y. Ozcan</u> : Crystal Structure of a Histidine Schiff Base	P.07.04.6(C306.105)   <u>S. Krachodnok</u> : A New Organically Tempered Vanadium Arsenate	P.07.04.17(C308.116)   <u>M. O. Awaleh</u> : Structural Relationships in the Coordination Complexes of Bis(phenylthio)methane (L1) and Bis(phenylthio)propane (L3) with Silver(I) Salts
P.06.07.12(C289.97)   <u>C. Massera</u> : Weak Intermolecular Interactions in Cavitands as Receptors for Mass Sensors	P.07.04.7(C306.106)   <u>K. Chainok</u> : Noncovalent Interactions in a Three Component Supramolecular Structure	P.07.04.18(C309.117)   <u>A. Ienco</u> : Supramolecular Interactions as Determining Factors of the Primary Geometry of Metallic Building Blocks
<b>07 CRYSTALLOGRAPHY OF ORGANOMETALLIC, COORDINATION AND MAIN GROUP COMPOUNDS</b> <b>2. Molecular Recognition Complexes</b>	P.07.04.8(C306.107)   <u>R. Puntharod</u> : Preparation and Characterization of NiCl(NO)(PPh <sub>3</sub> ) <sub>2</sub>	<b>5. Main Group Chemistry</b>
P.07.02.1(C304.98)   <u>É. Tozzo</u> : X-Ray Studies of some Tetradeятate Schiff Base Oxovanadium(IV) Complexes	P.07.04.9(C307.108)   <u>N. Khosavithkul</u> : Crystal Structure of [Sn(Bu) <sub>3</sub> (O=PPh <sub>3</sub> ) <sub>2</sub> ][BPh <sub>4</sub> ]	P.07.05.3(C309.118)   <u>A. Galindo</u> : Structural Features of Oxydiacetate and Thiodiacetate Complexes and crystal Structures of Magnesium Derivatives
<b>3. Fullerene Metal Complexes</b>	P.07.04.10(C307.109)   <u>T. D. Hamilton</u> : Supramolecular Decoration of Metal-Organic Hosts From Products of Template-Directed Synthesis	<b>08 STRUCTURE/PROPERTY RELATIONSHIP</b> <b>2. Chemical Crystallography of the Future</b>
P.07.03.1(C304.99)   <u>M. A. Petrukhina</u> : Metal Complexes of Fullerene Fragments	P.07.04.11(C307.110)   <u>X. Lu</u> : DB18C6 Sodium Polyoxometalate Supermolecular Complexes With $\alpha$ -Dawson and $\alpha$ -Keggin Structure	P.08.02.1(C316.119)   <u>H. D. Flack</u> : Is your Crystal

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

representative of the Bulk?

**P.08.02.2(C316.120)** | S.C. Capelli: Model Wave Function for Glycyl-L-Alanine from Experimental Diffraction Data

## 6. Phase Transitions

**P.08.06.1(C318.121)** | G. Puchkovska: Polymorphic Transitions in Even Paraffins  $n\text{-C}_{24}\text{H}_{50} \div \text{C}_{34}\text{H}_{70}$ . X-ray and Spectral Studies

**P.08.06.2(C319.122)** | B. Kulicka: Structure and Properties of  $[\text{4-NH}_2\text{C}_5\text{H}_4\text{NH}][\text{BiCl}_4]$

**P.08.06.3(C319.123)** | A.N. Bogdanova: Structure Transformations in the Saturated Hydrides  $\text{ZrV}_2\text{H}_{4-x}$

**P.08.06.4(C319.124)** | L. Kirpichnikova: Structure and Phase Transitions of Some crystals Containing  $[(\text{CH}_3)_2\text{NH}_2]^+$  and  $\text{MeCl}_4^-$

**P.08.06.5(C319.125)** | C. Sortais-Soulard: Striking Effect of Pressure and Temperature on  $\text{PdSe}_2$  Allotropes

**P.08.06.6(C320.126)** | A. Gagor: Diffusion Path Formation for  $\text{Cu}^+$  Ions in Superionic  $\text{Cu}_6\text{PS}_5\text{I}$  Single Crystal

**P.08.06.7(C320.127)** | V. Kopsky: Tensor Distinction of Domain States in Ferroic Phase Transitions

**P.08.06.8(C320.128)** | C. Capillas: Maximal Symmetry Transition Paths for Reconstructive Phase Transitions

**P.08.06.9(C320.129)** | A.F. Craievich: Melting and Freezing of Bi Nanoclusters Embedded in Glass

**P.08.06.10(C321.130)** | P. Gravereau: Jahn Teller

Transition Phase in  $\text{Cu}_{0.5}\text{Ti}(\text{PO}_4)$  Oxyphosphate

**P.08.06.11(C321.131)** | G.S. Nichol: A Temperature-Induced Phase Transition in Barbituric Acid Dihydrate

**P.08.06.12(C321.132)** | W. Somphon: An Order-Disorder Phase Transition in  $[\text{Ag}(\text{bipy})\text{NO}_3]_n$

**P.08.06.14(C321.133)** | A. Nazarenko: Re-examination of Phase Transitions in  $\text{KnbO}_3$

**P.08.06.15(C322.134)** | U. Amann: Substitution of Manganese by Iron or Gallium in Electron-doped Manganites

**P.08.06.16(C322.135)** | C. Du: Dynamic Phase Transition of the Charge-density Wave Lattice

**P.08.06.17(C322.136)** | C.K. Broder: Phase Transitions in Tetrachlorobenzene Studied by Neutron Powder Diffraction

**P.08.06.18(C322.137)** | J. Angel: Polyhedral Compressibilities Drive Structural Phase Transitions in Perovskites

**P.08.06.19(C323.138)** | S. Popovic: X-ray Diffraction Study of Thermal Properties of Titanium Oxide

**P.08.06.20(C323.139)** | J.M. Criado: Influence of Grinding and Atmosphere on the Crystallization of  $\text{ZrO}_2$  Gel

**P.08.06.21(C323.140)** | O. Cakir: Magnetic Study of Intermetallic  $\text{Ce}_{1-x}\text{Tb}_x\text{Mn}_2\text{Ge}_2$  ( $0 \leq x \leq 1$ ) Compounds

**P.08.06.22(C323.141)** | J.-C. Marmeggi: Phase Transitions and Crystal Dynamics at Low Temperature of Alpha-U

and  ${}^4\text{He}$

**P.08.06.23(C323.142)** | E. Haussuhl: Phase Transition of  $\text{C}_2\text{H}_5\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_3$   $\text{Zr} [\text{N}(\text{CH}_2\text{COO})_3]_2\text{H}_2\text{O}$

**P.08.06.24(C324.143)** | L. Fabian: Thermal transformations of some alicyclic  $\beta$ -amino acid hydrates

**P.08.06.25(C324.144)** | Y. Yoshimura: X-Ray Diffraction Study on the Phase Transitions of Barium Titanate

**P.08.06.26(C324.145)** | K. Ohwada: X-ray and Neutron Scattering Study of *as-grown*  $\text{Pb}(\text{In}_{1/2}\text{Nb}_{1/2})\text{O}_3$  Single Crystals

**P.08.06.27(C324.146)** | Y. Uchida: Phase Relationship of Two Polymorphs of a Diaminodicyanopyrazine Dye

**P.08.06.28(C325.147)** | J.M. Perez-Mato: Phase Transition Sequence in Ferroelectric Aurivillius Compounds

**P.08.06.29(C325.148)** | H.T. Stokes: New Graphical User Interface for Calculating Structural Distortions Using the ISOTROPY Software

**P.08.06.30(C325.149)** | D.M. Hatch: General Method for Determining Atomic Pathways in Reconstructive Phase Transitions: SiC and GaN

**P.08.06.31(C325.150)** | J.P. Chaminade: Phase Transition and Structures of the Phosphate  $\text{Zn}_{0.50}\text{Ti}_2(\text{PO}_4)_3$

**P.08.06.32(C325.151)** | J. Akimitsu: Two Phase Transitions in the Low-dimensional Quantum Spin System  $\text{TiOB}_3$

**P.08.06.33(C326.152)** | D. Lisovskytskij: Phase transition in

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

Li-Mn Spinels; *in situ* XRD and Impedance Spectroscopy Analysis

**P.08.06.34(C326.153)** | V. Dmitriev: Isosymmetric Phase Transitions in the Solid State

**P.08.06.35(C326.154)** | C. J. Howard: Synchrotron Powder Diffraction Study of Phase Transitions in Rutile Type Halides

**P.08.06.36(C326.155)** | S. Ravy: Displacive Transition Revisited by Coherent X-ray Diffraction

**P.08.06.37(C326.156)** | S. Yamamura: Bifurcation and Metastable States in Phase Transitions of Nucleotide Hydrates

**P.08.06.38(C327.157)** | K. Toriumi: Spin-Peierls Transition in Halogen-Bridged Mixed-Valence MMX Chain Compounds

**P.08.06.39(C327.158)** | H. Grove: Fe(II), Fe(III) and Co(II)-Complexes with Aromatic Nitrogen-Containing Ligands

**P.08.06.40(C327.159)** | D. Chernyshov: Spin Crossover in Solvates of an Iron(II) Complex with Solvent Mixtures

**P.08.06.41(C327.160)** | B. L. Pedersen: Dopant Atom Influence on the  $\alpha \rightarrow \beta$  Phase Transition in Thermoelectric Zn<sub>4</sub>Sb<sub>3</sub>

## 9. Structure and Chemical Reactivity

**P.08.09.1(C332.161)** | K. Molcanov: Structural Characterisation of *p*-semiquinone Radical in a Crystal : X-ray Structure and EPR Evidence

**P.08.09.2(C332.162)** | A. O. Tokareva: Crystal Structure and Synthesis of New Trinuclear 3d-metal Trifluoroacetates

**P.08.09.3(C333.163)** | M. F. Haddow: Structural and Electronic Properties of Carbenes as Ligands

**P.08.09.4(C333.164)** | J.-C. Daran: Chirality Control in 2,2'-biphosphole Ligands Leading to Enantio-pure Complexes

**P.08.09.5(C333.165)** | T. Ooga: Molecular Mechanism of ADP-ribose Pyrophosphatase from *Thermus thermophilus* HB8

**P.08.09.6(C333.166)** | P. Bénard-Rocherullé: Synthesis and Thermal Behaviour of New Lanthanide Oxalato-squares

**P.08.09.7(C334.167)** | D. V. Albov: Diffraction Study of Recyclization of Oxazolopyridinium Salts to Indolizines

**P.08.09.8(C334.168)** | A. Serpe: Structure and Properties of Safe and Powerful Noble-Metals Oxidation Reagents

**P.08.09.9(C334.169)** | J. M. Benito: Nickel(II) Carbosilane Dendrimers: Structure and Polymerization Catalysis

**P.08.09.10(C334.170)** | F. Montilla: Solid-state Formation of a Coordination Polymer Starting from a Monomeric Thiodiacetate Manganese Complex

**P.08.09.11(C335.171)** | E. Herrero-Gómez: Au(I)-arene Interactions

**P.08.09.12(C335.172)** | P. Velasco: Comparative Study of Structural Aspects of Monocyclopentadi-enyl Niobium and Tantalum Complexes. Synthesis and Reactivity

**P.08.09.13(C335.173)** | W. Oberhauser: Synthesis of cis,cis-1,2,3,4-tetrakis(diphenylphosphino)butadiene Exploiting the “Template Effect”

## 09 CRYSTAL ENGINEERING

### 6. Non Centrosymmetric Systems: Creation and Application

**P.09.06.1(C364.174)** | G. O. Lloyd: New Helical Host System Showing True Self-Inclusion

**P.09.06.2(C364.175)** | P. A. Plachinda: Comparative Study of Framework Borates Optical Non-linearities

**P.09.06.3(C364.176)** | M. M. R. Costa: Optical and Pyroelectric Properties and Structure of 2[K<sup>+</sup>H(C<sub>4</sub>H<sub>9</sub>O<sub>5</sub>)].C<sub>4</sub>H<sub>9</sub>O<sub>5</sub>

**P.09.06.4(C365.177)** | H. H.-Y. Sung: Geometric Analysis of Tartrate Coordination Modes from Crystallographic Data

## 12 SURFACES, INTERFACES, LIQUIDS AND THIN FILMS

### 11. Thin Films and Multilayers

**P.12.11.1(C413.178)** | S. Y. Choi: Evolution of Nanocrystallinity in Periodic Mesoporous Anatase Thin Films

**P.12.11.2(C413.179)** | A. Alemi: Sol-gel Synthesis and Study of LaPO<sub>4</sub> Doped with Cerium(III) and Ytterbium(III) Thin Films

**P.12.11.3(C413.180)** | J. Werckmann: Pulsed Laser Deposition Growth of Thin Hydroxyapatite Layers on Titanium Substrates

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

P.12.11.4(C414.181) | V. Kaganer: Strain-mediated Phase Coexistence at Phase Transitions in Epitaxial Films

P.12.11.5(C414.182) | Z. Sourek: Structural Properties of Ferromagnetic GaMnAs Layers

P.12.11.6(C414.183) | K. Fukuda: Estimation of Lattice Structure of Strained-Si Wafers Using Highly Parallel X-Ray Microbeam (I)

P.12.11.7(C414.184) | Y. Tsusaka: Estimation of Lattice Structure of Strained-Si Wafers Using Highly Parallel X-Ray Microbeam (II)

P.12.11.8(C414.185) | E. Rosendo: Study of Te Diffusion into Structure GaSb-n/GaSb-p on GaSb-n Substrate

P.12.11.9(C415.186) | H. Juarez Santiesteban: Density and Mobility of Carriers in AlGaSb and InGaAsSb Alloys Obtained by LPE

P.12.11.10(C415.187) | R. Kuzel: XRD Study of Strongly Textured and Stressed Thin Films

P.12.11.11(C415.188) | D. Balzar: Residual Stress in Tungsten Thin Films for Photon Counting Applications

P.12.11.12(C415.189) | J. A. Martin-Gago: Ordered SAMS of Peptide Nucleic Acids on Surfaces with DNA Recognition Capability

P.12.11.13(C415.190) | E. Holub-Krappe: Spin Reorientation in Thin Au/Co/Au Films: *in-situ* XMCD and EXAFS Study

17 CHARACTERIZATION OF DEFECTS,  
MICROSTRUCTURES AND TEXTURES

## 4. Diffraction

P.17.04.1(C448.191) | J. L. Garin: Quantitative X-ray Diffraction Study of Welded Joints in Heat-resistant Steels

P.17.04.2(C448.192) | H. Bezirganyan: Detection of Weak X-ray Waves Scattered by the Crystal Subsurface Inclusions

P.17.04.3(C448.193) | K. Nyilas: Dislocations and Crystallite Size in Forsterite Produced at 11 GPa and 1400 °C

P.17.04.4(C449.194) | K. Wieteska: X-Ray Synchrotron Studies of AlGaAs based Lasers Structures

P.17.04.5(C449.195) | W. Wierzchowski: Strain Profiles in the Insulated Buried Layers Obtained by He Implantation in AlGaAs

P.17.04.6(C449.196) | S. Dudarev: Huang Diffuse Scattering by Mesoscopic Interstitial Defects in BCC Metals

P.17.04.7(C449.197) | N. Budarina: XRD Peak Profiles in the Case of the Lognormal Crystallite Size Distribution

P.17.04.8(C449.198) | O. Boytsov: Evolution of Nanostructure States of Cu-powders Prepared by Ball Milling

P.17.04.9(C450.199) | P. Vagovic: Defects in  $\gamma$  Irradiated Cz-Si annealed under high pressure

P.17.04.10(C450.200) | A. Shalimov: X-Ray Diffuse Scattering on the First Type Defects in Semiconductors

P.17.04.11(C450.201) | S. Chakraborty: Structural and

Microstructural Studies of Synthetic and Naturally Occurring Hydroxyapatites using Powder Diffraction

P.17.04.12(C450.202) | A. K. Deb: An X-ray Diffraction Study on Dislocation Microstructure of as-prepared Al-Al<sub>2</sub>O<sub>3</sub> Composites

P.17.04.13(C451.203) | N. Audebrand: Strain-free Oxide Nanopowders, Facts and ex-Oxalate MgO Case

P.17.04.14(C451.204) | V. Klechkovskaya: Geterostructures of Bacterial Cellulose Acetobacter Xylinum Intercalated by Drug Materials

P.17.04.15(C451.205) | M. Hostettler: Honeycomb Diffuse Intensities in NaREF<sub>4</sub> Upconversion Materials

P.17.04.16(C451.206) | A. Kuznetsov: Stacking Faults and Internal Strains in DHCP Phase of La

P.17.04.17(C452.207) | N. Armstrong: X-Ray Line Profile Analysis of CeO<sub>2</sub> Nanoparticles

P.17.04.18(C452.208) | K. J. Roberts: Application of Molecular Modelling to Study Nucleation, Impurity Segregation, Solvent Adsorption and Polymorphic Transformation

P.17.04.19(C452.209) | J. te Nijenhuis: Development of Crystallographic Textures in Diamond Films

P.17.04.20(C452.210) | A. Rodriguez-Navarro: New Tools for Microstructure Analyses of Polycrystalline Materials using an X-ray Area Detector

## 18 ELECTRON MICROSCOPY

### 1. Application to Macromolecules

# THURSDAY, AUGUST 25, 2005 – POSTER SESSION

**P.18.01.1(C455.211)** | T. Miyata: Electron Microscopic Single Particle Analysis of the Clamp Loading Complex from *Pyrococcus furiosus*

**P.18.01.2(C455.212)** | L. Muzzolini: Correlation between Function and Oligomeric State of Human RECQL Helicase Revealed by Biochemical and Cryo-EM Analysis

## 2. Cryo-microscopy

**P.18.02.1(C455.213)** | W. Chiu: Electron Cryomicroscopy of Epsilon 15 Phage

## 19 ELECTRON DIFFRACTION

### 2. High Resolution Results

**P.19.02.1(C457.214)** | J.-G. Kim: 3-D Structure Determination of CAMoO<sub>4</sub> Using HVEM

**P.19.02.2(C457.215)** | P. Nakashima: Increasing the Precision of Quantitative CBED Structure Factor Measurements

## 21 SYMMETRY AND ITS GENERALISATIONS

### 1. General Symmetry: Theory

**P.21.01.1(C473.216)** | D. B. Litvin: VRML General Position Diagrams of non-Cubic Magnetic Space Groups

**P.21.01.2(C473.217)** | M. I. Aroyo: Database of the Subperiodic Rod Groups on the Bilbao Crystallographic Server

**P.21.01.3(C473.218)** | M. Samoilovitch: Fibration-defined Integer and Non-integer Axes

**P.21.01.4(C473.219)** | J. Z. Warczewski: A Fibre Bundle Approach to the Description of the Symmetry of Magnetic Structures in a 6-dimensional Space

## 3. Pseudo-Symmetry: Recognition and Applications

**P.21.03.1(C473.220)** | A. D. Rae: Validation of a Twinned Pseudo Symmetric Crystal using a Hierarchical Pathway

**P.21.03.2(C474.221)** | A. Collins: Relationships between Independent Molecules in Z'=2 Structures

**P.21.03.3(C474.222)** | G. Ferraris: Twinning Investigation via the Primitive Cell of Bravais Lattices

## 28 ART, CULTURAL HERITAGE AND CRYSTALLOGRAPHY

### 1. Art, Cultural Heritage and Crystallography

**P.28.01.1(C493.223)** | A. Haake: Applied Symmetry - Medieval Floor Tiles Excavated at the Castle of Kronberg.

**P.28.01.2(C493.224)** | F. Zaghis: A New Approach in Studying Ancient Cu-Sn Artifacts: Measure of Crystal Orientation and Phase Distribution by EBSD Analysis.

## 29 OTHER TOPICS

### 1. Crystallography and Forensic Science

**P.29.01.1(C495.225)** | M. Kotrly: Use the X-ray Diffraction in Forensic Science as a Device for Phase Analysis

## 3. Miscellanea

**P.29.03.2(C495.226)** | M. Sippl: Resolving Ambiguous

Side-chain Orientations of Asparagine and Glutamine

**FRIDAY, AUGUST 26, 2005 – KEYNOTE LECTURES****MORNING SESSION 8.30-9.30**

Michelangelo (**KN 11**)

**KN11.26(C3) | Andrej Sali:**

Structure of Protein Assemblies by Comparative Modeling and Electron Microscopy

*Chair: Douglas Ohlendorf*

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Botticelli (**KN 12**)

**KN12.26(C3) | Roberto Dovesi:**

Quantum mechanical simulation of the vibrational properties of garnets.

*Chair: Davide Viterbo*

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Cimabue (**KN 13**)

**KN13.26(C3) | Abraham Clearfield:**

In Situ X-Ray Study of Hydrothermally Prepared Titanates and Silicotitanates

*Chair: Roberto Fornari*

**AFTERNOON SESSION 17.30-18.30**

Michelangelo (**KN 14**)

**KN14.26(C3) | Deborah Fass:**

Catalysts of De Novo Disulfide Bond Formation

*Chair: Jennifer Martin*

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Botticelli (**KN 15**)

**KN15.26(C4) | A. Guy Orpen:**

Synthetic Crystallography

*Chair: Frank H. Allen*

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Cimabue (**KN 16**)

**KN16.26(C4) | John Tse:**

A perspective on the crystal structures of high pressure elements and their properties

*Chair: Werner F. Kuhs*

**FRIDAY, AUGUST 26 2005 – MORNING - MICROSYMPPOSIA**

<b>TIME</b>	<b>Michelangelo (MS 29)</b>	<b>Botticelli (MS 31)</b>	<b>Giotto (MS 32)</b>
10.00-10.05 Opening Remarks	<b>IMPROVING STRUCTURES USING BIO-INFORMATICS</b> <i>Chairs: P. E. Bourne, R. Sowdhamini</i>	<b>SUPRAMOLECULAR CHEMISTRY</b> <i>Chairs: F. Ugozzoli, C. Gervais</i>	<b>STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA (INORGANICS)</b> <i>Chairs: A. Altomare, H. Putz</i>
10.05-10.35	<b>MS29.26.1(C42)   H. M. Berman:</b> How the RCSB Validates PDB Structures	<b>MS31.26.1(C44)   J. L. Atwood:</b> Diffusion of Guests into Non-Porous Crystals	<b>MS32.26.1(C45)   L. Kocher:</b> Exploiting Preferred Orientation to Resolve the Intensities of Overlapping Reflections
10.35-11.05	<b>MS29.26.2(C42)   A. Godzik:</b> A Systematic Study of Flexibility in Protein Structures and its Implications in Protein Structure Prediction	<b>MS31.26.2(C44)   S. H. Dale:</b> Sandwiches and Cavities: The Supramolecular Chemistry of Hemimellitic Acid	<b>MS32.26.2(C45)   A.G. Moliterni:</b> New Strategies for the <i>Ab-initio</i> Structure Solution in EXPO2005
11.05-11.35	<b>MS29.26.3(C42)   B. Kojic-Prodic:</b> Bioinformatics Approach to Characterization of SGNH/GDSL-hydrolases	<b>MS31.26.3(C44)   A. Williams:</b> Supramolecular Coordination Chemistry – the Challenge of the Outer Sphere	<b>MS32.26.3(C45)   R. Dinnebier:</b> Are Well Known Phase Diagrams Really Well Known?
11.35-12.05	<b>MS29.26.4(C42)   M. J. Sippl:</b> Validation and Classification of Protein Structures	<b>MS31.26.4(C44)   J. W. Steed:</b> Structure Control by Hydrogen Bonding to Anions and Coordination to Cations	<b>MS32.26.4(C46)   T. Bataille:</b> Structure Solution of Thermal Decomposition Compounds Using Laboratory X-rays
12.05-12.35	<b>MS29.26.5(C42)   P. Gouet:</b> ESPrpt/ENDscript: Sequence and 3D Information from Protein Structures	<b>MS31.26.5(C45)   V. Balzani:</b> Molecular-level Devices and Machines	<b>MS32.26.5(C46)   P. Juhas:</b> Structure Solution of Single-Element Molecules from Pair Distribution Function

# FRIDAY, AUGUST 26 2005 - MORNING - MICROSYMPOSIA

Leonardo da Vinci ( <b><i>MS 33</i></b> )	Cimabue ( <b><i>MS 34</i></b> )	Donatello ( <b><i>MS 35</i></b> )	Michelangelo ( <b><i>MS 30</i></b> )
<b>SOFT CONDENSED ORGANIC-BIOLOGICAL MATERIALS UNDER PRESSURE</b> <i>Chairs:</i> R. Fourme, W. Poon	<b>ADVANCES IN COMPUTATIONAL METHODS FOR ELECTRON DENSITY STUDIES</b> <i>Chairs:</i> L. Farrugia, T. Koritsanszky	<b>POLYTYPOISM AND TWINNING</b> <i>Chairs:</i> G. Ferraris, E. Belokoneva	<b>ART AND CRYSTALLOGRAPHY</b> <i>Chairs:</i> E. Meyer, C. Acidini  <b><i>MS scheduled at 21.00</i></b>
<b>MS33.26.1(C46)</b>   <u>R. Winter</u> : Exploring the Configurational Landscape of Biomolecular Systems under Extreme Conditions	<b>MS34.26.1(C47)</b>   <u>R. Orlando</u> : <i>Ab-initio</i> Quantum-mechanical Calculation of Electron Charge-density in Crystals	<b>MS35.26.1(C48)</b>   <u>M. Nespolo</u> : Recent Aspects of the Theory of Oriented Crystal Associations	21.00 <u>C. Acidini</u> : Introductory Remarks
<b>MS33.26.2(C46)</b>   <u>T. Fujisawa</u> : Probing two Heads Configuration of Heavy Meromyosin by High-pressure SAXS Technique	<b>MS34.26.2(C47)</b>   <u>C. Gatti</u> : Beyond $\nabla^2 p_b$ : Chemical Bond Analysis using the Local Form of the Source Function	<b>MS35.26.2(C49)</b>   <u>R. Herbst-Irmer</u> : Non-merohedral Twinning in Small Molecule and Protein Crystallography	21.15 <b>MS30.26.1(C43)</b>   <u>M. Kemp</u> : Plastic Visions in Art and Science
<b>MS33.26.3(C46)</b>   <u>S. Finet</u> : SAXS Investigations of Conformation and Stability of Eye Lens Proteins under Pressure	<b>MS34.26.3(C48)</b>   <u>C. Johnson</u> : Thermal Motion Analysis via Modern Probability Methods	<b>MS35.26.3(C49)</b>   <u>C. Viti</u> : Additional Reflections and Polytypic Sequences in Polygonal Serpentine	21.45 <b>MS30.26.2(C43)</b>   <u>D. Schattschneider</u> : M.C. Escher and the Crystallographers
<b>MS33.26.4(C47)</b>   <u>E. Girard</u> : When Macromolecular Crystallography Meets High Pressure Techniques...	<b>MS34.26.4(C48)</b>   <u>D. Jayatilak</u> : Images of Unpaired Electron Density in Molecular Crystals Obtained using Experimentally Constrained Wavefunctions	<b>MS35.26.4(49)</b>   <u>D. Pinto</u> : Order-disorder, Polytypes and Twinning in the Crystal Structure of Vurorite	22.15 <b>MS30.26.3(C43)</b>   <u>G. Tsoucaris</u> : Ancient Crystalline Materials for the Arts of Beauty
<b>MS33.26.5(C47)</b>   <u>C. U. Kim</u> : High Pressure Cooling of Protein Crystals without Cryoprotectants	<b>MS34.26.5(C48)</b>   <u>P. G. Mezey</u> : Holographic Principles of Molecular Structure and Electron Density Calculations	<b>MS35.26.5(49)</b>   <u>A. Arakcheeva</u> : Simulation of a Polytypic Family from an Incommensurately Modulated Member	22.45 <b>MS30.26.4(C43)</b>   <u>E. Meyer</u> : Art in Crystallography in Art Closing Remarks

**FRIDAY, AUGUST 26 2005 - AFTERNOON - MICROSYMPOSIA**

<b>TIME</b>	<b>Michelangelo (MS 36)</b>	<b>Botticelli (MS 37)</b>	<b>Cimabue (MS 38)</b>
14.45-14.50 Opening Remarks	<b>COMBATING VIRUSES</b> <i>Chairs: E. Garman, M. Luo</i>	<b>INTRACELLULAR TRAFFICKING OF BIOMOLECULES</b> <i>Chairs: Y. Yoneda, D. Owen</i>	<b>CONTROLLED BUILDING OF CRYSTALS FROM NON-COVALENT INTERACTIONS</b> <i>Chairs: C. Aakeroy, A. Bacchi</i>
14.50-15.20	<b>MS36.26.1(C50)</b>   <u>M. James</u> : Non-nucleoside Inhibitors of NS5B Polymerase from HCV, Genotypes 1b and 2a	<b>MS37.26.1(C51)</b>   <u>E. Conti</u> : Transport out of the Nucleus and Beyond: Molecular Mechanisms	<b>MS38.26.1(C52)</b>   <u>R. Davey</u> : Understanding and Using Solution Chemistry to Direct Crystal Nucleation
15.20-15.50	<b>MS36.26.2(C50)</b>   <u>Z. Rao</u> : Crystal Structures of SARS Coronavirus Proteins	<b>MS37.26.2(C51)</b>   <u>A. Cook</u> : Cse1: the Structure of an Exportin in its Closed, Cytosolic State	<b>MS38.26.2(C52)</b>   <u>M.W. Hosseini</u> : Molecular Tectonics : from Tectons to Networks
16.50-16.20	<b>MS36.26.3(C50)</b>   <u>S. Curry</u> : Structure, Mechanism and Specificity of FMDV 3C Protease	<b>MS37.26.3(C51)</b>   <u>D. Kohda</u> : Cracking of the Targeting Signal Embedded in Mitochondrial Presequences	<b>MS38.26.3(C52)</b>   <u>C. Ruiz-Pérez</u> : Reliability of the Self-complementary Noncovalent Interactions: Supramolecular Implications and Supramolecular Design
16.20-16.50	<b>MS36.26.4(C50)</b>   <u>D. Stammers</u> : HIV Reverse Transcriptases: Structural Basis for Inhibition and Drug Resistance	<b>MS37.26.4(C51)</b>   <u>B. M. Collins</u> : Vps29: a Phosphoesterase Fold that Acts as an Interaction Scaffold in the Assembly of Retromer	<b>MS38.26.4(C53)</b>   <u>A. Comotti</u> : Recognition of Weak Interactions at the Gas-crystal Interface
16.50-17.20	<b>MS36.26.5(C51)</b>   <u>E. Arnold</u> : Structure-based Vaccine Design of Human Rhinovirus: HIV Chimeras as Candidate AIDS Vaccines	<b>MS37.26.5(C52)</b>   <u>C. S. Perez</u> : Crystallization of Molybdate-Binding Protein of Xanthomonas Citri	<b>MS38.26.5(C53)</b>   <u>C. H. Görbitz</u> : Peptide-Based Organic Microporous Materials

# FRIDAY, AUGUST 26 2005 - AFTERNOON- MICROSYMPOSIA

<b>Donatello (MS 39)</b>	<b>Leonardo da Vinci (MS 40)</b>	<b>Giotto (MS 41)</b>	<b>Brunelleschi (MS 42)</b>
<b>POWDER DIFFRACTION OF PROTEINS</b> <i>Chairs: R. H. Blessing, J. Cockcroft</i>	<b>COMPUTATIONAL CRYSTALLOGRAPHY APPLIED TO EXTREME CONDITIONS</b> <i>Chairs: G. Galli, A. Pavese</i>	<b>COMPUTATIONAL SOLUTIONS FOR HIGH-THROUGHPUT CRYSTALLOGRAPHY</b> <i>Chairs: D. E. McRee, J. Holton</i>	<b>COMPLEMENTARITIES OF NEUTRON AND X-RAYS METHODS IN MATERIAL SCIENCE</b> <i>Chairs: A. Schreyer, M. R. Daymond</i>
<b>MS39.26.1(C53)   R. Von Dreele:</b> Recent Developments in Protein Structure Analysis from Powder Diffraction Data	<b>MS40.26.1(C54)   M. Catti:</b> Structural Paths for the High-Pressure Phase Transitions of AgI	<b>MS41.26.4(C56)   M. Yamamoto:</b> Automated Operation of Protein Crystallography Beamlines at the SPring-8	<b>MS42.26.1(C56)   L. Edwards:</b> Integrated Use of Synchrotron and Neutron Diffraction to Monitor Residual Stress Evolution in Welded Aerospace Structures
<b>MS39.26.2(C53)   J. Wright:</b> Molecular Replacement With Powder Diffraction Data	<b>MS40.26.2(C54)   T. Ogitsu:</b> The Fifth Element in the Periodic Table, Boron: Do We Know the Ground State Structure?	<b>MS41.26.2(C55)   G. Wolf:</b> Parallel Data Processing for High Throughput X-ray Structure Determination	<b>MS42.26.2(C57)   H.-G. Brokmeier:</b> Crystallographic Texture of Semi-finished Products
<b>MS39.26.3(C54)   C. Gilmore:</b> Protein Powder Diffraction: Why Bother?	<b>MS40.26.3(C55)   S. Scandolo:</b> Oxides under Pressure: from Densified Silica to the Rheology of the Earth's Mantle	<b>MS41.26.1(C55)   S. Ness:</b> Crank - New Methods in Automated Structure Solution	<b>MS42.26.3(C57)   I. C. Noyan:</b> Dynamic Diffraction Effects in X-ray and Neutron Stress Analysis
<b>MS39.26.4(C54)   I. Margiolaki:</b> Development of Powder Diffraction Methods for Macromolecular Crystallography	<b>MS40.26.4(C55)   A. Oganov:</b> Novel High-pressure Phases: Theory and Experiment.	<b>MS41.26.5(C56)   W. Furey:</b> Automated Protein Structure Determination with <i>BnP</i>	<b>MS42.26.4(C57)   P. Bordet:</b> Charge Ordering and Magnetic Structure in $\text{Fe}_3\text{BO}_5$
<b>MS39.26.5(54)   S. Prugovecki:</b> Protein Measurements on a Laboratory Powder Diffractometer	<b>MS40.26.5(C55)   R. M. M. Wentzcovitch:</b> $\text{MgSiO}_3$ Post-perovskite at D" Conditions	<b>MS41.26.3(C56)   T. Terwilliger:</b> Iterative Model Building and Evaluation with Statistical Density Modification	<b>MS42.26.5(C57)   P. Lee:</b> Determining Pb/Bi Distributions using High-energy Resonant Scattering at K Edges

## **FRIDAY, AUGUST 26, 2005 – OTHER ACTIVITIES**

### **OPEN COMMISSION MEETINGS**

Leonardo da Vinci (12.35-14.35)

#### **OCM03 COMCIFS THE CURRENT STATUS AND FUTURE PROSPECTS OF CIF**

*Chair:* Ian David Brown

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##### **OCM03.26.1(CI27) | R. Grosse-Kunstleve:**

mmCIF and Modern Macromolecular Structure Determination Software: Status and Perspectives

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##### **OCM03.26.2(CI27) | H. Zheng:**

A Dictionary Approach to Translate Memory Variables from Crystallography Software to mmCIF Items

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##### **OCM03.26.3(CI27) | E. A. Merritt:**

Analysis and Visualization of TLS Motion in Proteins using the mmLib Toolkit

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##### **OCM03.26.4(CI27) | F. H. Allen:**

CIF Operations and Applications at the CCDC.

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##### **OCM03.26.5(CI28) | H. Nakamura:**

PDBML: the XML-based Database and its Applications

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##### **OCM03.26.6(CI28) | B. McMahon:**

Use of mmCIF in the Publication of Macromolecular Crystallography Communications

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##### **OCM03.26.7(CI28) | K. Henrick:**

mmCIF and Dictionary Driven Software with the MSD Database Production Pipeline

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##### **OCM03.26.8(CI28) | Z. Feng:**

mmCIF Applications at the RCSB Protein Data Bank

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Giotto (12.35-14.35)

#### **OCM04 COMMISSION ON BIOLOGICAL MACROMOLECULES**

*Chair:* Mitchell Guss

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##### **OCM04.26.1(CI29) | Z. Otwinowski:**

What is the Issue with Autodeposit?

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##### **OCM04.26.2(CI29) | T. Terwilliger:**

Harvesting Should Be A Complete and Repeatable Record of Experiment

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##### **OCM04.26.3(CI29) | H. Powell:**

Harvesting - from Data Collection to Deposition

## FRIDAY, AUGUST 26, 2005 – OTHER ACTIVITIES

**OCM04.26.4(C129)** | H. Einspahr:

Streamlining Data Bank Deposition and Manuscript  
Submission

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**COMPUTER FAYRE**

Ghirlandaio

(10.30-12.00)      R. Neder, T. Proffen:

Total Scattering: Software to Simulate Disordered  
Structures, Diffuse Scattering and Pair Distribution Functions

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(14.00-16.00)      H. T. Stokes, B. Campbell:

A new GUI for the ISOTROPY Software Package Designed  
Especially for Computing Structural Distortions

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**SPECIAL SEMINAR**

Brunelleschi (10.00-11.00)

Jan Boeyens:

The Crystallographic Game

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

## 01 INSTRUMENTATION AND EXPERIMENTAL TECHNIQUES

### 1. Conventional Sources of X-rays

**P.01.01.1(CI35.1)** | H. Schnablegger: SAXSess - An Analytical Tool for Nanostructured Materials

**P.01.01.2(CI35.2)** | L. Seijbel: Illuminating the Role of Brightness in X-ray Diffraction

**P.01.01.3(CI35.3)** | A. Mechaly: A Holder for Diffracting Crystals and Mesophases Straight from Crystallization Plates

### 2. Synchrotron Radiation I: Instrumentation and Techniques

**P.01.02.1(CI35.4)** | A. O. R. Baron: Applications of Bragg Backscattering from Crystalline Quartz

**P.01.02.2(CI35.5)** | R. Alkire: Development of a Real-time Timing-Shutter Delay Monitor

**P.01.02.3(CI36.6)** | S. L. G. Hushee: An X-ray Chopper for Time-resolved Crystallography

**P.01.02.4(CI36.7)** | E. Gozzo: Modeling the IRF of Synchrotron Powder Diffractometers with Focusing Optics

**P.01.02.5(CI36.8)** | N. Yasuda: Microcrystal X-ray Analyses Using LTV Camera at Spring-8 BL02B1 Beamline

**P.01.02.6(CI36.9)** | E. Duke: The Phase 1 Macromolecular Crystallography Beamlines on Diamond

**P.01.02.7(CI37.10)** | F. J. Rotella: Movement of Single-Crystal Protein Samples at Synchrotron Beamlines

**P.01.02.8(CI37.11)** | J. Hrdá: Harmonics-free Channel-cut X-ray Crystal Monochromator with Focussing Effect

**P.01.02.9(CI37.12)** | J. Hrdý: Aberrations of Bragg-case Diffractive-refractive Optics (Sagittal Focusing)

**P.01.02.10(CI37.13)** | B.-C. Wang: SER-CAT: The Advanced Photon Source's Latest Protein Crystallography Facility

**P.01.02.11(CI37.14)** | E. Weckert: PETRA III: a Low Emittance High Energy Synchrotron Radiation Source

**P.01.02.12(CI38.15)** | T. J. Gruber: Time-resolved and Charge-density Studies at ChemMatCARS

**P.01.02.13(CI38.16)** | T. Eriksson: A Comprehensive Environment for Doing Macromolecular Crystallography at SSRL

**P.01.02.14(CI38.17)** | N. Matsugaki: Development of Protein Crystallography Beamlines at the Photon Factory for Automated Experiment

**P.01.02.15(CI38.18)** | L. E. Berman: New Optical Design and Performance of the NSLS X21 X-Ray Wiggler Beamline

**P.01.02.16(CI39.19)** | V. Young: Microcrystallography at ChemMatCARS at the Advanced Photon Source

**P.01.02.17(CI39.20)** | R. Fischetti: GM/CA Canted Undulator Beamlines for Protein Crystallography

**P.01.02.18(CI39.21)** | M. Burghammer: Instrumentation for X-ray Scanning-Diffraction with Sub-micron Resolution

**P.01.02.19(CI39.22)** | A. Bombardi: I16: a Magnetic and Material Diffraction Beamline on Diamond

### 3. Synchrotron Radiation II: Applications

**P.01.03.1(CI39.23)** | S. F. S. Tada: Structural Characterization of a Small Heat-shock Protein from *Xylella fastidiosa*

**P.01.03.2(CI40.24)** | T. Koganezawa: Phase Determination Using a Wide-band Parallel Synchrotron Radiation Beam

**P.01.03.3(CI40.25)** | D. Ghisletti: Simultaneous XRPD-MS Study on Iron Oxides Supported on Spinel-like Aluminate.

**P.01.03.4(CI40.26)** | O. Svensson: Automation of MX Data Collection and Processing

**P.01.03.5(CI40.27)** | W. Clegg: Still Bad Crystals, but Good Data and Results from Synchrotron Facilities

**P.01.03.6(CI40.28)** | C. Paulmann: Recent Developments and Diffuse Scattering Studies at Beamline F1 (Hasylab/DESY)

**P.01.03.7(CI41.29)** | Y. Yamada: Efficiency of Light Atoms on the Low Energy SAD Phasing

### 4. New X-ray Sources

**P.01.04.1(CI41.30)** | R. Ruth: Testing the Compact Light Source: a Miniature Synchrotron for the Home Lab

**P.01.04.2(CI41.31)** | M. Navasardyan: On Forced Reflection and Transmission of Speech, Using X-Rays

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

P.01.04.3(CI41.32) | O. Mikhin: High Brilliance X-ray Laboratory System for Microdiffraction Studies

P.01.04.4(CI42.33) | N. Igarashi: BL-17: New Structural Biology Beam Line at the Photon Factory

## 7. X-ray Imaging

P.01.07.1(CI42.34) | M. Goncalves Hönnicke: X-ray Back-diffraction Wavefields Self-imaged with a CCD Detector

## 02 METHODS FOR STRUCTURE DETERMINATION

### 2. Direct Methods of Phase Determination

P.02.02.1(CI51.35) | B. Carrozzini: Sir2004: New Features for Ab-initio Crystal Structure Solution

P.02.02.2(CI51.36) | S. Selvanayagam: High Throughput Technique in Structural Bioinformatics

P.02.02.3(CI51.37) | Y. He: SAD Phasing at the Presence of Pseudo-translational Symmetry

P.02.02.4(CI52.38) | C. Weeks: Automated Web- and Grid-Based Protein Phasing with BnP

P.02.02.5(CI52.39) | A. B. Smith: A Deterministic Algorithm for Phasing Using Triplet and Quartet Invariants

P.02.02.6(CI52.40) | D. A. Langs: Neutron Structure Determination via Macromolecular H/D Derivatives

P.02.02.7(CI52.41) | J. Yao: A Modified ACORN to Solve Protein Structures at Resolutions of 1.7 Å or Better

## 12. Ab initio Powder Diffraction Solutions: Inorganic Compounds

P.02.12.3(CI58.4) | M. François: Structures in Mo-Ru-Si System by Powder and Anomalous X-Ray Diffraction

## 13. Ab initio Powder Diffraction Solutions: Electron Diffraction

P.02.13.1(CI59.42) | L. Meshi: New Tetragonal Phase in Al-Fe-U System

## 15. X-ray and Neutron Complementarity

P.02.15.1(CI59.43) | S. Sasaki: Magnetic Structure of BaFe12O19 Determined by Resonant X-ray Magnetic Scattering

P.02.15.2(CI59.44) | T. Hosoya: Neutron Diffraction Analysis of Photoisomerization of δ-Cyanobutyl Cobaloxime

## 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

### 1. Peptide and Protein Crystallisation

P.04.01.1(CI71.45) | B. Wu: Three-dimensional Structure of Human FKBP52

P.04.01.2(CI71.46) | P. Wilmann: Structural Investigations of GFP-like Proteins

P.04.01.3(CI71.47) | A. Izumi: Crystal Structure of Heme Bindig Enolase P46 from Bacteroides fragillis

P.04.01.4(CI71.48) | F. Rinaldi: Structural Studies of the Disulfide Oxidoreductases DsbA from *Xylella fastidiosa*

P.04.01.5(CI71.49) | M. Frank: Structure of MntC from Cyanobacteria

P.04.01.6(CI72.50) | A. Shahar: 3D Structure Determination of the Cpn60-2 protein from *Mycobacterium Tuberculosis*

P.04.01.7(CI72.51) | E. Santillana: Crystal Structure of OXA-24, a Novel Class Beta-lactamase with Carbapenemase Activity

P.04.01.8(CI72.52) | C. Rush: Crystallographic Studies of Human Methionine Adenosyltransferase (MAT)

P.04.01.9(CI72.53) | J. Wolfsova: Optimization of Crystallization of the Flavoprotein WrbA by Using Additives

P.04.01.10(CI73.54) | M. Spano-Budayova: Improving the Growth of Biomacromolecular Crystals for Neutrons and X-rays

P.04.01.11(CI73.55) | P. Schreiner: Crystallization of the TOM Complex from *Neurospora crassa* together with Monoclonal Antibodies

P.04.01.12(CI73.56) | C. Koerner: Crystallisation and Functional Analysis of Prokaryotic and Eukaryotic Rhomboid Proteases and Hsp70 Chaperones

P.04.01.13(CI74.57) | L. Roces: Preliminari Diffraction Study of the Full-legh Protein Hexokinase 2 of *Saccharomyces cerevisiae*

P.04.01.14(CI74.59) | A.-M. Lund Jensen: A New Crystal Form of the SR Ca<sup>2+</sup>-ATPase in the Ca2E1 State

P.04.01.15(CI74.60) | N. Asherie: Phase Behavior and

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

## Protein Interactions

**P.04.01.16(C174.61)** | I. Kuta Smatanova: Crystallization Study of Photosynthetic Proteins from *Pisum sativum*

**P.04.01.17(C174.62)** | K. Mizutani: The Crystal Structures of the Pseudouridine Synthases RluC and RluD

**P.04.01.18(C175.63)** | K. Kyunggon: Crystal Structure of PilF from *Pseudomonas aeruginosa*

**P.04.01.19(C175.64)** | A. Balan: Crystallization and Data Collection of *Xanthomonas citri* Maltose-Binding Protein

**P.04.01.20(C175.65)** | K. Tomoo: Crystal Structure of Ubiquitin-like Domain of Murine Parkin

**P.04.01.21(C175.66)** | L. Fonso: SERCA1a and Phospholamban Cocrystallisation

**P.04.01.22(C175.67)** | A.-M. Brandt: Structural Studies on Collagen Binding Integrin I domains

**P.04.01.23(C176.68)** | I. Laponogov: The Structure of the ParC Subunit of Topoisomerase IV from *Streptococcus pneumoniae*

**P.04.01.24(C176.69)** | X. Qiu: A Proposal to Engineer Protein Crystallization through Metal Ions

**P.04.01.25(C176.70)** | G. Lolli: The Crystal Structure of Human CDK7 and its Protein Recognition Properties

**P.04.01.26(C176.71)** | K. Hoffmann: Novel Vapour Diffusion Method

**P.04.01.27(C177.72)** | S. G. Goncalves: The Crystal Structure of Mannosylglycerate Synthase from

## Rhodothermus Marinus at 2.5 Å Resolution.

**P.04.01.28(C177.73)** | A. Armstrong: Local Conformational Similarity between Native and Denatured States

**P.04.01.29(C177.74)** | S. Hirano: Ubiquitin Binding Mechanism of Hrs-UIM

**P.04.01.30(C177.75)** | T. Satoh: Crystal Structures of the Carbohydrate Recognition Domain of Emp46p and Emp47p

**P.04.01.31(C178.76)** | M. Kawasaki: Molecular Mechanism of Ubiquitin Recognition by GGA3 GAT Domain

**P.04.01.32(C178.77)** | S. Rhee: Expression and Crystallization of Toxoflavin lyase(TflA) & TRP

**P.04.01.33(C178.78)** | A. Meents: Protein Crystal Quality Studies Using High Resolution X-ray Diffraction

**P.04.01.34(C178.79)** | G. Phillips: High-throughput Protein Crystallization at the Center for Eukaryotic Structural Genomics

**P.04.01.35(C178.80)** | M. Zimmerman: The Xtaldb System for Project Salvaging in High-throughput Crystallization

**P.04.01.36(C179.81)** | A. Lubambo: GIXD Investigation of GlnB of *H. Seropedicae* Adsorbed on Silicon.

**P.04.01.37(C179.82)** | J.-C. N. Poulsen: Using Multilayer Soft Lithography Formulator Chips to Map Precipitations Diagrams of Proteins

**P.04.01.38(C179.83)** | S. Simone: Metal Cations Effect on

## Membrane Crystallized Lysozyme

**P.04.01.39(C179.84)** | L. A. González-Ramírez: Mexicain, from the Crystal to the Structure: a Sixty Years Journey

**P.04.01.40(C180.85)** | A. Moreno: Do the Strong Magnetic Fields Modify the 3D Structure of Proteins?

## 3. Metallo-Enzymes

**P.04.03.6(C210.86)** | G. Oliva: Structure of Thi1: Thiamin Biosynthesis in *Arabidopsis thaliana*

## 11. Proteins of the Immune System

**P.04.11.1(C229.87)** | P. Mittl: The Crystal Structures of HcpB and -C: Two Proteins with SELL-like Repeat Architectures Involved in the Modulation of Innate Immune Response.

**P.04.11.2(C229.88)** | E. Debler: Structural Basis for Blue and Purple Fluorescence of Antibody-stilbene Complexes

**P.04.11.3(C230.89)** | P. A. Ramsland: Engineering Immune System Glycoproteins to Form Uniform Crystalline Lattices

**P.04.11.4(C230.90)** | M. Shiroishi: Crystal Structure of Leukocyte Ig-like Receptor 9 (LIR9/ILT11 /CD85f)

**P.04.11.5(C230.91)** | M. Koch: The Crystal Structure of Human CD1d with and without  $\alpha$ -Galactosylceramide Bound

**P.04.11.6(C230.92)** | T. J. Greenough: Structure, Function and Evolution of the Serum Pentraxins

**P.04.11.7(C230.93)** | K. Kitadokoro: Structural Studies of

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

<p>Human CD81 Extracellular Domain</p> <hr/> <p><b>16. Multi-domain Proteins</b></p> <p><b>P.04.16.1(C249.94)</b>   <u>D. Huang</u>: Identical Sets of Residues Produce Two Strikingly Different Dimers in NF-κB Family of Proteins</p> <hr/> <p><b>17. Structural Motifs</b></p> <p><b>P.04.17.1(C251.95)</b>   <u>R. Flraig</u>: Structural Basis for Cell-specific Activity of NGFI-B/Nurr1 Ligand-binding Domains</p> <p><b>P.04.17.2(C251.96)</b>   <u>Y. Hirano</u>: Structure of a Cell Polarity Regulator, an aPKC and Par6 PB1 Domain Complex</p> <hr/> <p><b>P.04.17.3(C252.97)</b>   <u>N. Pasquato</u>: The Allergenic Non-specific Lipid Transfer Protein from Peach:Structural Studies</p> <hr/> <p><b>P.04.17.4(C252.98)</b>   <u>T. Garrett</u>: LRRs: A Platform to Build a Protein Recognition Motif</p> <hr/> <p><b>24. Water and Other Solvent Structures In Macromolecules</b></p> <p><b>P.04.24.1(C261.99)</b>   <u>C. Carrell</u>: Comparative Study of Thrombin Binding of Potassium vs. Sodium</p> <hr/> <p><b>08 STRUCTURE/PROPERTY RELATIONSHIP</b></p> <p><b>10. Polymorphism and Isomorphism: Identification and Characterisation</b></p> <p><b>P.08.10.3(C336.100)</b>   <u>C. P. Brock</u>: The Many Crystal</p>	<p>Forms of [M(15-crown-5)(H<sub>2</sub>O)<sub>2</sub>](NO<sub>3</sub>)<sub>2</sub></p> <hr/> <p><b>15. No Sub-theme</b></p> <p><b>P.08.15.1(C351.101)</b>   <u>B. Courcot</u>: Approximate Reduced Density Matrix for Bioactive Systems: An <i>Ab-initio</i> Approach</p> <hr/> <p><b>P.08.15.2(C351.102)</b>   <u>E. Boanini</u>: Hydroxyapatite-bisphosphonate Nanocrystals</p> <hr/> <p><b>P.08.15.3(C352.103)</b>   <u>M. Hamadène</u>: The Ternary Fluoride Lithium at Low Temperature</p> <hr/> <p><b>14 CHARGE, SPIN AND MOMENTUM DENSITY</b></p> <p><b>7. Molecular and Crystal Properties From Charge Densities</b></p> <p><b>P.14.07.1(C425.104)</b>   <u>B. Rodrigues</u>: Experimental Electron Density of [Cu(phen)<sub>2</sub>Cl](NO<sub>3</sub>)(H<sub>2</sub>O)</p> <hr/> <p><b>P.14.07.2(C425.105)</b>   <u>E. Bendeif</u>: Phase Transition and Charge Density Study of the m-Carboxyphenyl Ammonium Phosphate</p> <hr/> <p><b>P.14.07.3(C425.106)</b>   <u>S. Novakovic</u>: Experimental Charge Density Study of Salicylaldehyde Thiosemicarbazone</p> <hr/> <p><b>P.14.07.4(C426.107)</b>   <u>M. Pitak</u>: Interactions in Selected Dicarboxylic Acids Derived from Electron Charge Density</p> <hr/> <p><b>P.14.07.5(C426.108)</b>   <u>G. Bogdanovic</u>: Experimental electron density distribution of Bis(thiosemicarbazide)-Zinc(II) Dinitrate</p> <hr/> <p><b>P.14.07.6(C426.109)</b>   <u>P. J. Becker</u>: Electron Density, the</p>	<p>Dirving Tool Towards Dynamics and Reactivity of Systems?</p> <hr/> <p><b>P.14.07.7(C426.110)</b>   <u>A. E. Whitten</u>: Estimating ADP's of Hydrogen Nuclei for Charge Density Analysis</p> <hr/> <p><b>P.14.07.8(C426.111)</b>   <u>D. Hashizume</u>: Bonding in 5-Membered Cyclic Alkynes: Charge Density in 1-Zirconacyclopent-3-yne</p> <hr/> <p><b>P.14.07.9(C427.112)</b>   <u>J. Kozisek</u>: Different Approaches to Absorption Corrections for Charge Density Analyses</p> <hr/> <p><b>P.14.07.10(C427.113)</b>   <u>K. Schwarz</u>: Chemical Bonding based on Charge Density Calculations for Solids</p> <hr/> <p><b>P.14.07.11(C427.114)</b>   <u>V. Tsirelson</u>: Electron-density Properties of the Functionally-Substituted Hydropyrimidines</p> <hr/> <p><b>P.14.07.12(C427.115)</b>   <u>Y.-C. Chuang</u>: Electron Density Study of 2,5-Dimethyl-3,4-trimethylene-6-a-thiophiphene Using XRD, XAS and DFT Calculations</p> <hr/> <p><b>P.14.07.13(C428.116)</b>   <u>S. Cameron</u>: An Examination of All the Inter-ion Interactions in (CH<sub>3</sub>)<sub>2</sub>N(H)CH<sub>2</sub>CH<sub>2</sub>N(H)(CH<sub>3</sub>)<sub>2</sub>(SCN)<sub>2</sub></p> <hr/> <p><b>P.14.07.14(C428.117)</b>   <u>G. Loupias</u>: Rb<sub>4</sub>C<sub>60</sub> Equation of States and Electronic Density Study by Compton Scattering</p> <hr/> <p><b>P.14.07.15(C428.118)</b>   <u>D. Wolstenholme</u>: An Examination of All the Inter-ion Interactions in Tetraphenylphosphonium Squarate</p> <hr/> <p><b>P.14.07.16(C428.119)</b>   <u>R. D. Poulsen</u>: X-ray Charge Density of a New Magnetic Metal Organic Framework,</p>
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# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

Mn<sub>3</sub>(C<sub>8</sub>O<sub>4</sub>H<sub>3</sub>)<sub>3</sub>(C<sub>5</sub>H<sub>11</sub>ON)<sub>2</sub>

P.14.07.17(C429.120) | D. Marabello: Charge Density of 1-Phenylpropane-1,2,3-Triyl Trinitrate

P.14.07.18(C429.121) | G. Gervasio: Ru<sub>3</sub>(CO)<sub>12</sub>. Why D<sub>3h</sub>?

P.14.07.19(C429.122) | C. M. Vande Velde: On the (Non)-Planarity of 1,2,4,5-Tetramethoxybenzene

## 16 CRYSTAL GROWTH: TECHNIQUES, INSTRUMENTATION AND APPLICATIONS

### 1. Systems that are Difficult to Crystallise

P.16.01.1(C437.123) | Y. Kim: Use of Reductive Methylation of Proteins to Increase Crystallization Efficiency at the Midwest Center for Structural Genomics

### 2. Industrial Mass Crystallisation

P.16.02.1(C437.124) | D. Frankel: Implementation of a Novel Protein Crystal Image Analysis Package

### 3. Crystal Growth from Solution and Gels

P.16.03.1(C437.125) | N. Piskunova: AFM Observation and Morphing-reconstruction of Dynamics of Crystal Growth

P.16.03.2(C437.126) | J. Novotny: Catalysed Growth of Doped TGS Single Crystals with Pt(IV) Ions

P.16.03.3(C437.127) | S. Kochetkov: Crystallization of Water-soluble Inorganic Salts in Microwave Field

P.16.03.4(C438.128) | N. Blagden: Monitoring Polymorphic Transformations in Solution

P.16.03.5(C438.129) | D. Vorontsov: Growth of the KDP Filamentary Crystals from Solution with Impurities

P.16.03.6(C438.130) | S. M. Dharmapakash: Crystal Growth and Characterization on Non-linear Optical L-Tyrosine Chloride

P.16.03.7(C438.131) | V. Manomenova: Growth of Cs<sub>2</sub>Ni(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O and Rb<sub>2</sub>Ni(SO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O and their Characteristics

P.16.03.8(C439.132) | A. Sanjoh: Protein Crystal Growth in Planar and Integrated Gel Interface Diffusion Device

P.16.03.9(C439.133) | M. Yamanaka: How to Optimize Gel-Tube Method

P.16.03.10(C439.134) | M. Sato: Optimized Crystallization Solution Analyzed From JAXA Cryoprotectant Database

P.16.03.11(C439.135) | S. Kaci: Optical and Morphological Properties of Lead Sulphide (PbS) Thin Films

P.16.03.12(C439.136) | Ö. Dogan: The Effect of Polyelectrolytes on Nano Hydroxyapatite Crystal Growth

P.16.03.13(C440.137) | E. Akyol: Morphological Control of Calcium Oxalate by Hydrophilic Block Copolymers

P.16.03.14(C440.138) | N. E. Chayen: Searching the Crystallisation Parameter Space using Evolutionary Algorithms

P.16.03.15(C440.139) | D. Suck: Crystallization Platform Integrating Screening & a Novel Optimization Strategy

4. Crystal Growth and Characterisation From the Melt

P.16.04.1(C440.140) | D. Ksenofontov:

Li<sub>3.17</sub>(P<sub>0.69</sub>Ge<sub>0.24</sub>Mo<sub>0.07</sub>)O<sub>4</sub>: Growth under Electrical Field and the Structure

P.16.04.2(C441.141) | S. K. Chaudhary: Phenomenon Of Polytypism In Melt Grown Layered Crystals Of CdI<sub>2</sub>, PbI<sub>2</sub> and CdBr<sub>2</sub>

P.16.04.3(C441.142) | K. Kokh: Nonstationary Heat Field as a New Approach in Bridgman Crystal Growth

P.16.04.4(C441.143) | F. Zavartsev: Growth and Crystal Structure of Bismuth Octaborate, α-Bi<sub>2</sub>B<sub>8</sub>O<sub>15</sub>

P.16.04.5(C441.144) | V. Mal'tsey: Flux Growth and Characterization of Gallium-substituted YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> Crystals

P.16.04.6(C441.145) | L. Ivleva: Characterization of Profiled LiNbO<sub>3</sub> and SBN Crystals by X-ray Diffraction

P.16.04.7(C442.146) | H. A. Dabkowska: Growth, Magnetic Behavior and Structure of Single Crystals of Pure and Mg Doped SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub>

### 5. Microgravity Crystallisation

P.16.05.1(C442.147) | M. Sato: JAXA-GCF Project -- High-quality Crystals Grown in Space for Structural Biology

P.16.05.2(C442.148) | H. Tanaka: Atomic Resolution Crystals Obtained in Viscous Crystallizing Condition in Space

### 6. Epitaxial Growth

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

P.16.06.1(C442.149) | V. Vonk: In-situ X-ray diffraction during Pulsed Laser Deposition

P.16.06.2(C443.150) | E. Volkova: Crystallization of RAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and R:YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> Single Crystal Layers

P.16.06.3(C443.151) | T. Ohachi: RHEED Observation of c-GaN on 3C-SiC/Si(001) Template Grown by RF-MBE

P.16.06.4(C443.152) | J. Olvera: Photoluminescence Study of Selenium Doped GaSb Layers Grown by Liquid Phase Epitaxy

## 7. Crystal Doping and Imperfections

P.16.07.1(C443.153) | L. H. Avanci: Substitutional and Interstitial Inclusions of Mn Additives onto the KDP Lattice

## 8. Self-assembled Crystals

P.16.08.1(C443.154) | A. Fiori: New Routes in Carbon Nanotube Synthesis by Means of a Modified Hot Filament Chemical Vapor Deposition Technique

## 10. Crystal Growth: Modelling, and Predicting Morphology

P.16.10.1(C444.155) | A. Askhabov: “Latent” Phase Clusters (Kvatarons) as Growth Units

P.16.10.2(C444.156) | C. Schvezov: Numerical Modeling of Interaction of Particles with Solidifying Crystals

P.16.10.3(C444.157) | N. Panina: Crystal Growth and Morphology Prediction of Two Quinacridone Polymorphs

P.16.10.4(C444.158) | H. Meekes: MONTY: an Algorithm for Predicting Growth Rates for any Crystal Structure in any Orientation.

## 12. Twinning: Acceptance and Avoidance

P.16.12.1(C445.159) | H. Grimmer: Lattice Aspects of Crystal Twinning

## 13. Polymorphism: Recognition and Applications

P.16.13.1(C445.160) | N. Shan: Selective Polymorph Transformation of Anthranilic Acid via Solvent-drop Grinding

P.16.13.2(C445.161) | S. Callear: Array Crystallisation for Functionalised Organics Using Different Variables

## 14. Low Temperature in situ Crystallisation

P.16.14.1(C445.162) | A. R. Choudhury: *In situ* Crystallization: Phase Transition and Polymorphism in Ionic Liquids

## 15. No Sub-theme

P.16.15.1(C446.163) | P. Nollert: Improved Crystal Detection of Protein Crystals by Bulk Contrast Enhancement

P.16.15.2(C446.164) | J.-P. Viola: How a New Chemical Compatibility Test Facilitates Protein’s Crystallization.

## 22 APERIODIC AND INCOMMENSURATE STRUCTURES

### 4. No Sub-theme

P.22.04.1(C477.165) | Q. Gu: Structural Study of Single Crystalline i-Zn-Mg-Dy at High Pressure and High

Temperature

P.22.04.2(C477.166) | H. Takakura: Framework Structure for Quasicrystal Models Based on Dense Icosahedral Sphere Packings

## 1. Data Collection and Structure Solution

P.22.01.1(C475.167) | J. Hadermann: Structure of LaSrCuO<sub>3.5</sub>

P.22.01.2(C475.168) | M. S. Rodriguez: HMT-Resorcinol: An Example of Modulated Structure in Substituted HMT Adducts.

P.22.01.3(C475.169) | I. Cisarova: The Way of Crystal of [cpMe<sub>2</sub>SiMe<sub>2</sub>N(t-Bu)]TiCl<sub>2</sub> from Disorder thru Modulation to Twinning

P.22.01.4(C475.170) | P. Oleynikov: Structure of the Pseudodecagonal Al-Co-Ni Approximant PD4

## 2. Identification and Refinement

P.22.02.1(C475.171) | M. Onoda: Diffuse Scattering from Composite Crystals Containing Stacking Faults

P.22.02.2(C476.172) | D. Deloudi: 5-D Modeling of the Co-rich Decagonal Al-Co-Ni Quasicrystal

P.22.02.3(C476.173) | L. Straver: Modulated Structure of [FeCl(DMPE)<sub>2</sub>(NCC<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>)][PF<sub>6</sub>] a Material for Use in NLO

P.22.02.4(C476.174) | R. Lifshitz: Dislocation Dynamics in a Dodecagonal Quasiperiodic System

## 3. Results and Applications

# FRIDAY, AUGUST 26, 2005 – POSTER SESSION

P.22.03.1(C476.175) | K. H. Hassdenteufel: Ab initio Simulations on the W-phase of the Al-Co-Ni system

P.22.03.2(C476.176) | B. Toudic: Interaction and Phase Transitions in a Pototype Self-assembled Supramolecular Aperiodic Crystal

## 25 INDUSTRIAL CRYSTALLOGRAPHY

### 1. Instrumentation and Techniques

P.25.01.1(C485.177) | A. Kitano: Characterization of Heteropoly Acids by X-ray Powder Diffraction at SPring-8

P.25.01.2(C485.178) | A. Lyuttsau: Convergent Beam Method in X-ray Diffractometry to Determine Single Crystal Cuts' Orientation

P.25.01.3(C485.179) | V. Kogan: New Model-free Method of Aberrations Correction for X-ray Powder Diffraction

### 2. Stress-Strain Analysis

P.25.02.1(C485.180) | T. Ishigaki: Residual Stress Measurements for Rocks by TOF Neutron Diffraction Methods.

P.25.02.2(C485.181) | P. Liu: Microstructural Evolution of Titanium Alloy (Ti-6Al-4V) after Metal Cutting Assisted by High Pressured Jet Cooling

### 3. On Line Diffraction Analysis

P.25.03.1(C486.182) | A. Gonzalez: New Tools to Integrate Data Analysis and Data Collection at SSRL: Web-Ice

### 7. Nanomaterials

P.25.07.1(C486.183) | S. K. Chatterjee: Study of Micro Structural Defect Parameters in Nickel Dispersed Silica Nano Composites by Warren-Averbach Method and Modified Rietveld Technique

P.25.07.2(C486.184) | D. Lamas: Synchrotron XRD Study of ZrO<sub>2</sub>-CeO<sub>2</sub> Nanopowders Synthesised by Gel-combustion

P.25.07.3(C486.185) | I. Dragomir-Cernatescu: Characterization of Individual Zincoxide Nano-belts by using X-Ray Nano-Diffraction Technique

P.25.07.4(C487.186) | M. Rossi: Structural Characterization of Hybrid Carbon Nanomaterials

P.25.07.5(C487.187) | V. Favre-Nicolin: Strain, Size and Composition of Buried GaN Quantum Dots in AlN Using Grazing Incidence Anomalous Diffraction

### 9. Thick Coatings

P.25.09.1(C487.188) | G. Lewis: Structure Indexing and Solution from Non-Ambient XRPD Data

### 10. Pharmaceutical Crystallography

P.25.10.1(C487.189) | N. Imayoshi: Structure Analysis of Pharmaceutical Compounds from Powder Diffraction Data

P.25.10.2(C488.190) | X. Solans: The Study on the Stability of a Drug. Can a Product Have Life?

P.25.10.3(C488.191) | S. Misaki: Ab-initio Structure Determination of Two Kinds of Forma for Adrenal Cortical Hormone, Prednisolone.

P.25.10.4(C488.192) | K. Suzuki: Crystal Structure of MC<sub>0.4</sub>-ACPT from *Thermus thermophilus* HB8

P.25.10.5(C488.193) | K. Miura: Pharmaceutical Application of Synchrotron X-ray Powder Diffraction at SPring-8

P.25.10.6(C489.194) | V. Giannellini: Mepivacaine Hydrochloride Polymorphs: a Drug Production Quandary

### 11. No sub-theme

P.25.11.1(C489.195) | H. J. Weyer: Retarding Effects of Cellulose Ethers on Early Portland Cement Hydration

P.25.11.2(C489.196) | A. Molenbroek: In situ studies of model High-Temperature Shift catalysts

## 26 CRYSTALLOGRAPHIC TEACHING

### 1. Changes in Teaching Methods for the Future

P.26.01.1(C491.197) | P. Kodess: Successfulness of a New Approach in Crystallographic Educator's Activity

P.26.01.2(C491.198) | J. Loehlin: Three Crystallographic Aids for Teaching Early Science Classes. Start Them Young!

### 4. Preparation for Publication; CIF Files; How Much?

P.26.04.1(C491.199) | A. Linden: Writing Papers for Section C of Acta Crystallographica

### 5. Crystallography on the World Wide Web

P.26.05.1(C491.200) | S. Stepanov: Internet-Based X-ray Server

SATURDAY, AUGUST 27, 2005 – KEYNOTE LECTURES

MORNING SESSION 8.30-9.30

Michelangelo (**KN 17**)

**KN17.27(C4)** | Harold Kroto:

Some New Insights in to the Mechanisms of  
Fullerene and Nanotube Formation

*Chair:* Ivano Bertini

AFTERNOON SESSION 17.30-18.30

Michelangelo (**KN 18**)

**KN18.27(C4)** | Louise N. Johnson:

Protein Kinase Inhibition and Substrate Recognition

*Chair:* John Helliwell

Botticelli (**KN 19**)

**KN19.27(C4)** | James A. Ibers:

Crystallography in Inorganic Solid-State Chemistry

*Chair:* Jan Boeyens

Cimabue (KN 20)

**KN20.27(C5)** | Michael Thackeray:

The Importance of Structure in the Design of Lithium  
Battery Materials

*Chair:* Peter G. Bruce

# SATURDAY, AUGUST 27 2005 – MORNING - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 44</b> )	Cimabue ( <b>MS 45</b> )	Brunelleschi ( <b>MS 46</b> )
10.00-10.05 Opening Remarks	<b>NUCLEIC ACIDS - TRANSCRIPTION, TRANSLATION AND REPAIR</b> <i>Chairs:</i> S. Neidle, E. Westhof	<b>PACKING OF ORGANIC MOLECULAR COMPOUNDS</b> <i>Chairs:</i> J. W. Steed, C. Brock	<b>IN-SITU OBSERVATION OF CRYSTAL GROWTH PROCESSES</b> <i>Chairs:</i> T. Ohachi, V. Kaganer
10.05-10.35	<b>MS44.27.1(C59)</b>   A.K. Aggarwal: Eukaryotic Translesion Synthesis DNA Polymerases: Structure and Function	<b>MS45.27.1(C60)</b>   L. Barbour: Porosity in Molecular Crystals	<b>MS46.27.1(C61)</b>   Y. Chu: Time-Resolved X-ray Topography Study on Growth of 180 Ferroelectric Domains
10.35-11.05	<b>MS44.27.2(C59)</b>   W. Yin: Mechanism for de Novo RNA Synthesis by T7 RNA Polymerase	<b>MS45.27.2(C60)</b>   C. Gervais: Exploring Structures and Structural Phenomena: The Derived Crystal Packing Model	<b>MS46.27.2(C61)</b>   W. Braun: <i>In-situ</i> Observation of Surface Kinetics During MBE Growth Using Synchrotron X-ray Diffraction
11.05-11.35	<b>MS44.27.3(C59)</b>   J. A. Doudna: Structural Basis for RNA-regulated Gene Expression	<b>MS45.27.3(C60)</b>   A. L. Gillon: Crystal Structure Analysis and Solid Form Selection in the Pharmaceutical Industry	<b>MS46.27.3(C62)</b>   G. Sazaki: <i>In-situ</i> Observation of Elementary Growth Steps on a Protein Crystal, Surface Diffusion of Protein Molecules and Dislocations Inside a Protein Crystal
11.35-12.05	<b>MS44.27.4(C59)</b>   R. Ficner: Structural Basis for Specific Recognition of the UsnRNP m <sub>3</sub> G-cap by Snurportin1	<b>MS45.27.4(C61)</b>   M. Kubicki: Different Reasons for Packing with Z'=2: 4-nitroimidazole Derivatives	<b>MS46.27.4(C62)</b>   E. Vlieg: Interface Crystallography of a Growing Interface: KDP{101} and {100}
12.05-12.35	<b>MS44.27.5(C60)</b>   E. C. M. Juan: Structural Basis for Antigene and Antisense Duplexes with Modified Nucleotides	<b>MS45.27.5(C61)</b>   L. R. Mac Gillivray: Directed Assembly and Covalent Capture of Supramolecular Architectures in the Solid State	<b>MS46.27.5(C62)</b>   A. Kharchenko: X-ray Diffractometer for <i>In-situ</i> and <i>Real-time</i> Monitoring of MOCVD

# SATURDAY, AUGUST 27 2005 – MORNING - MICROSYMPPOSIA

Leonardo da Vinci ( <b><i>MS 47</i></b> )	Giotto ( <b><i>MS 48</i></b> )	Donatello ( <b><i>MS 49</i></b> )	Botticelli ( <b><i>MS 43</i></b> )
<b>NOVEL MATERIALS UNDER HIGH PRESSURE</b> <i>Chairs: C. Pulham, N. Ross</i>	<b>MICROBEAM X-RAY SCATTERING</b> <i>Chairs: C. Riekel, A. Iida</i>	<b>CHARGE SPIN AND MOMENTUM DENSITIES IN MATERIAL SCIENCE</b> <i>Chairs: J. C. Spence, B. Iversen</i>	<b>EXTRACELLULAR PROTEINS AND CELLULAR ADHESION</b> <i>Chairs: A. Goldman, S. Narayana</i>
<b>MS47.27.1(C62)</b>   <u>T. Irifune</u> : Synthesis of Nano-polycrystalline Diamond and Related Hard Materials Using Multianvil Apparatus	<b>MS48.27.1(C63)</b>   <u>O. Paris</u> : Microbeam Diffraction of Hierarchical Nanocomposites	<b>MS49.27.1(C65)</b>   <u>T. Lippmann</u> : High-energy Synchrotron Radiation for Charge Density and Materials Science Experiments	<b>MS43.27.1(C58)</b>   <u>R. C. Liddington</u> : Integrins, Focal Adhesions and all That
<b>MS47.27.2(C62)</b>   <u>O. Degtyareva</u> : Combined Diffraction and Raman Studies on Incommensurately Modulated Host-guest Structures of Elements	<b>MS48.27.2(C64)</b>   <u>A. Cedola</u> : Engineered Bone from Bone Marrow Stromal Cells: a Structural Study by an Advanced X-ray Microdiffraction Technique	<b>MS49.27.2(C65)</b>   <u>B. Guillot</u> : Charge Density Studies of Ultra High Resolution Protein Structures	<b>MS43.27.2(C58)</b>   <u>G. Waksman</u> : The Chaperone-usher Pathway of Pilus Biogenesis: Structural Basis of the Assembly Process and of Host Recognition
<b>MS47.27.3(C63)</b>   <u>G. D. Gatta</u> : High-pressure Behavior of Feldspathoids: the Case of Analcite	<b>MS48.27.3(C64)</b>   <u>G. Ice</u> : Polychromatic Microdiffraction Measurements of Mesoscale Structure and Dynamics	<b>MS49.27.3(C65)</b>   <u>D. Stalke</u> : Hypervalency – Experimental Charge Density Uncovers a False Concept	<b>MS43.27.3(C58)</b>   <u>T. Izard</u> : Structural Relays in Adhesion Signaling
<b>MS47.27.4(C63)</b>   <u>D. Allan</u> : New High-pressure Forms of Simple Salts - Sulfates, Formates, and Acetates	<b>MS48.27.4(C64)</b>   <u>Y. Kagoshima</u> : SR X-Ray Microdiffraction Systems at SPring-8: Present Status and Applications	<b>MS49.27.4(C65)</b>   <u>J.-M. Zuo</u> : Measurements of Electron Densities in Solids	<b>MS43.27.4(C58)</b>   <u>S. Lea</u> : Complementing Pathogens or Structural Insights into Pathogen Evasion of the Complement System
<b>MS47.27.5(C63)</b>   <u>W. Mao</u> : Hydrogen Storage in Molecular Compounds	<b>MS48.27.5(C64)</b>   <u>C. Schroer</u> : Hard X-Ray Nanoprobe with Refractive X-Ray Lenses	<b>MS49.27.5(C65)</b>   <u>Y. Sakurai</u> : Orbital-wise Decomposition of Magnetic Compton Profiles and Spin Moments in UGe <sub>2</sub>	<b>MS43.27.5(C58)</b>   <u>J. Emsley</u> : Factor XI Structure Reveals a Novel Receptor Mediated Activation Pathway
			<b>MS43.27.6(C59)</b>   <u>A. Lundell</u> : Structural Studies of the CLD from Aggrecan

# SATURDAY, AUGUST 27 2005 - AFTERNOON- MICROSYMPOSIA

TIME	Michelangelo ( <i>MS 50</i> )	Cimabue ( <i>MS 51</i> )	Botticelli ( <i>MS 52</i> )
14.45-14.50 Opening Remarks	<b>ENZYMES AND ALLOSTERY</b> <i>Chairs: A. Wlodawer, S. Onesti</i>	<b>COMPLEMENTARY APPROACHES TO BIOLOGICAL STRUCTURE DETERMINATION</b> <i>Chairs: W. Chiu, L. Banci</i>	<b>INORGANIC-ORGANIC FRAMEWORK MATERIALS</b> <i>Chairs: C. Janiak, S. R. Batten</i>
14.50-15.20	<b>MS50.27.1(C66)</b>   <u>L. Lebioda</u> : Allostery and Heteroinhibition of Human Thymidylate Synthase	<b>MS51.27.1(C67)</b>   <u>R. F. Fischetti</u> : Estimating Protein Fold using Wide-angle Solution Scattering Data	<b>MS52.27.1(C68)</b>   <u>M. Schroder</u> : High Connectivity Framework Polymers: A New Co-ordination Chemistry
15.20-15.50	<b>MS50.27.2(C66)</b>   <u>M. Ishikawa</u> : Structural Basis for Substrate Channelling of a Fatty Acid $\beta$ -oxidation Multienzyme Complex	<b>MS51.27.2(C67)</b>   <u>J. Frank</u> : Cryo-electron Microscopy of the Ribosome: Methods of Fitting, and Inference of Dynamics	<b>MS52.27.2(C68)</b>   <u>J. Li</u> : Crystals and Nanostructures: A Unique Class of Tunable Inorganic-Organic Frameworks
16.50-16.20	<b>MS50.27.3(C66)</b>   <u>P. A. Williams</u> : Structural Biology of Cytochromes P450	<b>MS51.27.3(C67)</b>   <u>M. Schmid</u> : Structure of the Acrosomal Bundle, a Biological Machine, at 9.5 Å Resolution	<b>MS52.27.3(C68)</b>   <u>X.-M. Chen</u> : New Molecular Architectures of Copper Imidazolates and Triazolates
16.20-16.50	<b>MS50.27.4(C66)</b>   <u>W. Rypniewski</u> : The Structure of Yeast Phosphofructokinase 1	<b>MS51.27.4(C67)</b>   <u>C. Luchinat</u> : Beyond the Structure: How to Deal with Structural Disorder	<b>MS52.27.4(C69)</b>   <u>J. Pasán</u> : Influence of the Substituent in the Crystal Packing of Copper(II)-Malonates
16.50-17.20	<b>MS50.27.5(C67)</b>   <u>M. Rudolph</u> : Molecular Basis for MSD and Catalytic Mechanism of the Human Formylglycine Generating Enzyme	<b>MS51.27.5(C68)</b>   <u>G. Falini</u> : The Organization of the Organic Structural Framework in the Enamel Biominerization Processes	<b>MS52.27.5(C69)</b>   <u>O. Yaghi</u> : Hydrogen Storage in Metal-Organic Frameworks

# SATURDAY, AUGUST 27 2005 – AFTERNOON - MICROSYMPOSIA

Giotto ( <i>MS 53</i> )	Leonardo da Vinci ( <i>MS 54</i> )	Donatello ( <i>MS 55</i> )	Brunelleschi ( <i>MS 56</i> )
<b>MATERIALS FOR ENERGY CONVERSION AND STORAGE</b> <i>Chairs:</i> J. Irvine, T. Gustafsson	<b>CRYSTALLOGRAPHY AT CONDITIONS OF EARTH AND PLANETARY INTERIORS</b> <i>Chairs:</i> G. Fiquet, A. Oganov	<b>TIME RESOLVED DIFFRACTION</b> <i>Chairs:</i> J. Cao, H. Cailleau	<b>ANALYSIS COMBINING SANS AND SAXS EXPERIMENTS</b> <i>Chairs:</i> J. Teixeira, R. Triolo
<b>MS53.27.1(C69)</b>   <u>K. Edstrom</u> : Electrochemical Materials - Structure in Action	<b>MS54.27.1(C70)</b>   <u>T. Yagi</u> : Phase Transformation in FeO under Deep Mantle Conditions	<b>MS55.27.1(C71)</b>   <u>D. Boschetto</u> : Laser-Plasma X-ray Sources and their Applications	<b>MS56.27.1(C73)</b>   <u>M. Rawiso</u> : Hydrophobic Polyelectrolytes: Combined Small-angle Neutron and X-ray Scattering Studies
<b>MS53.27.2(C69)</b>   <u>J. Breger</u> : PDF and NMR Study of Ordering in the Positive Electrode Material Li(NiMn) <sub>0.5</sub> O <sub>2</sub>	<b>MS54.27.2(C70)</b>   <u>T. S. Duffy</u> : Compressibility and Structural Evolution of Post-perovskite Phase under Pressure	<b>MS55.27.2(C72)</b>   <u>K. Moffat</u> : How do Signaling Photoreceptors Respond to Light?	<b>MS56.27.2(C73)</b>   <u>G. Wignall</u> : The Utility of Absolute Calibration in SANS and SAXS Studies of Polymers and Colloids
<b>MS53.27.3(C70)</b>   <u>B. C. Hauback</u> : Hydrogen Storage in Light Complex Hydrides - Structural Studies	<b>MS54.27.3(C71)</b>   <u>A. Dewaele</u> : Refinement of High Pressure Metrology to 150 GPa	<b>MS55.27.3(C72)</b>   <u>R. J. D. Miller</u> : Femtosecond Electron Diffraction: Making the “Molecular Movie”	<b>MS56.27.3(C73)</b>   <u>D. Uhrikova</u> : The Structure of DNA+Cationic Liposome Aggregates Studied using SAXS and SANS
<b>MS53.27.4(C70)</b>   <u>P. Lacorre</u> : Structural Analysis of La <sub>2</sub> Mo <sub>2</sub> O <sub>9</sub> -based Fast Oxide-ion Conductors	<b>MS54.27.4(C71)</b>   <u>S. N. Luo</u> : Shock-Induced Superheating-Melting and Geophysical Implications	<b>MS55.27.4(C72)</b>   <u>X. Wang</u> : The Mechanism of Coherent Phonon Generation	<b>MS56.27.4(C73)</b>   <u>P. Callow</u> : The Subunit Arrangement of the Type I Restriction Modification Enzyme M.AhdI
<b>MS53.27.5(C70)</b>   <u>M. A. G. Aranda</u> : Interstitial Oxygen in Oxyapatites	<b>MS54.27.5(C71)</b>   <u>C. W. Glass</u> : Predicting Crystal Structures of New High-pressure Mineral Phases	<b>MS55.27.5(C72)</b>   <u>C. Curfs</u> : Time-resolved Diffraction Studies of the Combustion Synthesis of NiAl/TiC Composite	<b>MS56.27.5(C74)</b>   <u>A. Hoell</u> : Nanostructure and Ordering in Magnetic Liquids Probed by SAXS and SANS

## SATURDAY, AUGUST 27 2005 – OTHER ACTIVITIES

### OPEN COMMISSION MEETINGS

Brunelleschi (12.35-14.35)

#### OCM05 COMMISSION ON INORGANIC AND MINERAL STRUCTURE

*Chair:* Giovanni Ferraris

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**OCM05.27.1(C129) | E. Makovicky:**

Modular Aspects of Inorganic and Mineral Structures

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**OCM05.27.2(C130) | S. Merlino:**

OD Approach in Natural and Synthetic Inorganic Compounds: an Useful Tool in Structure Solving and Structure Modeling

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**OCM05.27.3(C130) | I. D. Brown:**

Graph Theory, Symmetry and Inorganic Solids

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**OCM05.27.4(C130) | R. Allmann:**

News about the Inorganic Crystal Structure Database ICSD

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**OCM05.27.5(C130) | M. Matsui:**

Pressure Calibration Standard at High Temperature and High Pressure

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**OCM06.27.6(C131) | D. Pushcharovsky:**

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Crystal Structures of Two Iron-containing Minerals:  
Sturmanite and Biraite-(Ce) (a New Mineral)

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Giotto (12.35-14.35)

#### OCM06 COMMISSION ON CHARGE, SPIN AND MOMENTUM DENSITIES

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*Chair:* Claude Lecomte

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Leonardo da Vinci (12.35-14.35)

#### OCM07 COMMISSION ON INTERNATIONAL TABLES OF CRYSTALLOGRAPHY

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*Chair:* Hartmut Fuess

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**OCM07.27.1(C131) | H. Fuess:**

International Tables. The Present and Future

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**OCM07.27.2(C131) | N. Ashcroft:**

International Tables for Crystallography Online

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**OCM07.27.3(C131) | D. B. Litvin:**

International Tables: Volume E

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**OCM07.27.4(C131) | A. Authier:**

Volume D of Int. Tables: "Physical Properties of Crystals"

## SATURDAY, AUGUST 27 2005 - OTHER ACTIVITIES

### **OCM07.27.5(C132) | U. Mueller:**

International Tables for Crystallography, Volume A1

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### **OCM07.27.6(C132) | S. R. Hall:**

Volume G: Definition and Exchange of Crystallographic Data

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### **OCM07.27.7(C132) | T. Hahn:**

Status of Volume A: Space-Group Symmetry

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### **OCM07.27.8(C132) | U. Shmueli:**

Status of Volume B: Reciprocal Space - Planned 3rd Edition

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### **OCM07.27.9(C132) | E. Arnold:**

Update on International Tables for Crystallography Volume F

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### **OCM07.27.10(C133) | E. Arnold:**

Intl Tables for Crystallography Vol F1, Space-Group Symmetry for Structural Biology

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## **ROUND TABLE ON DATA MINING FROM PDB**

Cimabue (12.35-14.35)

*Chairs: Helen Berman, Kim Henrick*

### **Speakers:**

#### Helen Berman:

An Introduction to the wwPDB

#### Kim Henrick:

Data Mining the PDB through the MSD Interface

#### Haruki Nakamura:

Data Mining the PDB through the PDBj Interface

#### Phil Bourne:

Data Mining the PDB through the RCSB Interface

## **Discussion**

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## **COMPUTER FAYRE Ghirlandaio**

(10.00-12.00)      J. Kopf:

GUI-design with the Qt C++ Class Library: Four crystallographic 'Open Source' Programs

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(15.00-17.00)      C. Weeks, W. Furey:

Automated Protein Phasing Program, BnP  
(two 1 hour sessions)

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

## 01 INSTRUMENTATION AND EXPERIMENTAL TECHNIQUES

### 10. Area Detectors (Multi-wire, Image Plate, CCD)

**P.01.10.1(C145.1)** | K. Sugimoto: A New Area Detector for Ultra-fast X-ray Diffraction Analysis

**P.01.10.2(C145.2)** | J. Hester: Obtaining Accurate Lattice Parameters from Debye-Scherrer Image Plate Data

**P.01.10.3(C145.3)** | K. Hasegawa: Data Collection System for Protein Crystallography using CMOS Image Sensor

**P.01.10.4(C145.4)** | N. Yagi: CMOS Flatpanel Detectors for SAXS/WAXS Experiments

**P.01.10.5(C146.5)** | M. Fransen: 1- and 2D Detectors and Sample Fluorescence in XRD.

**P.01.10.6(C146.6)** | C. Campana: Use of a Single Crystal Diffractometer and CCD Area Detector for Phase Identification

**P.01.10.7(C146.7)** | K. Tanaka: IP Slant-incidence Correction for Accurate Structure Factor Measurements

### 11. Data Accuracy and Detectors

**P.01.11.1(C146.8)** | N. BouDET: XPAD: a Pixel Detector for Material Sciences

**P.01.11.2(C147.9)** | B. N. Kodess: Metrological Assurance of the Substance and Materials Investigations by Diffraction Methods

**P.01.11.3(C147.10)** | I. Dix: The EU BIOXHIT Standard Test Crystal

**P.01.11.4(C147.11)** | A. Korsunsky: Strain Analysis Using

**B50**

## High Energy X-ray White Beam Diffraction

**P.01.11.5(C147.12)** | A. Coetze: Improving Data Quality without Having to Grow New Crystals

**P.01.11.6(C147.13)** | M. M. Benning: High Resolution Data Collection in the Home Lab

## 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

### 2. Enzymes and Enzyme Catalysis

**P.04.02.21(C185.14)** | R. Felts: The Crystal Structure of *Francisella tularensis* AcpA

**P.04.02.43(C190.15)** | D. Shi: Structures of A Novel N-acetyl-L-ornithine Transcarbamylase

**P.04.02.44(C190.16)** | Y.-J. Sun: Crystal Structure of Spermidine Synthase from *Helicobacter pylori*

**P.04.02.45(C190.17)** | K. Nishio: Helix-formation Due to the Binding of  $\alpha$ - with  $\beta_2$ -subunit of Tryptophan Synthase

**P.04.02.46(C190.18)** | W. Iwasaki: Structure of Stationary Phase Survival Protein SurE from *Thermus thermophilus*

**P.04.02.47(C191.19)** | Z. Fujimoto: Crystal structure of *Mortierella vinacea*  $\alpha$ -galactosidase I

**P.04.02.48(C191.20)** | K. Arita: Structural Basis for  $\text{Ca}^{2+}$ -induced Activation of Human PAD4

**P.04.02.49(C191.21)** | T. Nonaka: The Crystal Structure of a Novel Subtilisin-like Alkaline Serine Protease, KP-43

**P.04.02.50(C191.22)** | S. Watanabe: Crystal Structure of Atypical Cytoplasmic ABC-ATPase SufC

**P.04.02.51(C192.23)** | A. Gustchina: Comparisons of the Structures of Isolated Proteolytic Domains of Lon Proteases

**P.04.02.52(C192.24)** | H.-M. Chu: Structures and Function Studies of Microbial P-loop-containing Phosphatases

**P.04.02.53(C192.25)** | Y. Kezuka: Structure of a Two-domain Chitinase from *Streptomyces griseus*

**P.04.02.54(C192.26)** | R.-T. Guo: Structure-based Functional Analysis of Prenyltransferases: Trans-type OPPs from *T. maritima* and Cis-type UPPs from *E. coli*

**P.04.02.55(C193.27)** | Z. Fu: Crystal Structure of Human HMG-CoA Lyase

**P.04.02.56(C193.28)** | B. Mikami: Structural Analysis of Thr342 Mutants of Soybean  $\beta$ -Amylase: The Role of Conformational Changes of Two Loops in the Catalytic Mechanism

**P.04.02.57(C193.29)** | Y. Sato: Crystal Structure of the Haloalkane Dehalogenase DbjA

**P.04.02.58(C193.30)** | Z. Cao: Structure-Function Analysis of a Novel Mitochondrial Antioxidant Protein

**P.04.02.59(C193.31)** | H. J. Kang: Structural Studies on Novel Streptococcal Virulence Factors

**P.04.02.60(C194.32)** | K. Ida: Crystal Structure of L-phenylalanine Oxidase

**P.04.02.61(C194.33)** | T. Hisano: Crystal Structure of a Biopolyester-hydrolyzing Enzyme PHA Depolymerase

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

P.04.02.62(C194.34) | Y. Hagiwara: Crystal Structure of PcyA-biliverdin IX $\alpha$  complex

P.04.02.63(C194.35) | Y. Naoe: Structural Studies of Rat Calcineurin B Homologous Protein 1

P.04.02.64(C195.36) | H. Nii: Structure of  $\gamma$ -glutamylcysteine Synthetase Complexed with Buthionine Sulfoximine

P.04.02.65(C195.37) | T. Hibi:  $\gamma$ -glutamylcysteine Synthetase: Peptide Formation Coupling with ATP Hydrolysis

P.04.02.66(C195.38) | R. Jauch: Structures of Mnk-2 Reveal Novel Aspects of Kinase Regulation

P.04.02.67(C195.39) | A. Pearson: Tracking X-ray Derived Redox Changes Using Single Crystal Microspectrophotometry

P.04.02.68(C195.40) | N. Sekulic: Crystal Structures of Two Domains of Bifunctional Enzyme: Human PAPS Synthetase

P.04.02.69(C196.41) | Y. Umena: Structures of Arg-181 Mutant and Wild Type of L-lactate Oxidase from *A. viridans*

P.04.02.70(C196.42) | J. Ding: Structure of Small GTPase Human Rheb Provides a Structural Basis for its Unique Biological Function and Reveals a Novel GTP Hydrolysis Mechanism

P.04.02.71(C196.43) | E. Papinutto: Crystal Structure of Alkyl Hydroperoxide-reductase (AhpC) from *Helicobacter pylori*

P.04.02.72(C196.44) | M. Prabu-Jeyabalan: A Representation of a Possible Intermediate Step during Substrate Recognition of HIV-1 Protease: Crystal Structures of Substrate Bound Enzyme Exhibiting a Novel Flap Conformation.

P.04.02.73(C197.45) | C. De Ranter: Detecting the Structural Determinants of Glycosyl Hydrolase Family 11 Xylanase Inhibition

P.04.02.74(C197.46) | S. B. Gabelli: The Mechanism of *T. cruzi* FPPS Involves a Substrate Induced Conformational Change

P.04.02.75(C197.47) | M. Fujihashi: Crystallographic Analysis Identifies a Novel Enzymatic Reaction

P.04.02.76(C197.48) | K. Fukuyama: Structural Basis for the Methylation Mechanism in Methyl-transferase BchU Involved in Bacteriochlorophyll c Biosynthesis

P.04.02.77(C198.49) | T. Nakamura: Crystal Structure of hMTH1 in Complex with its Reaction Product, 8-oxo-dGMP

P.04.02.78(C198.50) | H. Tsuge: The Crystal Structure of L-proline Dehydrogenase in a Hyperthermophilic Archaeon

P.04.02.79(C198.51) | I. Miyahara: Double Substrate Recognition of Acetylornithine Aminotransferase

P.04.02.80(C198.52) | M. Senda: Detection of the Conformational Changes of FAD during the Catalysis

P.04.02.81(C198.53) | T. Senda: Crystal Structure of Biphenyl Dioxygenase

P.04.02.111(C205.54) | A. M. Silva: The Structure of *Yersinia pestis* Dehydroquinase

## 3. Metallo-Enzymes

P.04.03.14(C211.55) | I. M. Mavridis: Structure of the 2[4Fe-4S] Ferredoxin from *Pseudomonas aeruginosa* at 1.32 Å Resolution

## 7. Protein - RNA Interactions

P.04.07.3(C225.56) | Y. Maeda: Crystal Structure of *Sulfolobus tokodaii* Aspartyl-tRNA Synthetase

## 13. Viruses and Viral Proteins

P.04.13.1(C235.57) | S. Mario: Structural Differences Between B and F Subtypes of HIV PR

P.04.13.2(C235.58) | F. Akita: X-ray Crystallographic Structure of Virus like Particle from Hyperthermophilic Archaea *Pyrococcus furiosus*

P.04.13.3(C235.59) | T.-W. Lee: Structures of SARS Coronavirus Main Protease Bound by an Aza-peptide Epoxide

P.04.13.4(C236.60) | S. Violot: EED, a Cellular Partner of the Viral Proteins MA, IN and Nef from HIV-1

P.04.13.5(C236.61) | K. Ratia: Kinetic and Crystallographic Analyses of SARS Coronavirus 3CLpro Inhibitors

P.04.13.6(C236.62) | R. Jokiah: Crystallization of Recombinant HIV-1 Nef

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

<p><b>P.04.13.7(C236.63)</b>   C.-H. Hsu: Structural and Immunological Characterization of the Fusion Core of the SARS-coronavirus Spike Protein</p>	<p><b>Compounds</b></p>	<p><b>P.08.14.14(C344.80)</b>   E. Tyunina: The Bond Valence Model and Point Defects in Langasite Family</p>
<p><b>P.04.13.8(C237.64)</b>   C. Bourne: Structural Study of Hepatitis B Virus Capsid Polymorphism and Stabilization</p>		<p><b>P.08.14.15(C344.81)</b>   B. Muktha: Synthesis, Structure and Photocatalysis in LiBi<sub>4</sub>Ta<sub>3</sub>O<sub>14</sub> and LiBi<sub>4</sub>Nb<sub>3</sub>O<sub>14</sub></p>
<p><b>18. Organelles</b></p>		<p><b>P.08.14.16(C344.82)</b>   N. Van Tri: Peculiarities of the Electronic Structure and Dynamics in the Nanosystems</p>
<p><b>P.04.18.1(C252.65)</b>   M. Igura: Cracking of the Targeting Signal Embedded in Mitochondrial Presequences</p>		<p><b>P.08.14.17(C344.83)</b>   J. Haines: High-temperature Structural Disorder in <math>\alpha</math>-Quartz-Type Piezoelectric Materials</p>
<p><b>26. No sub-theme</b></p>		<p><b>P.08.14.18(C344.84)</b>   G. Kuz'micheva: Unusual Structural Properties of (Na,Gd,Yb)WO<sub>4</sub> and (Na,La,Ce,Er)MoO<sub>4</sub></p>
<p><b>P.04.26.7(C266.208)</b>   U. Honisch: Advanced High-Throughput Platforms for Protein Crystallography</p>		<p><b>P.08.14.19(C345.85)</b>   H. Homeida: Lattice Parameters Measurements of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-<math>\delta</math></sub> Superconductors Prepared under Various Forming Pressures using X-ray Diffraction Technique</p>
<p><b>08 STRUCTURE/PROPERTY RELATIONSHIP</b></p>		<p><b>P.08.14.20(C345.86)</b>   S. A. Barannikova: On a New Wave Type Generated in Deforming Metal Crystals</p>
<p><b>13. Hydrogen Bonding Studies</b></p>		<p><b>P.08.14.21(C345.87)</b>   L.-C. Wu: Structure and Magnetic Properties of 3-substituted-5-(2-pyridyl) Pyrazole Metal(II) Complexes</p>
<p><b>P.08.13.10(C340.66)</b>   M. T. Duarte: From Carboxylic Precursors to Thioxanthones: Interplay of Hydrogen Bonds, Br<sup>-</sup>Nitro, S<sup>-</sup>Carbonyl and <math>\pi</math><sup>-</sup><math>\pi</math> Stacking Interactions</p>		<p><b>P.08.14.22(C345.88)</b>   Y.-C. Lin: X-ray Absorption Studies of Fe-btr Spin Crossover Complexes</p>
<p><b>14. Structure Property Relationship</b></p>		<p><b>P.08.14.23(C345.89)</b>   V. Ilyasov: Change of Structure and Properties of System WC-Ti at Mechanical Activation</p>
<p><b>P.08.14.1(C340.67)</b>   T. Bezrodna: Structure Peculiarities of Polydisperse TiO<sub>2</sub> Particles with Metal-modified Surface</p>		<p><b>P.08.14.24(C346.90)</b>   J. Scherer: Search for Polarons in Li<sub>1-<math>\delta</math></sub>Nb<sub>1-<math>\delta</math></sub>O<sub>3-<math>\delta</math></sub>. Structural Investigation of the Defect Structure in Thermally Reduced Single Crystals</p>
<p><b>P.08.14.2(C341.68)</b>   O. Alekseeva: Structural Conditionality of Physical Properties in Nb or Sb Doped KTP Crystals</p>		
<p><b>P.08.14.3(C341.69)</b>   A. V. Vologzhanina: Lanthanides Stereochemistry in the Structure of Oxygen containing</p>		

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

**P.08.14.25(C346.91)** | R. E. Gladyshevskii: Structural Origin of the Low Superconducting Anisotropy of Bi,Pb-2212 Crystals

**P.08.14.26(C346.92)** | D. Capsoni: Structure Investigation of Pure and Cr Doped Li<sub>2</sub>VO<sub>4</sub>

**P.08.14.27(C346.93)** | S. Vachieri: Structures of *C. perfringens* *a*-toxin mutant, T74I, that Affects its Activity

**P.08.14.28(C347.94)** | I. A. Guzei: An Improved Method for Calculating Ligand Solid Angles

**P.08.14.29(C347.95)** | C.-H. Lee: The Perpendicular Magnetic Anisotropy Effect and the Directional Structure Ordering of CrPt<sub>3</sub> the Epitaxial Films

**P.08.14.30(C347.96)** | M. Suzuki: Distribution of Sr Ions in Tungstenbronze-type-like (Ba<sub>1-x</sub>Sm<sub>x</sub>)<sub>6-3x</sub>R<sub>8+2x</sub>Ti<sub>18</sub>O<sub>54</sub> (*R* = Sm, Nd) Solid Solutions

**P.08.14.31(C347.97)** | I. Leban: Structural Investigation of Cyclamic Acid and Related Cyclamates

**P.08.14.32(C347.98)** | H. Ohsato: Structure and Microwave Dielectric Properties on *ALa*<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub> (*A* = Ba, Sr and Ca)

**P.08.14.33(C348.99)** | H. N. Bordallo: Extraordinary Negative Thermal Expansion in the Smallest Chiral Amino Acid, Alanine

**P.08.14.34(C348.100)** | S. Mazumder: Structure Evolution and Magnetoelectricity in BaO-TiO-FeO-CoO system at R.T.

**P.08.14.35(C348.101)** | X. Chen: Negative Refraction: an

## Intrinsic Property of Uniaxial Crystals

**P.08.14.36(C348.102)** | M. Helliwell: Unravelling the Mechanism of the Bathochromic Shift in the Lobster Carapace

**P.08.14.37(C348.103)** | Y. Kado: Crystal Structure of Hematopoietic Prostaglandin D Synthase Complexed of HQL-79

**P.08.14.38(C349.104)** | F. Arod: Polymorphism and Photochromism of Salicylideneaniline

**P.08.14.39(C349.105)** | F. Cargnoni: Structure, Chemical Bonding and Thermoelectric Performance of Zn<sub>4</sub>Sb<sub>3</sub>

**P.08.14.40(C349.106)** | I. G. Lesci: Synthetic Chrysotile: Effect of Foreign Ions on the Hydrothermal Synthesis

**P.08.14.41(C349.107)** | E. L. Thomas: Structural Comparisons of Three Intermetallic Antimonide Families

**P.08.14.42(C350.108)** | J. N. Millican: The Crystal Growth and Structure and Property Relationships of Pr-Ni-Ga Phases

**P.08.14.43(C350.109)** | M. Shiina: Structural Basis for the Diverse DNA Sequence Recognition by C/EBPâ Homodimer

**P.08.14.44(C350.110)** | S. Cenedese: *Ab-initio* Modeling of Electronic Transport Properties: A Structural Informer

**P.08.14.45(C350.111)** | C. H. Schwalbe: Crystal Structures and Physical Properties of Flurbiprofen Salts

**P.08.14.46(C351.112)** | I. C. Santos: The Role of Cation on the Crystal Packing of the Molecular Conductors Based

## on Ni(dcdmp)<sub>2</sub>

**P.08.14.47(C351.113)** | F. Artizzu: Structure and Emission Properties of Erbium Quinolinolate Complexes

## 10 INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES 5. Minerals: Characterisation Methods and Structures

**P.10.05.1(C375.114)** | Y. A. Golubev: Research of Nanostructurized X-ray Amorphous Minerals by AFM

**P.10.05.2(C376.115)** | M. C. Dalconi: Distinct Local Environments for Ca in Pyrope-Grossular Garnets: A New Model based on XRD and EXAFS Studies

**P.10.05.3(C376.116)** | O. A. Blatova: Analysis of Microporous Crystal Structures with Voronoi-Dirichlet Polyhedra

**P.10.05.4(C376.117)** | E. Domoroshchina: Langasite Crystals: Growth, Composition and Physical Properties

**P.10.05.5(C376.118)** | H. Boller: Ponomarevite, K<sub>4</sub>Cu<sub>4</sub>OCl<sub>10</sub>, a Naturally Occurring Mineral with a [Cu<sub>4</sub>O] Core – Ancestor of Many Synthetic Cluster Compounds

**P.10.05.6(C377.119)** | F. M. Michel: Resolving Structure and Size of Amorphous Mineral Precipitates by PDF Analysis

**P.10.05.7(C377.120)** | T. Echigo: Crystal Structures of Rb<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>H<sub>2</sub>O and Tl<sub>2</sub>(C<sub>2</sub>O<sub>4</sub>): Application of Valence Matching Rule

**P.10.05.8(C377.121)** | D. S. Sergeev: Structure and Composition Properties of Mica from Ilmen Reserve Granite Pegmatites

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

P.10.05.9(C377.122) | G. Capitani: XRD and HRTEM

Structural Analyses of Antigorite Polysomes

P.10.05.10(C378.123) | F. Nishi: Two kinds of

Superstructures of (Ge, Si) Wollastonite

P.10.05.11(C378.124) | A. Kyono: Light-Induced

Degradation Dynamics in Realgar ( $\text{As}_4\text{S}_4$ )

P.10.05.12(C378.125) | R. Oberti: A Revision of the

Structure and Crystal-Chemistry of the Arrojadite-Group

P.10.05.13(C378.126) | S. Geiger: Supramolecular

Arrangement of Tensioactive Molecules in Interlayer  
Spaces of Organophilic Clays

P.10.05.14(C378.127) | E. Mesto: Ti-Investigation by XPS

of Biotite from Metapelites of El Joyazo (Spain)

P.10.05.15(C379.128) | B. Lavina: Mg, Al, Si, Ca -

Bearing Magnetite from Korshunovskoe, East Siberia

P.10.05.16(C379.129) | J. Rius: Analysis of Structure

Factors of 2D-connected Crystal Structures

P.10.05.17(C379.130) | R. I. Kassimova: The Spinsels Unit

Cell Parameter as Diamond Potentially Indicator

P.10.05.18(C379.131) | M. Pósfai: Variations in the

morphologies and magnetic properties of magnetite  
crystals in bacteria

P.10.05.20(C380.133) | F. Liziero: Crystal Structure of

Non-Metamict Minerals of Chevkinite Group

11 CRYSTALLOGRAPHY IN MATERIAL SCIENCE

1. Superconducting and Semi-Conducting Materials

P.11.01.1(C385.134) | G. Schuck: Structure/Properties Relationships in doped  $\text{MgB}_2$  Single Crystals

P.11.01.2(C385.135) | A. Soshnikov: The Investigation of

Crack Propagation in Cleavage Directions on the Surface of  $\text{SiC}$  by Sclerometry

P.11.01.3(C385.136) | E. Giannini: Superstructures of Pb-

free and Pb-doped  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$  Superconducting Phases

P.11.01.4(C385.137) | J. E. Lorenzo: Presence of an ionic

charge ordering at the Verwey transition in  $\text{Fe}_3\text{O}_4$ : a Resonant X-ray Diffraction Study

P.11.01.5(C385.138) | W. Wong-Ng: Crystal Chemistry

and Crystallography of the  $\text{Ba}_2\text{RCu}_3\text{O}_{6+x}$  -  $\text{SrTiO}_3$  System

P.11.01.6(C386.139) | O. Dyachenko: New Molecular

Conductors based on  $[\text{Ni}(\text{dmid})_2]$  with TMTTF, TTF and ET as Cations

P.11.01.7(C386.140) | R. Tazaki: Novel Style of Structure

Determination for  $\pi$ -d System by Synchrotron X-ray Diffraction

P.11.01.8(C386.141) | H. Wondergem: Twin Formation in InP Nanowires Epitaxially Grown on Germanium and Silicon

P.11.01.9(C386.142) | F. Duc: Low Temperature

Structural Investigations of the  $J_1$ - $J_2$  Model System  $\text{VOMoO}_4$

P.11.01.10(C387.143) | B. Papadopoulos: Comparison and

Analysis of the Samples with same Synthesis of  $\text{Bi-Sr-Ca-Cu-O}$ , Prepared by Different Ways of Heating

P.11.01.11(C387.144) | C. Stergiou: Crystallographic Study of Superconducting Series  $\text{Nd}_{1+x}\text{Ba}_{2-x}\text{Cu}_3\text{O}_y$  ( $x = 0, 0.0, 0.2, 0.4, 0.6$ ), Prepared at 850°C and 860°C

P.11.01.12(C387.145) | S. Yilmaz: Crystallographic Study of Samples Produced from Mixtures  $\text{La}_{1+x}\text{Ba}_{2-x}\text{Cu}_3\text{O}_y$  ( $x = 0.0, 0.2, 0.4, 0.6$ ), Heated at 850°C and 860°C

## 3. Giant Magneto Resistance Materials

P.11.03.1(C387.146) | H. L. Bhat: Growth and Structural Investigations on Lead-doped  $\text{NdMnO}_3$  Single Crystals

P.11.03.2(C387.147) | S. Hosokawa: Atomic Image of Diluted Magnetic Semiconductor  $\text{Zn}_{1-x}\text{Mn}_x\text{Te}$  Obtained by X-ray Fluorescence Holography

P.11.03.3(C388.148) | Y. Elerman: Investigation of  $\text{LaMn}_{2-x}\text{Fe}_x\text{Si}_2$  ( $0 \leq x \leq 1.2$ ) by Magnetic Measurements and Neutron Diffraction

P.11.03.4(C388.149) | A. Balagurov: Structural Reasons for the Giant Oxygen Isotope Effect in  $\text{Re}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$  Perovskites

## 5. Non-crystalline Materials

P.11.05.1(C388.150) | O. Kovaleva: X-ray Study of the Native Solid Hydrocarbons Transformation

P.11.05.2(C388.151) | D. Kamashov: The Influence of Synthesis Conditions on the Packing of the Spherical Particles of Silica in a Supramolecular Structure

P.11.05.3(C389.152) | T. Grygar: Quantitative Analysis of Poorly Crystalline  $\text{Fe}_2\text{O}_3$  Specimens

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

P.11.05.4(C389.153) | G. Navarra: Revisitation of the Structural Models for Ferrihydrites

## 6. Ceramics, Glasses and Amorphous Materials

P.11.06.1(C389.154) | F. Capitelli: Crystal Structure of New Lanthanide Diphosphates

P.11.06.2(C389.155) | I. N. Robu: Roman Ceramics in the Transylvanian Basin (Romania)

P.11.06.3(C390.156) | J. Popovic: Cobalt Incorporation in Mullite

P.11.06.4(C390.157) | A. Meden: Rietveld Refinement of Solid Solutions of La<sub>2</sub>TiO<sub>5</sub> and La<sub>4</sub>Ga<sub>2</sub>O<sub>9</sub>

P.11.06.5(C390.158) | A. Thalal: Comparative Study between Synthesized Zn<sub>2-x</sub>Co<sub>x</sub>SiO<sub>4</sub> and Cobalt-base Pigments

P.11.06.6(C390.159) | L. Bucio: Rietveld Analysis in Biological Apatite Composite Tissues

P.11.06.7(C390.160) | J. Martinez: Structural Characterization of CdCO<sub>3</sub>-CdS by X-ray

## 8. Polymers

P.11.08.3(C391.161) | Y. Nozue: Deformation Process of Polymer Spherulite Observed with Microbeam-SAXS and -WAXS

## 10. Nonlinear Optical and Electronic Materials

P.11.10.1(C393.162) | E. Kharitonova: Growth and Properties of KTiOPO<sub>4</sub> Single Crystals Doped with Er and Nd

P.11.10.2(C393.163) | A. Forni: Second-Order Nonlinear Optical Properties of Tetradentate Schiff base Complexes

P.11.10.3(C393.164) | R. Ochrombel: Temperature Dependence of Refractive Indices in Selected Borates

P.11.10.4(C393.165) | L. Bayarjargal: Nonlinear Optical Properties of Lithium Sulfate Monohydrate, Li<sub>2</sub>SO<sub>4</sub>•H<sub>2</sub>O

P.11.10.5(C394.166) | C. G. Pozzi: Neutron Diffraction Study of 4-Nitroaniline at 100 K

P.11.10.6(C394.167) | S. Hara: Cation Distribution in Eu<sup>2+</sup>- and/or Eu<sup>3+</sup>-Containing Inorganic Compounds

P.11.10.7(C394.168) | E. Borca: Synthesis and Characterization of Nanocrystalline Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub> derived by a Sol-Gel Method

P.11.10.8(C394.169) | E. Tkalcic: Structural Study of Sn-doped In<sub>2</sub>O<sub>3</sub>

P.11.10.9(C395.170) | J. C. M. Gustafsson: Electron Density in Ga doped RTP

P.11.10.10(C395.171) | B. Grzeta: Structural Changes of Sol-Gel derived Sn-doped In<sub>2</sub>O<sub>3</sub> due to Annealing at 1000 C

P.11.10.11(C395.172) | L. Pilia: Push-Pull Mixed-Ligand d<sup>8</sup>-Metal Dithiolene Complexes

## 12. Ferroic and Ferroelectric Structures

P.11.12.1(C398.173) | P. Pacek: Lattice Parameters of the PZT 90/10 Ceramic doped with La

P.11.12.2(C398.174) | D. Swain: Structural Phase Transitions and Hydrogen Bonding in Rb<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub>

P.11.12.3(C398.175) | K. Taibi: Relaxor Ferroelectric Behaviour of Ba<sub>1-x</sub>A<sub>x</sub>(Ti<sub>0.7</sub>Zr<sub>0.3</sub>)O<sub>3</sub> compositions (A=Ca,Sr)

P.11.12.4(C398.176) | H. Kasatani: Ferroelectric Phase Transition Mechanism in C<sub>5</sub>H<sub>6</sub>NBF<sub>4</sub> by X-ray Crystal Analysis

P.11.12.5(C399.177) | Y. Noda: Magnetism, Ferroelectricity and Lattice modulation of RMn<sub>2</sub>O<sub>5</sub>

P.11.12.6(C399.178) | E. H. Kisi: Crystal Structure, Phase Transitions and Negative Thermal Expansion in the Relaxor Ferroelectric PZN

P.11.12.7(C399.179) | F. Mo: Rochelle Salt - A Structural Reinvestigation with Improved Tools

P.11.12.8(C399.180) | J. S. Forrester: Temperature-Composition Phase Diagram of PZN-PT Studied by High Resolution Neutron Powder Diffraction

P.11.12.9(C400.181) | R. Schierholz: Local Symmetry in PbZr<sub>x</sub>Ti<sub>1-x</sub>O<sub>3</sub> Ceramics

P.11.12.10(C400.182) | A. Pietraszko: Local Order in the PSN, PST and PSNT Ferroelectric Relaxors

P.11.12.11(C400.183) | H. Fuess: In-situ Electric Field Synchrotron Diffraction of PbZr<sub>(x)</sub>Ti<sub>(1-x)</sub>O<sub>3</sub> Microdomains

P.11.12.12(C400.184) | Y. P. Mascalenhas: Analysis of the Crystalline Phases of PLZT doped with Nd, Ho, Er, Tm, Yb

## 13. Battery and Fuel Cell Materials

# SATURDAY, AUGUST 27, 2005 – POSTER SESSION

P.11.13.1(C400.185) | R. V. Martins: In-situ Study of Residual Strain in Solid Oxide Fuel Cells

P.11.13.2(C401.186) | D. Grossie: A Crystallographic Examination of Dilithium Phthalocyanine

P.11.13.3(C401.187) | T. Ohno: Site Preference of Valence Ions in  $\text{Fe}_{1+x}\text{Co}_{2-x}\text{O}_4$  ( $0 \leq x \leq 1$ )

P.11.13.4(C401.188) | S. Schmid: Structures of Defect Perovskites Suitable for Li Ion Intercalation

## 14. Residual Stress Measurements

P.11.14.1(C401.189) | A. Carradò: Residual Stress Distribution Near HA Coating Interface on Titanium Alloy Substrate

P.11.14.2(C402.190) | K. Khor: A New, Rapid 3D Tomographic Energy Dispersive Diffraction Imaging System for Materials Characterisation and Object Imaging (Rapid TEDDI)

## 15. Pore Framework Materials

P.11.15.1(C402.191) | H. Park: Synthesis and Structural Characterization of Novel Metal-Organic Frameworks

P.11.15.2(C402.192) | N. F. Sciortino: Spin-Crossover and Nanoporosity: Magnetic, Structural and Guest-Exchange Studies

P.11.15.3(C402.193) | J. J. Bevitt: In situ Control of Guest Exchange in Single Crystal X-ray Diffraction

P.11.15.4(C402.194) | Z. Yuan: Two new Inorganic-organic Hybrids with Framework Gallium 1,2-

ethylenediphosphonates Containing Pyridine

P.11.15.5(C403.195) | H. Imura: Mechanism of Phase Transition Caused by Water Absorption in FAPO-34

P.11.15.6(C403.196) | Y. Kubota: Direct Observation of Hydrogen Molecules adsorbed in a Coordination Polymer

P.11.15.7(C403.197) | G. Punte: Magnetic and Structural Properties of Rare Earth Hybrid Frameworks

P.11.15.8(C403.198) | F. A. Almeida Paz: Novel Modular Coordination Frameworks

P.11.15.9(C404.199) | M. C. A. Fantini: Structure Fingerprints of Ordered Mesoporous Silica

P.11.15.10(C404.200) | K. O. Kongshaug: Design of Porous Bilayer Compounds Containing 1D Channels

## 18 ELECTRON MICROSCOPY

### 3. New Techniques and New Instrumentation

P.18.03.1(C455.201) | F. Gramm: Using Transmission Electron Microscopy (TEM) to Complement Powder Diffraction Data

P.18.03.2(C456.202) | K. Saitoh: Detection of Interstitial Atoms by Hollow-Cone Illumination HAADF-STEM

## 19 ELECTRON DIFFRACTION

### 3. Other Applications and Advances

P.19.03.1(C458.203) | M. Nickolsky: Relation of Local and Integral Intensities of Reflections on Oblique Texture Electron Diffraction (OTED) Pattern

P.19.03.2(C458.204) | V. Hansen: Structure Determination

of Embedded Precipitates by Precession Electron Diffraction and Synchrotron Radiation: a Comparison

P.19.03.3(C458.205) | Y. Zhu: Measurements of Valence Electron Distribution in Perovskite  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$

P.19.03.4(C458.206) | H. Klein: A Complex  $\text{PbMnO}_{2.75}$  Phase Solved by Electron Crystallography

## 4. No sub theme

P.19.04.1(C459.207) | P. Dasgupta: Effect of Sonication and Grinding on the Structure of Hydrogenated Amorphous Carbon

SUNDAY, AUGUST 28 2005 - KEYNOTE LECTURES

MORNING SESSION 8.30-9.30

Michelangelo (*KN 21*)

**KN21.28(C5)** | Michael Parker:  
Pore-forming Toxins

*Chair:* William L. Duax

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Cimabue (*KN 22*)

**KN22.28(C5)** | Malcolm Mc Mahon:  
Pressure Induced Complexity in the Elements

*Chair:* Osamu Shimomura

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Botticelli (*KN 23*)

**KN23.28(C5)** | Mark A. Spackman:  
Electrostatic and Related Properties from Accurate  
Charge Density Analyses

*Chair:* Vladimir Tsirelson

AFTERNOON SESSION 17.30-18.30

Michelangelo (*KN 24*)

**KN24.28(C5)** | Nenad Ban:  
Structural and Functional Studies of Large  
Macromolecular Assemblies

*Chair:* Sherry Mowbray

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Cimabue (*KN 25*)

**KN25.28(C6)** | Lawrence Margulies:  
Micro Beam Diffraction Using High Energy  
Synchrotron Radiation

*Chair:* Stefano Lagomarsino

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Botticelli (*KN 26*)

**KN26.28(C6)** | Dmitri Svergun:  
New Possibilities for Structure Determination of  
Biomolecular Complexes

*Chair:* Giuseppe Zanotti

# SUNDAY, AUGUST 28 2005 – MORNING - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 57</b> )	Giotto ( <b>MS 58</b> )	Cimabue ( <b>MS 59</b> )
10.00-10.05 Opening Remarks	LARGE PROTEIN ASSEMBLIES - FORMING AND ANALYSING COMPLEXES <i>Chairs:</i> K. Miki, D. Stuart	CRYSTALLOGRAPHY AND UNDERSTANDING OF CULTURAL HERITAGE <i>Chairs:</i> S. Siano, H. Schenk	APPLICATIONS OF SYNCHROTRON AND NEUTRON FACILITIES IN STRUCTURAL CHEMISTRY <i>Chairs:</i> P. Raithby, T. Forsyth
10.05-10.35	<b>MS57.28.1(C75)</b>   <u>S. V. Strelkov</u> : Intermediate Filaments: from the Elementary Dimer Structure to the Complete Filament Architecture	<b>MS58.28.1(C76)</b>   <u>D. Visser</u> : An Archaeometric Study of Lead-White Pigment and its Production using Neutron Diffraction	<b>MS59.28.1(C77)</b>   <u>R. E. Morris</u> : Microcrystal X-ray Diffraction and MAS NMR Studies of Zeolties
10.35-11.05	<b>MS57.28.2(C75)</b>   <u>D. Tomchick</u> : Structural Basis of Actin Filament Nucleation and Processive Capping by a Formin Homology 2 Domain	<b>MS58.28.2(C76)</b>   <u>E. Dooryhée</u> : Powder Diffraction in Art and Archaeology	<b>MS59.28.2(C77)</b>   <u>W. Scherer</u> : Combined X-ray and Neutron Charge Density Studies on C-H activation catalysts
11.05-11.35	<b>MS57.28.3(C75)</b>   <u>R. Frank</u> : Active Site Coupling in Multienzyme Complexes	<b>MS58.28.3(C76)</b>   <u>V. Simova</u> : X-ray Powder Microdiffraction: Useful Tool in Investigation of Wall Painting Layers	<b>MS59.28.3(C77)</b>   <u>A. Albinati</u> : Structure and Dynamics of Co-ordination Compounds by Neutron Scattering
11.35-12.05	<b>MS57.28.4(C75)</b>   <u>R. Cogdell</u> : The Structure of the RC-LH1 'Core' Complex from <i>Rhodopsuedomonas Palustris</i>	<b>MS58.28.4(C76)</b>   <u>R. Arletti</u> : Colouring and Opacifying Agents in Roman Glass: a Multi-technique Analytical Approach	<b>MS59.28.4(C77)</b>   <u>R. Bau</u> : Location of a 4-coordinate H Atom via Neutron Diffraction.
12.05-12.35	<b>MS57.28.5(C75)</b>   <u>M.G. Rossmann</u> : 3D Rearrangement of Proteins in the Tail of Bacteriophage T4 on Infection of its Host	<b>MS58.28.5(C77)</b>   <u>G. Chiari</u> : Maya Blue: a Long Lasting Mystery Revealed	<b>MS59.28.5(C78)</b>   <u>M. P. Blakeley</u> : Neutron Cryocrystallography of Proteins

# SUNDAY, AUGUST 28 2005 – MORNING - MICROSYMPOSIA

Brunelleschi ( <b><i>MS 60</i></b> )	Leonardo da Vinci ( <b><i>MS 61</i></b> )	Botticelli ( <b><i>MS 62</i></b> )	Donatello ( <b><i>MS 63</i></b> )
<b>MICROSTRUCTURAL PROPERTIES FROM POWDER DIFFRACTION DATA</b> <i>Chairs:</i> D. Balzar, P. Scardi	<b>STRUCTURES PHASE TRANSITIONS AND PROPERTIES AT HIGH PRESSURE</b> <i>Chairs:</i> M. Mezouar, N. Hamaya	<b>ADVANCES IN COMPUTATIONAL METHODS FOR PROTEIN CRYSTALLOGRAPHY</b> <i>Chairs:</i> P. Gros, K. D. Cowtan	<b>CHEMICAL INSIGHTS FROM ELECTRON DENSITY STUDIES AND WAVEFUNCTIONS</b> <i>Chairs:</i> N. E. Ghermani, P. Blaha
<b>MS60.28.1(C78)</b>   T. Ungar: Subgrain Size-Distributions, Dislocation Structures, Stacking- & Twin Faults and Vacancy Concentrations in Crystalline Materials Determined by X-ray Line Profile Analysis	<b>MS61.28.1(C79)</b>   L.F. Lundegaard: Single Crystal Studies of the Incommensurate Composite Structure of Rb-IV	<b>MS62.28.1(C81)</b>   R. Read: New Likelihood-based Phasing Methods in Phaser	<b>MS63.28.1(C82)</b>   R. F. W. Bader: Quantum Mechanical Basis of Conceptual Chemistry
<b>MS60.28.2(C78)</b>   M. Leoni: Microstructural Studies of Nanocrystalline Materials using WPPM	<b>MS61.28.2(C79)</b>   F. Datchi: Structural and Vibrational Studies of Solid Ammonia to 120 GPa	<b>MS62.28.2(C81)</b>   M. Schiltz: Broken Symmetries in Macromolecular Crystallography	<b>MS63.28.2(C82)</b>   J.-M. Gillet: Construction or Refinement of Approximate Reduced Density Matrices
<b>MS60.28.3(C79)</b>   R. Kuzel: Structural Studies of Nanocrystalline Metals	<b>MS61.28.3(C80)</b>   L. Dubrovinsky: Phase Transitions in Transition Metal Monooxides: Interplay Between Structural, Magnetic, and Electronic Properties	<b>MS62.28.3(C81)</b>   H. Xu: Statistical Direct Methods of Phase Determination	<b>MS63.28.3(C82)</b>   P. Luger: Atomic and Bond Topological Properties of Strained Carbon Ring and Cage Systems.
<b>MS60.28.4(C79)</b>   N. Popa: Size Anisotropy and Lognormal Size Distribution in the Powder Diffraction whole Pattern Fitting	<b>MS61.28.4(C80)</b>   T. Watanuki: Successive Alteration of the Propagation Direction of the Inner Shell Ordering by Pressure in a Cd-Yb 1/1 Approximant Crystal	<b>MS62.28.4(C81)</b>   P. Skubak: Direct Use of SAD Phase Information in Automated Model Building and Refinement	<b>MS63.28.4(C82)</b>   A. Korlyukov: Chemical Bonding in Hypervalent Silicon and Germanium Compounds
<b>MS60.28.5(C79)</b>   N. Armstrong: Development of a NIST SRM 1979 Nano-Crystallite Size Standard for Broadening of X-Ray Line Profiles	<b>MS61.28.5(C80)</b>   P. Dera: Combining Laue Diffraction with White-beam Single-crystal EXAFS	<b>MS62.28.5(C81)</b>   R. Grosse-Kunstleve: Hybrid Programming in Crystallography: Phenix.refine and phenix.hyss	<b>MS63.28.5(C83)</b>   A. Ø. Madsen: Ribitol and Xylitol: Explaining the Differences in Physical Chemical Properties

**SUNDAY, AUGUST 28 2005 – AFTERNOON - MICROSYMPPOSIA**

TIME	Botticelli ( <b><i>MS 64</i></b> )	Michelangelo ( <b><i>MS 65</i></b> )	Cimabue ( <b><i>MS 66</i></b> )
14.45-14.50 Opening Remarks	DIFFICULT PHASING AND DIFFICULT STRUCTURES IN STRUCTURAL BIOLOGY <i>Chairs:</i> B.-C. Wang, A. Urzhumtsev	PROTEIN INTERACTIONS WITH OTHER BIOLOGICAL MACROMOLECULES <i>Chairs:</i> Z. Rao, B. W. Matthews	TOPOLOGY OF CRYSTAL STRUCTURES: NETS, KNOTS AND SURFACES <i>Chairs:</i> D. M. Proserpio, J.-G. Eon
14.50-15.20	<b>MS64.28.1(C83)</b>   A. Wlodawer: How to Deal with Pathological Crystals of Macromolecules	<b>MS65.28.1(C84)</b>   E. Y. Jones: Protein-protein Complexes in Cell Adhesion	<b>MS66.28.1(C85)</b>   M. O'Keeffe: Self-dual Tilings and Interpenetrating Periodic Nets
15.20-15.50	<b>MS64.28.2(C83)</b>   R. Caliandro: Phasing at Resolution Higher than the Experimental One	<b>MS65.28.2(C84)</b>   C. Hill: Activating the Molecule of Mass Destruction	<b>MS66.28.2(C85)</b>   E. Koch: Sphere Packings with Exceptional Properties
16.50-16.20	<b>MS64.28.3(C83)</b>   E. Rudiño-Piñera: A Challenging 90 Residue Problem: the <sup>2</sup> F1- <sup>3</sup> F1 Module Pair of Human Fibronectin	<b>MS65.28.3(C84)</b>   D. Wigley: Structure and Mechanism of RecBCD	<b>MS66.28.3(C85)</b>   S. Hyde: Knotted Nets and Weavings – from 2D Hyperbolic to 3D Euclidean Patterns
16.20-16.50	<b>MS64.28.4(C83)</b>   S. Trapani: NCS and Normal Modes Ensembles Solve Difficult MR Problem.	<b>MS65.28.4(C84)</b>   Y.-S. Heo: Molecular Basis for the Allosteric Inhibition of JNKs by the Peptide Fragment from the Scaffolding Protein JIP1	<b>MS66.28.4(C85)</b>   S. Batten: The Nomenclature of Interpenetration
16.50-17.20	<b>MS64.28.5(C84)</b>   T. Yeates: Disorder and Twinning: New Equations/Applications to Protein Structure Determination from the Carboxysome Shell	<b>MS65.28.5(C85)</b>   H. S. Yuan: Structural and Functional Insight into Cell-defending Non-specific Nucleases	<b>MS66.28.5(C86)</b>   V. A. Blatov: Computer Analysis and Classification of Entanglements in Crystal Structures

# SUNDAY, AUGUST 28 2005 – AFTERNOON - MICROSYMPOSIA

Donatello ( <b><i>MS 67</i></b> )	Leonardo da Vinci ( <b><i>MS 68</i></b> )	Giotto ( <b><i>MS 69</i></b> )	Brunelleschi ( <b><i>MS 70</i></b> )
<b>NON-AMBIENT POWDER DIFFRACTION AND KINETIC STUDIES</b> <i>Chairs:</i> I. R. Evans, R. Boese	<b>LIQUIDS AND AMORPHOUS SYSTEMS AT HIGH PRESSURE</b> <i>Chairs:</i> C. Tulk, D. Klug	<b>ELECTRON CRYSTALLOGRAPHY ON ORGANIC CRYSTALS AND BIOMOLECULES</b> <i>Chairs:</i> H. Hebert, U. Kolb	<b>NEW SAS FRONTIERS</b> <i>Chairs:</i> G. Kostorz, T. Narayanan
<b>MS67.28.1(C86)</b>   P. Chupas: Simultaneous Local and Long Range Structure Determination: Application to In-Situ Studies	<b>MS68.28.1(C87)</b>   C. Benmore: Intermediate Range Chemical Ordering in H <sub>2</sub> O, Si and Ge under Pressure	<b>MS69.28.1(C88)</b>   U. Weierstall: Electron Diffraction from a Beam of Laser-aligned Proteins: Progress Report	<b>MS70.28.1(C89)</b>   G. Beaucage: <i>In situ</i> X-ray Scattering Studies of Nanomaterial Growth Dynamics in Aerosols
<b>MS67.28.2(C86)</b>   R. Suryanarayanan: Qualitative and Quantitative Applications of Non-ambient X-ray Diffractometry	<b>MS68.28.2(C87)</b>   R. Martonak: Evolution of the Structure of Amorphous Ice - from LDA through HDA to VHDA.	<b>MS69.28.2(C88)</b>   A. Philippse: Methods Development and Software Engineering for 2D Electron Crystallography	<b>MS70.28.2(C89)</b>   M. Gradzinski: Dynamics of Amphiphilic Systems Probed by Highly Time-resolved
<b>MS67.28.3(C86)</b>   R. Guinebretiere: <i>In-situ</i> High Temperature Microstructural Transformations of Oxide Epitaxial Thin Films	<b>MS68.28.3(C87)</b>   S. Kohara: Structure of High-pressure Liquids: X-ray Diffraction and RMC Modelling	<b>MS69.28.3(C89)</b>   P. Holm: Atomic Model of Microsomal Glutathione Transferase 1 from Electron Crystallography	<b>MS70.28.3(C89)</b>   E. Kondrashkina: Cytochrome c and αTS Folding Probed by Submillisecond Continuous-Flow SAXS
<b>MS67.28.4(C87)</b>   K. W. Chapman: Anomalous Thermal Expansion in Cyanide-Bridged Molecular Framework Materials	<b>MS68.28.4(C88)</b>   S. Falconi: X-ray Diffraction Study in Liquid Cs up to 9.8 GPa	<b>MS69.28.4(C89)</b>   A. Kawaguchi: Structural Features of Inclusion Complexes of Cyclodextrins	<b>MS70.28.4(C90)</b>   B. Roessli: Spin Chirality in Non-centrosymmetric MnSi as Probed by Polarised Neutrons
<b>MS67.28.5(C87)</b>   G. Artioli: <i>In-situ</i> Synchrotron XRD Studies of Combustion Processes	<b>MS68.28.5(C88)</b>   V. Degtyareva: CdSb under Pressure: Compound Decomposition, New Phase Formation and Amorphization	<b>MS69.28.5(N.A.)</b>   P. Purhonen: Electron crystallography of membrane-bound transport proteins	<b>MS70.28.5(C90)</b>   M. Giglio: Near Field Heterodyne X-Ray Speckles

## SUNDAY, AUGUST 28 2005 – OTHER ACTIVITIES

**COMPUTER FAYRE** Ghirlandaio

(10.00-12.00)      V. Favre-Nicolin:

FOX Free Objects for Xtallography

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(14.00-16.00)      S. Coles

Grid Computing and Crystallography

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**IUCr GENERAL ASSEMBLY**

Cimabue (19.00-22.00)

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

## 01 INSTRUMENTATION AND EXPERIMENTAL TECHNIQUES

### 8. Neutron Scattering I: Techniques and Instrumentation

**P.01.08.1(CI42.1)** | H.-C. Hu: A High Quality Bent Crystal Monochromator Based on Asymmetric Laue Geometry

**P.01.08.2(CI43.2)** | P. Mikula: High-Resolution Neutron Diffraction Monochromators

**P.01.08.3(CI43.3)** | P. F. Henry: Isotopic Substitution Neutron Diffraction for Enhanced Structural Information from Crystalline Powder Materials

**P.01.08.4(CI43.4)** | W. Klooster: The New Quasi-Laue Diffractometer at the Australian OPAL Research Reactor

**P.01.08.5(CI43.5)** | L. Keller: Design of a Neutron Diffractometer at SINQ Using Monte Carlo Simulations

**P.01.08.6(CI43.6)** | C. B. Ramos Parente: The IPEN-CNEN/SP PSD Neutron Diffractometer

**P.01.08.7(CI44.7)** | M. Meven: The New Single Crystal Diffractometer HEiDi at the FRM-II and its Applications

**P.01.08.8(CI44.8)** | F. Grazzi: The Italian Neutron Experimental Station (INES) at ISIS: Status and Development

**P.01.08.9(CI44.9)** | P. Thiagarajan: Design of a High Resolution Macromolecular Neutron Diffractometer (MaNDi) for Structural Biology Research at the SNS

**P.01.08.10(CI44.10)** | C. Hoffmann: Advances in Neutron Single Crystal Diffraction towards a Smaller Sample Sizes

## 9. Neutron Scattering II: Applications

**P.01.09.1(CI45.11)** | T. F. Koetzle: Single-Crystal Neutron Diffraction on Sigma Complexes: Recent Results from IPNS

### 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

#### 3. Metallo-Enzymes

**P.04.03.26(C214.12)** | K. Nagata: Crystal Structure of Carboxypeptidase 1 from *Thermus thermophilus*

#### 14. Macromolecular Assemblies

**P.04.14.1(C237.13)** | C. T. Webb: Structural Determination of the hTIM10 Complex

**P.04.14.2(C237.14)** | M. Dines: Structure Determination of Proteins Involved in the Stability of Phycobilisomes during Environmental Stress

**P.04.14.3(C237.15)** | J. Dohnalek: Cage-like Hexamers of Cold-active  $\beta$ -galactosidase from *Arthrobacter* sp. C2-2

**P.04.14.4(C238.16)** | A. Kita: Crystal Structure of a Cyanobacterial BLUF Protein, Tll0078

**P.04.14.5(C238.17)** | A. Nakagawa: SR Beamline for Macromolecular Assembly Crystallography Operated by IPR at SPring-8

**P.04.14.6(C238.18)** | E. Krissinel: Calculation of Biological Units from Protein Crystallography Data

**P.04.14.7(C238.19)** | G. Montoya: X-ray Structure of Recombinant Core 8D of the Nuclear Chaperone Nucleoplasmin

**P.04.14.8(C238.20)** | F. Sica: Hinge Peptide and Intersubunit Interface in Domain Swapping

**P.04.14.9(C239.21)** | I. Pechik: Molecular Mechanisms of Thrombin-Mediated Fibrin Assembly

**P.04.14.10(C239.22)** | G. Buchwald: The Complex of the Polycomb Group Proteins Ring1B (RNF2) and Bmi1 –A Structure-function-analysis

**P.04.14.11(C239.23)** | N. Numoto: Structure of a Giant Hemoglobin of the Gutless Beard Worm *Oligobrachia mashikoi*

**(C237.24)** | D. M. A. Guérin: Structure of an inter-ring allosteric GroEL mutant (E461K) at 3.3 $\text{\AA}$  resolution

**P.04.14.12(C239.25)** | L. Terradot: Structural Biology of Type IV Secretion System

**P.04.14.13(C240.26)** | H. Matsunami: Crystallization and X-ray Analysis of a Flagellar Hook Capping Protein

**P.04.14.14(C240.27)** | D. Borek: High Symmetry Involved in Cellular Regulation

**P.04.14.15(C240.28)** | Y. Li: Nanotubular Structures of Microtubule Complexes with Spermine and Lipid Membrane

**P.04.14.16(C240.29)** | A. Cabo: Structure of an Inter-ring Allosteric GroEL Mutant (E461K) at 3.3 $\text{\AA}$  Resolution

**P.04.14.17(C241.30)** | O. Pasternak: Structure of Cytokinin-specific Binding Protein in Complex with Plant Hormone

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

**P.04.14.18(C241.31)** | M. J. Romão: Modular Assembly of complexed Forms of the Cellulosome Revealed by X-ray Crystallography

## 15. Macromolecular Based Drug Design

**P.04.15.1(C241.32)** | G. A. Hall: Structural Studies of Thioredoxins and Associated Inhibitor Based Complexes

**P.04.15.2(C241.33)** | C. L. Gee: A Dramatic Side Chain Movement in Adrenaline-Synthesising PNMT: Implications for Drug Design

**P.04.15.3(C241.34)** | L. Parker: Structural Studies of Glutathione S-transferase Inhibitors – A Promising Target for Anti-cancer Drug Design

**P.04.15.4(C242.35)** | A. Casini: X-ray Crystallography of the Antiepileptic Drug Zonisamide with CA II

**P.04.15.5(C242.36)** | S.-Y. Ku: Structures of 5-methylthioribose Kinase: Catalytic Mechanism and Drug Design

**P.04.15.6(C242.37)** | I. Sanchez: Dobexilate as Lead Compound in Angiogenesis Inhibition Search

**P.04.15.7(C242.38)** | J. Hasek: HIV Protease Inhibition Seen by X-ray Diffraction and Molecular Dynamics.

**P.04.15.8(C243.39)** | T. Skalova: Series of HIV-1 Protease Nanomolar Inhibitors; Binding to WT and Mutant Protease

**P.04.15.9(C243.40)** | S. B. Patel: Crystallization and X-ray Analysis of the Catalytic Domain of Human PDE 3B

**P.04.15.10(C243.41)** | H.-J. Yoon: Crystal Structure of Nicotinic Acid Mononucleotide Adenyllyltransferase from *Pseudomonas aeruginosa* in its Apo and Substrate-

**B64**

complexed Forms

**P.04.15.11(C243.42)** | J. Watermeyer: Structure of a Glycosylation Mutant of Testis ACE Bound to a Novel Inhibitor

**P.04.15.12(C244.43)** | B. Calamini: Structural Basis for Potent Inhibition of COX by Resveratrol-A Natural Product in Wine

**P.04.15.13(C244.44)** | H. U. Ahmed: Structural Studies on Human  $\alpha$ -thrombin

**P.04.15.14(C244.45)** | T. Kinoshita: Active Structure of FR901451, a Potent Macrocyclic Elastase Inhibitor

**P.04.15.15(C244.46)** | A. Dawson: Structure of Pteridine Reductase (PTR1) from *Trypanosoma brucei*

**P.04.15.16(C244.47)** | N. Demitri: Crystallography as a Tool to Identify the Best Inhibitor in a Complex Mixture

**P.04.15.17(C245.48)** | P. Kaur: Crystal Structure of a Disintegrin Heterodimer from *Echis carinatus* at 1.9 Å Resolution

**P.04.15.18(C245.49)** | H. Yang: Structure-assisted Design of Inhibitors Targeting Coronavirus Main Proteases

**P.04.15.19(C245.50)** | J. E. Debreczeni: Structural Insights into the Substrate Binding Mechanism, Inhibition and Regulation of Pim-1

**P.04.15.20(C245.51)** | S. Di Marco: Interdomain Communication in HCV Polymerase Abolished by Small-Molecule Inhibitors

**P.04.15.21(C246.52)** | E. Pyetan: Structural Parameters

Influencing the Affinities and Effectiveness of Ribosomal Antibiotics

**P.04.15.22(C246.53)** | B. L. Staker: Multiple Inhibitor Co-crystal Structures of the Human Topoisomerase I Covalent DNA Complex Bound to a Series of Structurally Diverse Anti-cancer Compounds

**P.04.15.23(C246.54)** | A. Cleasby: Fragment-based Screening by X-ray Crystallography: an Alternative to High Throughput Screening

**P.04.15.24(C246.55)** | R. Battistutta: Inspecting the Pharmacophore of Protein Kinase CK2 with Tetrabromobenzimidazoles

**P.04.15.25(C247.56)** | T. Pauly: Structure of Guinea Pig 11 $\beta$  Steroid Dehydrogenase 1 with Glycyrhetic Acid

**P.04.15.26(C247.57)** | K. Kavanagh: Farnesy Pyrophosphate Synthase: Clinical Target for Bone Diseases

**P.04.15.27(C247.58)** | Y. Kusakabe: Structure of S-Adenosyl-L-Homocysteine Hydrolase from *Plasmodium falciparum*

**P.04.15.28(C247.59)** | A. Ruf: Crystal Structure of Oxido Squalene Cyclase

**P.04.15.29(C247.60)** | N. Tanaka: Crystal Structure of the N-terminal Ankyrin Repeat Domain of Human RNase L

**P.04.15.30(C248.61)** | K. Aoki: Crystal Structures of Autocrine Motility Factor Complexed with Inhibitors

**P.04.15.31(C248.62)** | T. Hori: LTB4 12-hydroxydehydrogenase/15-oxo-PG 13-reductase and

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

## Indomethacin Complex

**P.04.15.32(C248.63)** | C. Vonrhein: Automated Structure Refinement for High-throughput Ligand Detection with BUSTER-TNT

**P.04.15.33(C248.64)** | D. Tondi: Crystallographic Studies of Novel Inhibitors of  $\beta$ -Lactamases

**P.04.15.34(C249.65)** | D. M. Himmel: X-ray Structure for an RNase H Inhibitor Bound to HIV-1 Reverse Transcriptase

**P.04.15.35(C249.66)** | G. Labesse: Crystal Structure of the NAD Kinase from *Listeria monocytogenes*

## 25. Hot Macromolecular Structures

**P.04.25.1(C262.67)** | T. Nakamura: Crystal Structure of Hyperthermstable Thioredoxin Peroxidase from *Aeropyrum pernix* K1

**P.04.25.2(C262.68)** | U. Kosinska: Thymidine Kinase of Mycoplasmic Origin – An Enzyme With Lasso

**P.04.25.3(C262.69)** | Z. Chen: Structure of Heterotetrameric Sarcosine Oxidase (TSOX) at 1.85 Å Resolution

**P.04.25.4(C262.70)** | N. Suzuki: Structure of Plant ATG12, a Ubiquitin-like Modifier Essential for Autophagy

**P.04.25.5(C263.71)** | J. Jeyaraman: Crystal Structure of Novel Cyan-emitting Fluorescent Protein from *Acropora* Stony Coral

**P.04.25.6(C263.72)** | M. Matsushita: Structural Study of Atg5 and Atg16 Essential for Autophagy

**P.04.25.7(C263.73)** | E. Fukumura: Crystal Structure of Novel Orange-emitting Fluorescent Protein from Stony Coral

**P.04.25.8(C263.74)** | S. Jenko Kokalj: Proline Isomerization in Stenf B: a Crucial Step Towards Amyloid Fibril Formation

**P.04.25.9(C264.75)** | E. Chabriere: Serendipitous Discovery and X-Ray Structure of a Human Phosphate Binding Apolipoprotein

**P.04.25.10(C264.76)** | A. Kikuchi: Structural Basis for Cyan-Emitting Mechanism in a Cyan Fluorescent Protein

**P.04.25.11(C264.77)** | M. Guerin: Structural Basis of Glycogen Synthesis

**P.04.25.12(C264.78)** | P. Curmi: Dramatic structural Change in CLIC1: Globular Protein that Forms an ion Channel

**P.04.25.13(C265.79)** | H. Unno: Crystal Structure Analysis of Maize Glutamine Synthetase

**P.04.25.14(C265.80)** | C. Frazao: The Sulfur Oxygenase Reductase from *Acidianus ambivalens*

## 26. No sub-theme

**P.04.26.1(C265.81)** | K. kulkarni: Structural Basis for Carbohydrate Specificity of Basic Winged Bean Lectin

**P.04.26.2(C265.82)** | R. Owen: Experimental Tests of the Theoretical Dose Limit for Cryocooled Protein Crystals

**P.04.26.3(C266.83)** | N. Paterson: Structural Studies on

MsmE, a Sugar Binding Lipoprotein, from *S. pneumoniae*

**P.04.26.4(C266.84)** | M. Aslanas: Macromolecular Crystallography at Room Temperature: Wavelength Dependence Radiation Sensitivity and Damage

**P.04.26.5(C266.85)** | M. Kozak: Solution Scattering Studies of Xylanase XYNII from *Trichoderma longibrachiatum*

**P.04.26.6(C266.86)** | A. Vogel: Towards the Structure Determination of the HtrA1 Protein from *Staphylococcus aureus*

**P.04.26.8(C267.88)** | E. Fioravanti: Lactate Dehydrogenases from Extremophile Organisms: Clues for Radio-resistance?

**P.04.26.9(C267.89)** | A. W. Roszak: Interactions of Phospholipids with Integral Membrane Proteins; Use of Brominated Lipids

**P.04.26.10(C267.90)** | T. Ohtsuki: Structural Studies of Water-soluble Chlorophyll Protein from *Chenopodium album*

**P.04.26.11(C267.91)** | D. Goldstone: Structure of the C-terminal Domain of DipZ from *Mycobacterium tuberculosis*

**P.04.26.12(C268.92)** | K. Shiozawa: Structure of the N-terminal Domain of PEX1 AAA-ATPase

**P.04.26.13(C268.93)** | P. Harris: Hyperthermstable Ferredoxin from *Pyrococcus furiosus*

**P.04.26.14(C268.94)** | M. Momma: Crystal Structure of the NgcE Protein of the *Streptomyces* ABC transporter

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

P.04.26.15(C268.95) | K. Miyazono: Crystal Structure and Structural Stability of Acylphosphatase from Hyperthermophilic Archaea *Pyrococcus horikoshii* OT3

P.04.26.16(C269.96) | M. D. Bennett: The Structure of an Ester Synthesising Peptidase

P.04.26.17(C269.97) | B. Schoenborn: Protein Crystallography with Spallation Neutrons

P.04.26.18(C269.98) | M. A. Bianchet: Crystal Structure of *Moronis saxatilis* F-lectin

P.04.26.19(C269.99) | P. Stephens: Producing Diffraction Quality Powders from Soluble Lysozyme and Thaumatin.

P.04.26.20(C269.100) | D. Horigome: A Novel Chlorophyll-Binding Mode Of Water-Soluble Chlorophyll Protein (WSCP)

P.04.26.21(C270.101) | E. Warkentin: Group-subgroup Relations, Twinning, and Rigid-body Vibration (TLS) in a Bio-crystal: Analogy to Inorganic Structures

P.04.26.22(C270.102) | F. Moraes Ferreira: Phasing with Iodine and an X-ray Home Source.

P.04.26.23(C270.103) | F. Zein: Structural Comparison and Analysis of the Substrate Specificities of Purine Nucleoside Phosphorylases

P.04.26.24(C270.104) | J. M. Choi: Examination of the Mechanism of Carbamate Kinase by Structural Analyses

P.04.26.25(C271.105) | A. Wagner: The First Structure from Ultralente Insulin Microcrystals

P.04.26.26(C271.106) | M. Norrman: Characterization of Insulin NPH Microcrystals in Pharmaceutical Suspensions

P.04.26.27(C271.107) | M. Kashii: Femtosecond Laser Processing of Protein Crystals

P.04.26.28(C271.108) | Y. Vekhter: Validation of the Molecular Replacement Solutions with the OMIT Procedure

P.04.26.29(C271.109) | S. Geremia: Estimate the Time of Soak Simulating Small Molecule Diffusion in Protein Crystal

## 1 INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES

### 1. General Geosciences

P.10.01.1(C367.110) | N. P. Yushkin: Crystallosymmetric Structure and Evolution of the Mineral World

### 2. Systematics of Inorganic Compounds

P.10.02.13(C369.111) | O. Oeckler: Order-Disorder Phenomena in Nitridosilicates and Nitridophosphates

P.10.02.15(C370.112) | E. Tillmanns: Rb<sub>5</sub>In(MoO<sub>4</sub>)<sub>4</sub>: Crystal Structure of a Possible Laser Material

### 4. High Pressure and High Temperature Studies

P.10.04.1(C372.113) | J. M. Zaug: White Phosphorous: The Equation of State and Pressure-Induced Transitions

P.10.04.2(C372.114) | I. Korolkov: X-ray Study of the Iridium-Osmium System

P.10.04.3(C372.115) | A. Lysiuk: Crystal Phases in Glasses

P.10.04.4(C373.116) | A. Zadesenets: Synthesis and X-ray Study of [Pt(NH<sub>3</sub>)<sub>4</sub>](ReO<sub>4</sub>)<sub>2</sub> Thermolysis Products

P.10.04.5(C373.117) | H. M. Park: Crystal Structure of KLiSO<sub>4</sub> at High Temperatures

P.10.04.6(C373.118) | D. Y. Jung: *Ab initio* Treatment of Minerals at Extreme Conditions

P.10.04.7(C373.119) | K. Funakoshi: Viscosity Measurements of Fe-FeS Melts under High Pressures

P.10.04.8(C374.120) | M. Okube: Accommodation Mechanism of Kr Trapped in Terrestrial and Planetary Materials

P.10.04.9(C374.121) | J.-J. Lee: Pressure-Induced Electron Transfer in Cobalt-Iron Prussian Blue Complex Studied by RIXS

P.10.04.10(C374.122) | M. Kunz: ALS Beamline 12.2.2, A High-Pressure X-ray User Facility at the US-West-Coast.

P.10.04.11(C374.123) | C. L. Bull: High Pressure Single-Crystal Neutron Diffraction of DKDP

P.10.04.12(C375.124) | Y. Ohishi: Compression of Oxygen Vacancy Type Al-bearing MgSiO<sub>3</sub> Perovskite

P.10.04.13(C375.125) | K. Hagiya: New High-pressure Phase of Calcite at Room Temperature

P.10.04.14(C375.126) | S. Nazzareni: High-pressure Single-crystal Study of Chlorite

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

## 5. Minerals: Characterisation Methods and Structures

**P.10.05.19(C380.219)** | M. Pérez-Prieto: Going Inside Fettelite, a Hg-Sulfosalt Mineral

## 6. Zeolites (Natural and Synthetic)

**P.10.06.1(C380.127)** | A. Ivanova: Structure of New Rare-Earth Borates  $\text{Ln}[\text{B}_6\text{O}_9(\text{OH})_3]$  and its Relation to Boracites

**P.10.06.2(C380.128)** | M. C. Betti: Zeolites Gismondine and Li-ABW Under Pressure: Synchrotron XRPD and MD Simulations

**P.10.06.3(C381.129)** | P. Gavrilenko: The Crystal Structure of Chabasite-K

**P.10.06.4(C381.130)** | L. Robu: Crystallochemistry of Natural Zeolites from 'Tuful de Dej' (Romania)

**P.10.06.5(C381.131)** | X. Zou: Open-framework Germanates by Organic Templating

**P.10.06.6(C381.132)** | C.-Y. Cheng: Synthesis and Characterization of Highly Dispersed Tungsten Oxide into SBA Molecular Sieve

**P.10.06.7(C382.133)** | K. Byrappa: Hydrothermal Crystallization and Characterization of  $\text{R}^{+3}\text{:AlPO}_4$  Zeolites, where R = Ce, Pr and Nd

**P.10.06.10(C382.134)** | P. Ballirano: The Crystal Structure of Sacrofanite, the 74 Å Phase of the Cancrinite Group

## 8. No sub-theme

**P.10.08.1(C382.135)** | T. Mihajlović:  $\text{BaZn}_2(\text{AsO}_4)_2\text{H}_2\text{O}$ : A Framework Structure Related to Feldspar

<b>P.10.08.2(C383.136)</b>   <u>Z. Mayerová</u> : Slabs from Cubic $\text{Sb}_2\text{O}_3$ Interspersed Between Puckered BN-type $\text{CuCl}_x\text{Br}_{1-x}$ Layers	the Layered Compound $\text{Sr}_3\text{NdFe}_3\text{O}_9$
<b>P.10.08.3(C383.137)</b>   <u>C. Röhr</u> : New Intermetallic Compounds Forming the $\text{Ca}_{11}\text{Ga}_7$ Structure Type	<b>P.11.11.7(C397.147)</b>   <u>R. Tellgren</u> : Synthesis, Nuclear Structure, and Magnetic Properties of Some Doped Perovskites
<b>P.10.08.4(C383.138)</b>   <u>S. Schnabel</u> : Structure and Bonding in Thioxovanadates $\text{A}_3\text{VS}_x\text{O}_{4-x}$ ( $\text{A} = \text{Na}, \text{K}; x = 1 - 4$ )	<b>P.11.11.8(C397.148)</b>   <u>P. Paufler</u> : On the Initial Stage of Plastic deformation of $\text{SrTiO}_3$
<b>P.10.08.5(C383.139)</b>   <u>G. Frisch</u> : New Oxoferates of the Alkali Metals	<b>P.11.11.9(C397.149)</b>   <u>E. Dooryhée</u> : Nano-Structure of PLD-Grown Epitaxial $\text{PbTiO}_3/\text{BaTiO}_3$ Superlattices by Synchrotron X-ray Diffraction
<b>P.10.08.6(C383.140)</b>   <u>M. Bostrom</u> : Rietveld Refinement of the Crystal Structure of the Novel Compound $\text{Ir}_4\text{Ga}_{11}$	<b>P.11.11.10(C397.150)</b>   <u>S. Misture</u> : Tolerance Factors and Solid Solutions in Three-Layer Aurivillius Ceramics
<b>11 CRYSTALLOGRAPHY IN MATERIAL SCIENCE</b>	
<b>11. Perovskite Materials</b>	
<b>P.11.11.1(C395.141)</b>   <u>J. Guevarra</u> : Structures of Perovskite-related layered $\text{A}_n\text{B}_n\text{O}_{3n+2}$	<b>P.11.16.1(C404.152)</b>   <u>K. Nakajima</u> : Si Crystal Mirrors Prepared by Plastic Deformation for Solar Cell Systems
<b>P.11.11.2(C395.142)</b>   <u>N. Rotiroli</u> : Structural Phase Transition of $\text{La}_{0.815}\text{Ba}_{0.185}\text{MnO}_3$ studied by X-ray Diffraction and Maximum Entropy Method	<b>P.11.16.2(C404.153)</b>   <u>V. V. Pustovalov</u> : Low Temperature Anomaly of Plasticity and a Local Arrangement in Pb-In Alloys
<b>P.11.11.3(C396.143)</b>   <u>J. I. da Silva</u> : Comparison of $\text{Ba}_{0.05}\text{Sr}_{0.95}\text{RuO}_3$ and $\text{Ca}_{0.05}\text{Sr}_{0.95}\text{RuO}_3$ Structures	<b>P.11.16.3(C405.154)</b>   <u>E. Kudrenko</u> : Phase States Cycling Sequence in Complex Oxides Received by Decomposition of the Melt-Solution of the Simple Oxides (Nitrates) in $\text{NH}_4\text{NO}_3$
<b>P.11.11.4(C396.144)</b>   <u>P. Karen</u> : Verwey Transition in a Perovskite-Type Structure	<b>P.11.16.4(C405.155)</b>   <u>L. A. Pajdzik</u> : Three-dimensional Birefringence Imaging with a Microscope Tilting Stage
<b>P.11.11.5(C396.145)</b>   <u>P. Teslenko</u> : Nanostructural Effects at $\text{KNbO}_3$ Synthesis	<b>P.11.16.5(C405.156)</b>   <u>K. Schmid-Rausch</u> : Dynamic method for Measurement of Piezo-optic Coefficients
<b>P.11.11.6(C396.146)</b>   <u>D. Pelloquin</u> : Crystal Structure of	

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

P.11.16.6(C405.157) | C. Giannini: X-ray Powder Diffraction Characterization of Nanoparticles

P.11.16.7(C406.158) | K. Nomura: Conduction Path and Disorder of Oxide Ions in LaGaO<sub>3</sub>-Based Fast Oxide-ion Conductors

P.11.16.8(C406.159) | C.-T. Liu: Spin Crossover Iron complexes in 2D and 3D frameworks

P.11.16.9(C406.160) | D. P. Riley: "Trigger" Mechanisms of Ultra-Fast Reactions

P.11.16.10(C406.161) | L. Male: Investigations on Metal Alanates Using X-Ray and Neutron Powder Diffraction

P.11.16.11(C406.162) | C.-F. Sheu: Structural Characterization and LIESST Properties of Spin Crossover Complex *trans*-[Fe(abpt)<sub>2</sub>(NCS)<sub>2</sub>] Polymorph D (abpt = 4-Amino-3,5-bis(pyridin-2-yl)-1,2,4-triazole)

P.11.16.12(C407.163) | H. E. Du Plessis: The Crystal Structures of the Iron Carbides

P.11.16.13(C407.164) | S. M.-C. Manuel: Classification of White Marble Varieties by Monocrystal X-ray Diffraction

## 13 FIBRE DIFFRACTION

### 2. Structure Determination of Fibres

P.13.02.1(C417.165) | A. Immirzi: Studying Fibrous Structures with Use of Internal Coordinates

## 20 NON-AMBIENT CONDITIONS

### 1. High Pressure Crystallography I: Extremes of Temperature and Pressure

P.20.01.1(C461.166) | L. Fontana: Study of the High P-T Phase Diagram of Crystalline Polyethylene

P.20.01.2(C461.167) | P. Pruzan: Vibrational Dynamics and Phase Diagram of KNbO<sub>3</sub> up to 30 GPa and from 10 to 500 K

### 2. High Pressure Crystallography II: Physical Properties Under Pressure

P.20.02.1(C461.168) | V. Pischedda: Compressibility and Evidence of Amorphisation of 6 nm TiO<sub>2</sub> Nano-anatase

P.20.02.2(C461.169) | A. Lennie: A Novel Facility for Diamond Anvil Cell Diffraction at the SRS, Daresbury, UK

P.20.02.4(C462.170) | Y. Nakamoto: The Phase Transition of Hydrogen-bonded Ferroelectric PbHPO<sub>4</sub> under High Pressure

P.20.02.3(C462.171) | A. Wosylus: High Pressure Synthesis of EuGa<sub>2-x</sub>Si<sub>4+x</sub> [x = 1.3(1)]

### 3. High Pressure Crystallography III: Phase Transitions and High Pressure

P.20.03.1(C462.172) | W. A. Crichton: High Pressure Structures and Compressibilities of YF<sub>3</sub> and LaF<sub>3</sub>

P.20.03.2(C462.173) | S. Ivashevskaya: Isosymmetric Reversible Phase Transition in Sodium Oxalate.

P.20.03.3(C462.174) | A. Davidson: Isostructural Transformation and Polymorphism of Thiourea Dioxide at High Pressure

P.20.03.4(C463.175) | S. A. Moggach: The Effect of Pressure, and Formation of New Polymorphs of the Amino Acids L-Cysteine and L-Serine

P.20.03.5(C463.176) | R. Gajda: Absence of Halogen Bonding in the High-pressure Structure of Chlorotrimethylsilane

P.20.03.6(C463.177) | A. Budzianowski: High-pressure Crystal Phase of 1,2-ethylenediamine

P.20.03.7(C463.178) | F. Fabbiani: Probing Polymorphism with High Pressure

P.20.03.8(C464.179) | R. Nelmes: Complex Structures in Barium at High Pressure

P.20.03.9(C464.180) | T. Bovornratana: Structures and Phase Transitions of CuInSe<sub>2</sub> under High Pressure

P.20.03.10(C464.181) | G. Rousse: Resolution of the Intermediate High Pressure Phase of PbTe

P.20.03.11(C464.182) | K. Takemura: Structural Study of Solid Mercury at High Pressures

P.20.03.12(C464.183) | S. Aoyagi: High Pressure Effect on Bonding Nature in KMnF<sub>3</sub>

P.20.03.13(C465.184) | M. Colligan: High Pressure X-ray Diffraction Studies of Purely Siliceous Zeolites

P.20.03.14(C465.185) | V. Giordano: High Pressure High Temperature Carbon Dioxide

P.20.03.15(C465.186) | M. Santoro: High P-T Phase Diagram of Solid Benzene, and Transformation to an Extended Amorphous State

# SUNDAY, AUGUST 28, 2005 – POSTER SESSION

P.20.03.16(C465.187) | D. Adams: Molecular Dynamics Simulations of Cubic CaSiO<sub>3</sub> at Lower Mantle Conditions

P.20.03.17(C466.188) | T. Ogitsu: First-principles Simulations of LiH: Towards the B2 Phase

P.20.03.18(C466.189) | T. Yamanaka: Pressure-induced Structure Change of Ferroelectric KNbO<sub>3</sub> using SR

P.20.03.19(C466.190) | N. Casati: High Pressure Study of Co<sub>2</sub>(CO)<sub>6</sub>(XPh<sub>3</sub>)<sub>2</sub> (X=As,P) Phase Transitions via SXRD

P.20.03.20(C466.191) | C. Hejny: Incommensurate Structures in the Group VIA Elements above 100 GPa

P.20.03.21(C467.192) | O. Degtyareva: Charge-density Wave in the Incommensurate Phase of Metallic Sulfur at Megabar Pressure

P.20.03.22(C467.193) | A. Kurnosov: Phase Transitions in the O<sub>2</sub> – H<sub>2</sub>O System at High Pressures

P.20.03.23(C467.194) | A. Uodome: Hexagonal Diamond from Highly Crystalline Graphite Film

P.20.03.24(C467.195) | M. Mc Mahon: Chain Melting at HT/HP in Incommensurate Rb-IV

P.20.03.25(C468.196) | L. Oswald: High Pressure Studies of Molecular Systems at the ESRF

## 4. High Pressure Crystallography IV: Data Acquisition and Analysis

P.20.04.1(C468.197) | D. Yufit: 'Poor-men' High Pressure Cell for Single Crystal X-ray Crystallography

## 6. High Pressure Crystallography VI: New Frontiers

P.20.06.1(C468.198) | P. A. Wood: The Effect of High Pressure on the Topology of Organic Systems

P.20.06.2(C468.199) | T. Okuchi: Hydrogen Bonding and Dynamics of Methanol by High-pressure Diamond Anvil Cell NMR

P.20.06.3(C468.200) | J. S. Loveday: Structural Relationships Between Amorphous Ices at High Pressure

## 7. High Temperature Crystallography: Instrumentation, Techniques and Applications

P.20.07.1(C469.201) | S. Petrova: High-temperature X-ray Study of Zn-substituted Cu<sub>2</sub>V<sub>2</sub>O<sub>7</sub>

P.20.07.2(C469.202) | O. Leynaud: A Furnace for *in situ* Time Resolved Diffraction with Gas Flow

## 8. Low Temperature Crystallography: Instrumentation, Techniques and Applications

P.20.08.1(C469.203) | L.R. Evans: A Parametric Approach to Single Crystal Diffraction Data Analysis

## 9. Phase Transitions I: Characterisation and Applications

P.20.09.1(C469.204) | M. Milanesio: A Combined Raman-X-ray Powder Diffraction Study at Non-ambient Condition

P.20.09.2(C470.205) | L.E. Depero: Phase Transitions of Alluminosilicate Refractories by Temperature Resolved XRD

P.20.09.3(C470.206) | M. Haluska: Characterization of

Shape-Preserving Diatom Displacement Reactions using High Temperature X-ray Diffraction

P.20.09.4(C470.207) | H. Borrmann: Low-temperature Phase Transitions for Solid Solutions of TbVO<sub>4</sub>/DyVO<sub>4</sub>

## 10. Phase Transitions II: Magnetic and Structural Identification

P.20.10.1(C470.208) | O. Makarova: Magneto-structural Phenomena in Hydrides with Unusual Topology of Spin Lattice

P.20.10.2(C470.209) | A. Schoenleber: Low Temperature Structures of the Metal Oxyhalides MO<sub>X</sub>: M = Ti, V and X = Cl, Br

P.20.10.3(C471.210) | A. Venter: Studies of the Magnetic Ordering in Polycrystalline Cr-Ru Alloys by Neutron Powder Diffraction

P.20.10.4(C471.211) | A. Yucel: Magnetic Transitions in ErCo<sub>10</sub>Mo<sub>2-x</sub>M<sub>x</sub> (M=Si and V)

P.20.10.5(C471.212) | T. Inami: X-ray Diffraction and Absorption Study under Strong Pulsed Magnetic Fields

P.20.10.6(C471.213) | V. Pecharsky: Magnetic Field Induced Polymorphism of R<sub>5</sub>T<sub>4</sub> Compounds

## 12. Crystallography of Excited States

P.20.12.1(C471.214) | J. Bjernemose: When 2+2 isn't 4

P.20.12.2(C472.215) | T. L. Savarese: Synthetic and Structural Studies on Photoactivated Complexes

P.20.12.3(C472.216) | K. Kato: Charge Density Study of

## SUNDAY, AUGUST 28, 2005 – POSTER SESSION

Photo-Excited State in Spin Crossover Complex

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P.20.12.4(C472.217) | A. Thompson: Thermal and Light-  
Induced Polymorphism in Fe(II) Spin Crossover Materials

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### 23 CRYSTALLOGRAPHY TOPOLOGY 4. Networks

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P.23.04.2(C479.218) | H.-J. Klein: Non-redundant Graph  
Representation of Polyhedral Networks

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**MONDAY, AUGUST 29 2005 - KEYNOTE LECTURES****MORNING SESSION 8.30-9.30**

Botticelli (**KN 27**)

**KN27.29(C6) | Michael Murphy:**  
Bound Ligands to Probe the Activity of Type 2  
Copper Sites in Proteins

*Chair: Carrie Wilmot*

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Cimabue (**KN 28**)

**KN28.29(C6) | Tim White:**  
Crystallochemical Basis of Synthetic Mineral  
Immobilisation

*Chair: Ekkehart Tillmanns*

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Michelangelo (**KN 29**)

**KN29.29(C7) | Gerhard Klebe:**  
Molecular Recognition Principles in Protein-Ligand  
Interactions as a Prerequisite for the Design of  
Specific and Selective Leads

*Chair: Hans-Beat Buergi*

**AFTERNOON SESSION 17.30-18.30**

Michelangelo (**KN 30**)

**KN30.29(C7) | Janet Smith:**  
Structural Studies of Macromolecular Complexes:  
Cytochrome b6f

*Chair: Mitchell Guss*

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Botticelli (**KN 31**)

**KN31.29(C7) | Myunghyun Paik Suh:**  
Metal-Organic Frameworks: Assembly and Crystal  
Dynamics of Functional Materials

*Chair: Antonio Tiripicchio*

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Cimabue (**KN 32**)

**KN32.29(C7) | Michiyoshi Tanaka:**  
Nano Structures Studied by Convergent Beam  
Electron Diffraction

*Chair: Yuji Ohashi*

# MONDAY, AUGUST 29 2005 – MORNING - MICROSYMPOSIA

TIME	Botticelli (MS 71)	Michelangelo (MS 72)	Giotto (MS 73)
10.00-10.05 Opening Remarks	<b>STRUCTURAL BIOLOGY AND THE IMMUNE SYSTEM</b> <i>Chairs: D.Rose, M. Degano</i>	<b>HOT STRUCTURES IN PROTEIN CRYSTALLOGRAPHY</b> <i>Chairs: G. Oliva, A. H.-J. Wang</i>	<b>MOLECULAR CRYSTALS WITH NOVEL PHYSICAL PROPERTIES</b> <i>Chairs: C. Ruiz-Perez, A. Powell</i>
10.05-10.35	<b>MS71.29.1(C91)</b>   <u>L. A. Wilson</u> : Structural Basis of HIV-1 Neutralization: Implications for Vaccine Design	<b>MS72.29.1(C92)</b>   <u>C. Kerfeld</u> : Structural Studies on Carboxysomes	<b>MS73.29.1(C93)</b>   <u>M. Andruh</u> : New Synthetic Approaches Towards Supramolecular Multimetallic Systems with Interesting Magnetic Properties
10.35-11.05	<b>MS71.29.2(C91)</b>   <u>A. K. Shrive</u> : Structural Basis of Ligand Recognition by the Collectins	<b>MS72.29.2(C92)</b>   <u>M. J. Marcaida</u> : Structure and Function of RNase E and the RNA Degradosome Assembly	<b>MS73.29.2(C93)</b>   <u>V. Maravaud</u> : High Spin and Photomagnetic High Spin Molecules
11.05-11.35	<b>MS71.29.3(C91)</b>   <u>V. Streltsov</u> : Do Sharks Have a New Antibody Lineage?	<b>MS72.29.3(C92)</b>   <u>S. Wakatsuki</u> : Crystal Structures of Proteins Involved in Membrane Traffic	<b>MS73.29.3(C93)</b>   <u>C. Rovira</u> : Crystal Structure-Mobility Correlation in TTF Based Organic Field-Effect Transistors
11.35-12.05	<b>MS71.29.4(C91)</b>   <u>M. Dunstone</u> : The Structure of CD3 in Complex with the Therapeutic Antibody, OKT3	<b>MS72.29.4(C92)</b>   <u>T. Eneqvist</u> : The Structure of a Mitochondrial Peptidasome	<b>MS73.29.4(C94)</b>   <u>B. Zhang</u> : Dual-function Molecular Crystal with $[\text{Fe}^{\text{III}}(\text{C}_2\text{O}_4)\text{Cl}_2]^-$ chain Anion
12.05-12.35	<b>MS71.29.5(C91)</b>   <u>P. Gros</u> : Structural Insights into the Central Complement Component C3	<b>MS72.29.5(C93)</b>   <u>W. Hol</u> : Molecular Machines and Tropical Pathogens	<b>MS73.29.5(C94)</b>   <u>M. U. Schmidt</u> : Crystal Engineering on Organic Pigments

# MONDAY, AUGUST 29 2005 – MORNING - MICROSYMPOSIA

Leonardo da Vinci ( <b>MS 74</b> )	Brunelleschi ( <b>MS 75</b> )	Cimabue ( <b>MS 76</b> )	Donatello ( <b>MS 77</b> )
<b>TOTAL SCATTERING AND LOCAL ORDER</b> <i>Chairs: D. Louca, D. Keen</i>	<b>SURFACES</b> <i>Chair: L. D. Marks</i>	<b>NEW ALGORITHMS FOR STRUCTURE PREDICTION</b> <i>Chairs: P. Erk, S. Motherwell</i>	<b>PERSPECTIVE OF NEUTRON CRYSTALLOGRAPHY AT HIGH POWER SOURCES</b> <i>Chairs: M. Arai, I. Anderson</i>
<b>MS74.29.1(C94)</b>   <u>T. Egami</u> : Static & Dynamic Pair Correlation Functions Determined by Neutron Scattering and Inelastic Correction to Total Scattering	<b>MS75.29.1(C95)</b>   <u>M. A. Navasardyan</u> : Electromagnetic Wave Tunneling Through a Barrier With Periodical Structure	<b>MS76.29.1(C96)</b>   <u>G. M. Day</u> : Assessing Lattice Energy Minimisation for Crystal Structure Prediction	<b>MS77.29.1(C97)</b>   <u>C. A. Tulk</u> : Prospects for Neutron Diffraction under Extreme Pressure Conditions
<b>MS74.29.2(C94)</b>   <u>M. Guthrie</u> : The Local Structure of Ice VII Determined by Neutron Total Scattering	<b>MS75.29.2(C95)</b>   <u>D. Saldin</u> : Holographic methods for surface crystallography	<b>MS76.29.2(C96)</b>   <u>M. A. Neumann</u> : A Hybrid Method for the Accurate Energy Ranking of Molecular Crystals	<b>MS77.29.2(C98)</b>   <u>P. G. Radaelli</u> : ISIS Crystallography on TS-II: What Can We Do with 60 kW?
<b>MS74.29.3(C94)</b>   <u>Ii-K. Jeong</u> : Medium Range Ordering of Local Polarizations in Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	<b>MS75.29.3(C96)</b>   <u>J. Stangl</u> : X-Ray Diffraction From Semiconductor Nanostructures	<b>MS76.29.3(C97)</b>   <u>P. Raiteri</u> : Exploring Polymorphism: the Case of Benzene	<b>MS77.29.3(C98)</b>   <u>N. Niimura</u> : Hydrogen and Hydration Sensitive Structural Biology
<b>MS74.29.4(C95)</b>   <u>M. Tucker</u> : Getting the most from Total Scattering	<b>MS75.29.4(C96)</b>   <u>Z. Kaszkur</u> : Interaction of NO and CO with Surface of Pd Nanoclusters Studied by XRD	<b>MS76.29.4(C97)</b>   <u>P. Karamertzanis</u> : Progress in Crystal Structure Prediction for Diastereomeric Salts	<b>MS77.29.4(C98)</b>   <u>T. Kamiyama</u> : Shaping the Future of Neutron Powder Diffraction
<b>MS74.29.5(C95)</b>   <u>R. B. Neder</u> : Characterisation of Nanoparticles	<b>MS75.29.5(C96)</b>   <u>R. Feidenhans'l</u> : Three Dimensional Charge Density Measurements at Surfaces	<b>MS76.29.5(C97)</b>   <u>A. Le Bail</u> : Inorganic Structure Prediction with GRINSP	<b>MS77.29.5(C98)</b>   <u>J. R. Helliwell</u> : Neutron Protein Crystallography Development: Higher Molecular Weight Capability

# MONDAY, AUGUST 29 2005 – AFTERNOON - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 78</b> )	Botticelli ( <b>MS 79</b> )	Cimabue ( <b>MS 80</b> )
14.45-14.50 Opening Remarks	<b>STRUCTUROMES – STRUCTURES OF RIBOSOMES NUCLEOSOMES AND OTHER -OMES</b> <i>Chairs:</i> A. Liljas, W. Hendrickson	<b>INORGANIC AND MINERAL STRUCTURES SOLVED AND REFINED BY POWDER DIFFRACTION DATA</b> <i>Chairs:</i> J. Rius, E. Antipov	<b>STRUCTURAL KNOWLEDGE AND CATALYSIS</b> <i>Chairs:</i> J.-C. Daran, P. Gómez-Sal
14.50-15.20	<b>MS78.29.1(C99)</b>   T. Richmond: Nucleosome Core and Compact Nucleosome Array Structures	<b>MS79.29.1(C100)</b>   H. Gies: NMR and PXRD Analysis of the Structure of a New Hydrous Layer Silicate	<b>MS80.29.1(C101)</b>   A. Galindo: Structural Diversity and Properties of Oxydiacetate and Thiodiacetate Mn Complexes
15.20-15.50	<b>MS78.29.2(C99)</b>   K. Morikawa: Structural View of the Clamp-loading Mechanism onto DNA	<b>MS79.29.2(C100)</b>   J. Kaduk: Adventures in Solving Structures of Inorganic Compounds Using Powder Diffraction Data	<b>MS80.29.2(C101)</b>   T. Imamoto: Structure and Sense of Enantioselection of Rhodium Complexes of P-Chiral Diphosphines
16.50-16.20	<b>MS78.29.3(C99)</b>   J. Cate: X-ray Crystal Structures of the <i>E. coli</i> ribosome	<b>MS79.29.3(C100)</b>   K. Vidal: New Cathodes for Solid Oxide Fuel Cells Studied by Powder Diffraction: the System (Al-xA'x)FeO <sub>3</sub>	<b>MS80.29.3(C101)</b>   A. Mezzetti: Understanding Stereoselective Atom-transfer Reactions of Chiral Ruthenium Complexes
16.20-16.50	<b>MS78.29.4(C99)</b>   M. C. Wahl: Structural Analysis of the L7/L12 Ribosomal Stalk	<b>MS79.29.4(C100)</b>   D. N. Argyriou: Crystal Structure of Superconductivity in the Layer Cobaltite Na <sub>x</sub> CoO <sub>2</sub> yD <sub>2</sub> O	<b>MS80.29.4(C102)</b>   W. Baratta: 14-Electron Metal Complexes Stabilized by M $\eta^3$ -H <sub>2</sub> C Agostic Interactions
16.50-17.20	<b>MS78.29.5(C99)</b>   D. Baram: Ribosomal Crystallography Reveals Co-translational Trafficking by Eubacterial Trigger Factor	<b>MS79.29.5(C101)</b>   V. P. Ting: Structural Studies of the A <sub>3</sub> CoNb <sub>2</sub> O <sub>9</sub> “1.2” Ordered Perovskites (A = Ca <sup>2+</sup> , Sr <sup>2+</sup> , Ba <sup>2+</sup> )	<b>MS80.29.5(C102)</b>   G. Gainsford: Asymmetric Hydrogenation: Novel Rh(I) Catalysts & Predictive DFT Calculations

# MONDAY, AUGUST 29 2005 – AFTERNOON - MICROSYMPOSIA

Leonardo da Vinci ( <b>MS 81</b> )	Donatello ( <b>MS 82</b> )	Giotto ( <b>MS 83</b> )	Brunelleschi ( <b>MS 84</b> )
<b>TIME-RESOLVED POWDER DIFFRACTION FOR MATERIALS PRODUCTION AND PROCESSING</b> <i>Chairs:</i> E. Kisi, P. Barnes	<b>X-RAY CHARACTERIZATION OF NANOSTRUCTURES</b> <i>Chairs:</i> U. Valbusa, T. Baumbach	<b>COMPUTATIONAL PROBLEMS AND SOLUTIONS FOR APERIODIC CRYSTALS</b> <i>Chairs:</i> C. Svensson, V. Favre-Nicolin	<b>THEORETICAL METHODS FOR ANALYSES OF DATA FROM SOLUTIONS</b> <i>Chairs:</i> S. Vass, S. Ciccarello
<b>MS81.29.1(C102)</b>   T. Hansen: Investigating Fast Solid State Reactions with Time-resolved Constant Wavelength Neutron Powder Diffraction at D20	<b>MS82.29.1(C103)</b>   C. Teichert: Quantitive Morphological Characterization of Nanostructure Arrays by Scanning Probe Microscopy	<b>MS83.29.1(C104)</b>   M. Dusek: Towards the Routine Application of Computing System Jana2000	<b>MS84.29.1(C106)</b>   J. S. Pedersen: Analysis of Small-angle Scattering Data from Block Copolymer Micelles using Models based on Monte Carlo
<b>MS81.29.2(C102)</b>   Å. Kvick: Time-resolved Studies on Materials Using Synchrotron Radiation at the ESRF	<b>MS82.29.2(C103)</b>   J. Grenzer: Ripple Structure of Ion Beam Induced Si Wafers	<b>MS83.29.2(C105)</b>   S. van Smaalen: Modulation Functions of Aperiodic Crystals Determined by the Maximum Entropy Method	<b>MS84.29.2(C106)</b>   C. Burger: Theoretical Treatment and Practical Aspects of Systems with Preferred Orientation
<b>MS81.29.3(C102)</b>   N. Scarlett: <i>In-situ</i> X-ray Diffraction Studies into Pressure Acid Leaching of Lateritic Ores	<b>MS82.29.3(C104)</b>   H. Sawa: Direct Observation of a H <sub>2</sub> Molecule Swallowed by Open-mouthed C <sub>60</sub>	<b>MS83.29.3(C105)</b>   L. Palatinus: Ab Initio Solution of Incommensurately Modulated Structures by Charge Flipping	<b>MS84.29.3(C106)</b>   P. Vachette: Structural Biology Studies Coupling SAXS with Crystallography and NMR
<b>MS81.29.4(C103)</b>   R. Ibberson: <i>In-situ</i> Measurement of Cation Ordering in Electroceramics	<b>MS82.29.4(C104)</b>   V. Holý: Anomalous X-ray Scattering Methods for Structure Investigations of Semiconductor Nanostructures	<b>MS83.29.4(C105)</b>   Z. Izaola: Pyrrhotites Revisited in Superspace with <i>ab-initio</i> Calculations Insights.	<b>MS84.29.4(C106)</b>   M. Petoukhov: Methods for Quaternary and Domain Structure Analysis by Small Angle Scattering
<b>MS81.29.5(C103)</b>   R. Cerny: Phase Transitions in Metal Hydrides by <i>In-situ</i> Synchrotron Powder Diffraction with High Time-resolution	<b>MS82.29.5(C104)</b>   G. Srájer: Magnetic Imaging of Biquadratic Coupling in Ferromagnetic Bilayers	<b>MS83.29.5(C105)</b>   I. Orlov: New Tool Based on the Superspace Concept to Discover Structure Relations	<b>MS84.29.5(C107)</b>   R. Kranold: The Long-Wavelenght Limit of the Structure Factor of Mixed Metaphosphate Glasses

## **MONDAY, AUGUST 29 2005 – OTHER ACTIVITIES**

## **OPEN COMMISSION MEETINGS**

Beato Angelico (14.00-16.00 and 16.30-18.30)

## OCM08 COMMISSION ON HIGH PRESSURE

Chair: Martin Kunz

OCM08.29.1(CJ33) | P. Dera:

# Exploring Novel Synchrotron Approaches to Structure Determination by Single-crystal XRD

OCM08.29.2(CJ33) | C. Hejny:

## Single Crystal Studies Using the 9.8 Station at SRS Daresbury

OCM08.29.3(Cl33) | M. Guthrie

## High Pressure Single Crystal Studies Using Neutrons

OCM08.29.4(C134) | L. Goncharenko

## Single Crystal Neutron Experiments under Pressures up to 38 GPa

OCM08.29.5(C134) | M. Mezouar:

# Development of a New State-of-the-art Beamline Optimised for Single Crystal and Powder X-ray Diffraction under Extreme Conditions at the ESRF

OCM08.29.5(C134) | T. Katsura:

# Recent Progress in Large-volume High P-T in situ X-ray Observation at SPring-8

**OCM08.29.6(C134)** | J.-P. Rueff:

## High-pressure Magnetic Collapse in Transition-metal Oxides

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**COMPUTER FAYRE** Ghirlandajo

(10.00-12.00)  
OASIS-2004

(14.00-16.00) L. J. Farrugia  
The WinGX Suite of Programs

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IUCr GENERAL ASSEMBLY

### Cimbahue (19.00-20.00)

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

## 02 METHODS FOR STRUCTURE DETERMINATION

### 9. Liquid Structure Determination

P.02.09.1(C155.1) | L. Fu: X-ray Scattering Measurements of Liquid Water

### 12. Ab initio Powder Diffraction Solutions: Inorganic Compounds

P.02.12.1(C158.2) | M. Grzywa: Preparation and Crystal Structure of Tetraperoxo Complexes

P.02.12.2(C158.3) | C. Cuocci: Space Group Determination by EXPO2005

P.02.12.4(C158.5) | L. Lutterotti: Algorithms for Solving Crystal Structure Using Texture

## 03 COMPUTERS IN ANALYSIS, MOLECULAR MODELLING AND MOLECULAR DESIGN

### 7. Structure Simulations: Protein Folding Studies

P.03.07.1(C167.6) | V. Pletnev: 3d Model of Ternary Complex of Human 3 $\beta$ -HSD type I. Rational Mutagenesis.

P.03.07.2(C167.7) | M. Kuty: Force Field Parameters for the Photosystem II Reaction Center

### 8. Map Fitting and Modification

P.03.08.1(C167.8) | D. Turk: MAIN 2004: Model Building beyond 100 Residues per Minute.

P.03.08.2(C168.9) | D. Risal: Automated de novo Electron Density Map Tracing for the Structural Genomics Era

### 10. Homology Modelling, Structural Families and Doc

P.03.10.1(C168.10) | R. Rathore: Elucidation of Structural Models of Formyl Peptide Receptors, FPR & FPR2, and Identification of Features, Responsible for their Differential Ligand-Binding Affinities

P.03.10.2(C168.11) | L. Caracelli: Structural and Docking Studies of  $\beta$ -lapachone Derivatives

P.03.10.3(C168.12) | A. Moutran: Homology Modeling of Xanthomonas Citri Molybdate-binding Protein

P.03.10.4(C169.13) | A. Seal: Specificities of Binding of Different Inhibitors of Cathepsins

## 11. Use Of Genetic Algorithms and Other Optimisation Methods

P.03.11.1(C169.14) | Z. Otwinowski: Multi-component Analysis of Raw Diffraction Data

## 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

### 3. Metallo-Enzymes

P.04.03.1(C208.15) | T. Yokoyama: Novel Mechanisms of pH Sensitivity in Tuna Hemoglobin

P.04.03.2(C209.16) | M. Ferraroni: Substrate Specificity of Three New Intradiol Dioxygenases: an X-ray Characterization

P.04.03.3(C209.17) | Y. Kitagawa: Crystal Structure of Iron Superoxide Dismutase from Obligate Anaerobic Bacterium

P.04.03.4(C209.18) | G. K.-W. Kong: Understanding How the Alzheimer's Amyloid Precursor Protein Binds Copper

## Ions

P.04.03.5(C209.19) | B. Johnson: Dioxygen Activation in *Hansenula polymorpha* Amine Oxidase

P.04.03.7(C210.20) | R. Hoeft: Analysis of Mutants of an Active Site Base in a Non-heme Extradiol Dioxygenase

P.04.03.8(C210.21) | S. Tom-Yew: Anion-independent Iron Binding by *Campylobacter jejuni* Ferric Binding Protein

P.04.03.9(C210.22) | V. Malashkevich: Tat System of *Escherichia coli*: Zn<sup>2+</sup>-bound Structures of tatD, ycfH and yjjV

P.04.03.10(C211.23) | A. K. Rohr: A Tri-nuclear Metal Cluster in Reduced Mouse Ribonucleotide Reductase R2 Subunit

P.04.03.11(C211.24) | T. Saitoh: Structural Analysis of the Interaction between Plant Sulfite Reductase and Ferredoxin

P.04.03.12(C211.25) | M. Podobnik: Rv0805: Cyclic Nucleotide Phosphodiesterase from *M. tuberculosis*

P.04.03.13(C211.26) | S. H. Oakley: Manganese Superoxide Dismutases and Substrate Mimic Derivatives

P.04.03.15(C212.27) | Y. Kawano: Dynamic Structures and Reaction Mechanism of Active Fe-type Nitrile Hydratase.

P.04.03.16(C212.28) | M. Nardini: Structural Studies on *Cerebratulus lacteus* Mini-Hb K(E10)W and L(G12)A Mutants

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

P.04.03.17(C212.29)   N. Adir: Structure of the MntC Protein: Mn <sup>2+</sup> Import in Cyanobacteria is Redox Controlled	P.04.03.29(C215.40)   H. Sugimoto: Crystal Structure of Human Indoleamine 2,3-dioxygenase	Reveals a Novel Fold and Provides Insights into its Biological Functions
P.04.03.18(C212.30)   I. Muñoz: Crystal Structure of Eukaryotic FeSODs Suggests Intersubunit Cooperation during Catalysis	P.04.03.30(C215.41)   M. Makino: High Resolution Structure of Cytoglobin Reveals the Extra Helix in N-terminus	P.04.12.2(C231.51)   S. Muraoka: Crystal Structure of the Small G Protein M-Ras and Its Implications
P.04.03.19(C213.31)   T. Karlberg: Towards the Crystal Structure of <i>Saccharomyces cerevisiae</i> Frataxin	P.04.03.31(C215.42)   V. Alterio: The Crystal Structure of the (Zn/Zn)bLAP/Zofenoprilat Complex	P.04.12.3(C231.52)   M. Booth: Structural Studies of Plant RKIP/PEBP Family Members
P.04.03.20(C213.32)   P. Grochulski: The Crystal Structure of NEP and its Complexes with Inhibitors	P.04.03.32(C216.43)   A. Di Fiore: The Crystal Structure of Human CA II Bound to a Strong Benzenesulfonamide Inhibitor	P.04.12.4(C231.53)   O. Sleator: Inwardly Rectifying Potassium Channels
P.04.03.21(C213.33)   M. Sugishima: Crystal Structures of Cyanobacterial Heme Oxygenases	P.04.03.33(C216.44)   Y. Higuchi: Role of the Non-protein Ligand at the Ni-Fe Active Site of [NiFe] Hydrogenase	P.04.12.5(C232.54)   A. Nagata: Structural and Functional Analysis of SHPS-1, a Receptor-type Membrane Protein
P.04.03.22(C213.34)   A. O. Tastan Bishop: Crystal Structure of Nitrile Hydratases: Possible Industrial Usage	P.04.03.34(C216.45)   M. Kusunoki: Crystal Structure of Mouse Carnosinase CN2 at 1.8 Å Resolution	P.04.12.6(C232.55)   N. Burton: Interaction between Raf Kinase and Raf Kinase Inhibitor Protein
P.04.03.23(C214.35)   H. Chida: Crystal Structure and Stability of Red Alga <i>Porphyra yezoensis</i> Cytochrome <i>c</i> <sub>6</sub>	P.04.03.35(C216.46)   T. Santos-Silva: Class III Superoxide Reductase from <i>Treponema pallidum</i>	P.04.12.7(C232.56)   A. Wehenkel: Structural Studies of Mycobacterial Protein Kinases and Phosphatases
P.04.03.24(C214.36)   H.-P. Hersleth: Structure of the Intermediates in the Myoglobin-peroxide Reaction	P.04.03.36(C216.47)   C. Bonifacio: Crystal Structures of Cytochrome c Peroxidases from <i>Ps. nautica</i> and <i>Ps. stutzeri</i>	P.04.12.8(C232.57)   M. Vijayan: Banana Lectin, a β-prism I Fold Lectin with Two Carbohydrate-binding Sites
P.04.03.25(C214.37)   G. Hagelüken: Crystal Structure of PA0740, a Novel Zinc Hydrolase of <i>Pseudomonas aeruginosa</i>	P.04.03.37(C217.48)   A. Tochowicz: Structures of Matrix Metalloproteinase - 9 in Complex with Pharmacological Inhibitors	P.04.12.9(C233.58)   C. Wiesmann: Crystal Structure of the HGF β-chain in Complex with the Sema Domain of the Met Receptor
P.04.03.27(C214.38)   V. Calderone: Mimicking Evolution from Inactive <i>Bacillus subtilis</i> SOD-like Protein to Active Mutants	P.04.03.38(C217.49)   A. Halavaty: Ru(bpy)2(mbpy)-Adx(1-108) Complex: Photoreduction and Crystal Structure	P.04.12.10(C233.59)   T. Ishigaki: Crystal Structure of Human C-type Lectin-like Oxidized LDL Receptor 1(LOX-1)
P.04.03.28(C215.39)   L. Vitagliano: Structural Characterization of the Oxidation Pathway of Antarctic Fish Hemoglobins	<b>12. Receptor and Signal Transduction Proteins</b>	P.04.12.11(C233.60)   M. Milani: The ‘Active-like’ Structure of the Unphosphorylated Response Regulator StyR
	P.04.12.1(C231.50)   P. Zhang: Structure of MRG15	P.04.12.12(C233.61)   M. Lawrence: Insecticide Selectivity: Structure of a Lepidopteran Ecdysone

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

## Receptor LBD

**P.04.12.13(C233.62)** | A. K. Padyana: Structural Basis for Autoinhibition and Activation of eIF2 $\alpha$  Protein Kinase GCN2

**P.04.12.14(C234.63)** | C. Kasper: Domain Closure of the Ligand-binding Core of the AMPA Receptor GluR2: Insights from Agonist and Antagonist Complexes

**P.04.12.15(C234.64)** | J. S. Kastrup: Structural Studies of Kainate Receptor GluR5 Ligand-binding Core Complexes

**P.04.12.16(C234.65)** | S. Covaceuszach: Unraveling the Binding Mode of the Neutralizing Neuroantibody aD11 to NGF

**P.04.12.17(C234.66)** | F. Paletti: Towards a Comprehension of the Structure of Mouse proNGF

**P.04.12.18(C235.67)** | C. Chan: Structural Basis for the Activity and Allosteric Control of Diguanylate Cyclase

## 16. Multi-domain Proteins

**P.04.16.2(C249.68)** | E. Sauvage: Crystal structure of the *Actinomadura* R39 DD-peptidase (PBP4)

**P.04.16.3(C249.69)** | C.-J. Chen: Sulfur SAD Structure of Heparin-Binding CRISP from *Naja atra* Reveals Protease and Ion Channel Blocking Domains

**P.04.16.4(C250.70)** | T. Akiba: Structure of Parasporin-1, a Novel Bacterial Cytotoxin against Human Cancer Cells

**P.04.16.5(C250.71)** | N. Shibata: Structure of Diol Dehydratase Reactivating Factor – A Novel Molecular Chaperone

**P.04.16.6(C250.72)** | M. Sevanna: Structural and Functional Analysis of PDI-related Proteins

**P.04.16.7(C250.73)** | M. Jinek: TPR Repeat Domain of O-linked GlcNAc Transferase: Similarities to Importin Alpha

**P.04.16.8(C251.74)** | E. Soriano: Structural Studies of Quinolinate Synthase

**P.04.16.9(C251.75)** | L. M. Podust: A Second FMN-binding Site in Yeast CPR Suggests a Novel Mechanism of Electron Transfer by Diflavin Reductases

**P.04.16.10(C251.76)** | D. Han: Identification and Purification of a Soluble Region of BubR1

## 19. Diseases and Toxicity

**P.04.19.1(C252.77)** | K. Kitano: Crystal Structure of Decameric Peroxiredoxin (AhpC) from *Amphibacillus xylinus*

**P.04.19.2(C253.78)** | H. Lewis: Structures of CFTR NBD1 Suggest a Molecular Mechanism for Cystic Fibrosis

**P.04.19.3(C253.79)** | E. Horjales: Amyloidosis: Structure of a  $\lambda$  6 Light Chain Antibody Fragment.

**P.04.19.4(C253.80)** | P. Rigolet: Structural and Functional Study of the Bloom Syndrome Protein

**P.04.19.5(C253.81)** | K. Hirata: Molecular Basis for Antitumor Effect of Actin-aplyronine A Complex

**P.04.19.6(C254.82)** | H. M. Baker: Crystal Structure of SSL11, a Superantigen-related Toxin from *Staphylococcus aureus*

**P.04.19.7(C254.83)** | J. Schulze: Crystal Structure of 5-Aminolevulinate Synthase of *Rhodobacter capsulatus*

**P.04.19.8(C254.84)** | M. Becker: Structures of *B. burgdorferi* OspB Alone, and in Complex with a Bactericidal Fab

**P.04.19.9(C254.85)** | J. Arndt: Crystal Structure of Botulinum Neurotoxin Type G Light Chain

## 23. High Resolution Protein Structures

**P.04.23.1(C260.86)** | R. Gordon: Structural Insights into GnT-I Substrate Recognition & Specificity

**P.04.23.2(C260.87)** | A. Urzhumtsev: On the Incompleteness of Atomic Models

**P.04.23.3(C260.88)** | N. Shimizu: Ultra-high Resolution Measurement at BL41XU of SPRing-8

**P.04.23.4(C260.89)** | M. Takata: A Challenge to Bonding Nature Study in Protein Crystallography

**P.04.23.5(C261.90)** | M. Biadene: Opening of the Safety-belt Loop of Human Aldose Reductase

**P.04.23.6(C261.91)** | D. V. Tamu: Crystal Structure of *Caenorhabditis elegans* Spermidine Synthase: in Preparation

**P.04.23.7(C261.92)** | E. Mitchell: Structure of *Ralstonia Solanacearum* Fucose Binding Lectin at 0.94Å Resolution

**P.04.23.8(C261.93)** | M. Diaconu: Crystal Structures of Ribosomal Protein L10 in Complex with L7/12 N-

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

## Terminal Domains

### 07 CRYSTALLOGRAPHY OF ORGANOMETALLIC, COORDINATION AND MAIN GROUP COMPOUNDS

#### 1. Metal Atom Complexes (N = 1-3) and Metal Clusters (N>3)

**P.07.01.1(C295.94)** | R. Kia: Synthesis and Structure of the 1.1 Adducts of Copper (I) Halides with Bis-(benzophenone)ethylenediimine

**P.07.01.2(C295.95)** | S. Ghammamy: Synthesis and Structural Analysis of a Number of Hexacoordinate Heteroleptic Non-VSEPR Molybdenum and Tungsten Complexes

**P.07.01.3(C295.96)** | J. Costamagna: Crystal and Molecular Structure of Bis-N-Octyl-hydroxy-naphthaldiminato Cu(II). A Study Including Magnetic Properties of Also N-Dodecyl and N-Octadecyl Derivatives

**P.07.01.4(C295.97)** | L. Zhao: Silver Complexes Containing 1,3-Butadiynediide C<sub>4</sub><sup>2-</sup> and Ar(C≡C)<sub>n</sub> (n = 1, 2)

**P.07.01.5(C296.98)** | J. F. Van der Maelen Uria: Mn- and Cr-highly Electrophilic Carbenes: Calculated vs Experimental Parameters

**P.07.01.6(C296.99)** | I. V. Medrish: Structure of New Different-ligand Uranyl Complexes

**P.07.01.7(C296.100)** | E. A. Kiseleva: Polymorphism of Yttrium Threemethylacetate

**P.07.01.8(C296.101)** | G. Marinoni: Unconventional

#### Distribution of Hydrides in Hydrido Rhenium Carbonyl Clusters

**P.07.01.9(C296.102)** | B. M. Draskovic: C-H•••π Interactions in the Novel Ni(II) Complex with Tetradentate Thiosemicarbazide Based Ligand

**P.07.01.10(C297.103)** | R. Baggio: Isolation and Characterization of a Ferromagnetic Gadolinium (III) Citrate Chain

**P.07.01.11(C297.104)** | B. Tinant: Novel water-soluble Peroxo Complexes of Nb(V) and Ta(V)

**P.07.01.12(C297.105)** | K. Guille: Studies in the Structural Chemistry of Complexes between Nucleobases and *s*-Block Metals

**P.07.01.13(C297.106)** | K. Andjelkovic: Structure of Pd(II) Complex with a 2-(diphenylphosphino)benzaldehyde Derivative

**P.07.01.14(C298.107)** | M. Di Vaira: From P<sub>4</sub> to PH<sub>3</sub> Metal Complexes by Plane Hydrolysis

**P.07.01.15(C298.108)** | F. Balegroune: New Polymeric Barium(II)2,2'-diphenyldicarboxylate Complex

**P.07.01.16(C298.109)** | W.-T. Wong: Fabrications of Carbon Nanotube Coated with Os-Pd Mixed-metal Nanoparticles

**P.07.01.17(C298.110)** | J. P. Lau: Synthesis and Structural Characterization of a Series of High-hydride Content Osmium-Rhodium Carbonyl Complexes

**P.07.01.18(C298.111)** | R. Spagna: Scorpionate Complexes with the Main Group Elements Ca, Ba, Sr

**P.07.01.19(C299.112)** | V. S. Jevtovic: Synthesis and Crystal Structure of [Co(HL)]CH<sub>2</sub>OH (H<sub>2</sub>L = Pyridoxal S-methylisothiosemicarbazone)

**P.07.01.20(C299.113)** | M. Parvez: Novel Five-membered B-N-C Heterocycles

**P.07.01.21(C299.114)** | Z. Xi-Rui: A new Trinuclear Europium(III) Complex

**P.07.01.22(C299.115)** | E. Herdtweck: Non Classical vs. Classical Metal•••H<sub>3</sub>C-C Interactions: A Neutron Diffraction Study of a 14-Electron Ruthenium(II) System

**P.07.01.23(C300.116)** | P. Martín-Zarza: Order-Disorder Phase Transition in Hexakis(Imidazole)Metal(II) Complex

**P.07.01.24(C300.117)** | C. Kazak: Bis-(5,5'-diethylbarbiturato)copper(II) and cadmium(II) Complexes with Ethylenediamine

**P.07.01.25(C300.118)** | W.-S. Wu: Crystal Structure of N-picoloylhyclazide and its Binuclear Palladium Complex

**P.07.01.26(C300.119)** | N. Lah: Copper-imidazole-chloride/bromide complexes

**P.07.01.27(C300.120)** | M. Ramos Silva: Bis(bis(μ<sub>2</sub>-dimethylglycine-O,O')-tetrachlorocuprate-dicopper(II)) Hydrate

**P.07.01.28(C301.121)** | H. Pasaooglu: Spectroscopic and Structural Investigation of ZnI<sub>2</sub>(nicotinamide)<sub>2</sub>, [Zn(H<sub>2</sub>O)<sub>2</sub>(picolinamide)<sub>2</sub>]I<sub>2</sub> and Zn I<sub>2</sub>(isonicotinamide)<sub>2</sub>

**P.07.01.29(C301.122)** | M. R. Bond: Green-yellow Thermochromism of (N-methyl-2,6-lutidinium)<sub>2</sub> CuCl<sub>4</sub>

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

**P.07.01.30(C301.123)** | T. Yamagata: Structure of Hydrido(carboxylato)Ir(III) Complexes and Catalytic Symmetric Hydrogenation of Imines

**P.07.01.31(C301.124)** | L. Tatar Yildirim: Synthesis, Characterization and Crystal Structure of new Transition Metal Compounds of Thiocyanate

**P.07.01.32(C301.125)** | N. Kanehisa: Crystal Structure of Trimethyltin hydroxide,  $(\text{CH}_3)_3\text{SnOH}$

**P.07.01.33(C302.126)** | N. Yoshikawa: Crystal Structure of  $[\text{RuCl}(\text{dpphen})(\text{terpy})]\text{PF}_6$  and  $[\text{Ru}(\text{CH}_3\text{CN})(\text{phen})(\text{terpy})]\text{PF}_6$

**P.07.01.34(C302.127)** | M. Monari: Structural Studies on Copper(II) Carboxylate Complexes Containing Pyrazole

**P.07.01.35(C302.128)** | A. Kapor: Crystal Packing of Three-Aqua Sodium Maleate

**P.07.01.36(C302.129)** | D. Swenson: Structural Parameters of Several Lanthanide Clusters

**P.07.01.37(C303.130)** | K. W. Törnroos: Unit Cellmates: the *Cis* and *Trans* Isomers of an Iron(II) Complex Co-crystallize

**P.07.01.38(C303.131)** | L. Marchiò: Influence of the R Group in  $[\text{Mo}_2(\mu-\text{R})(\mu-\text{PCy}_2)(\text{CO})_2\text{Cp}_2]$ , R=H,  $\text{CH}_3$ , Ph, Bz

**P.07.01.39(C303.132)** | D. Yakhvarov: Synthesis and X-ray Study of the P<sub>5</sub>-polyphosphorus Rhodium Complex  $[(\text{dpmp})(\text{Ph}_2\text{PCH}_2\text{P}(\text{Ph}_2)\text{PPPP})\text{Rh}]\text{OTf}$

**P.07.01.40(C303.133)** | M. L. Martin-Albina: Structural Analysis of New Early-late Heterobimetallic Tetranuclear

## Metallamacrocycles

**P.07.01.41(C304.134)** | M. J. Fabra-Caro: Structural Aspects of Pyridyl-pyrazole Dinuclear Rh and Ir Complexes

**P.07.01.42(C304.135)** | J. Cirera: Spin State and Stereochemistry in Tetracoordinate Complexes of d<sup>n</sup> Transition Metals

**P.07.01.43(C304.136)** | U. Baisch: Structure Determination of Twinned and Disordered Cyclopentadienyl Complexes

## 11. No Sub-Theme

**P.07.11.2(C313.137)** | L. Vendier: X-ray Structural Study of σ-borane and Dhydridoborate Ruthenium Complexes

## 08 STRUCTURE/PROPERTY RELATIONSHIP

### 3. Dynamic Properties in Molecular Crystal

**P.08.03.1(C316.138)** | S. Yoneda: Dynamics of Nucleoside and Nucleotide Hydrates by MD Simulation

**P.08.03.2(C317.139)** | B. Vangdal: A Novel Spin Transition Curve in  $[\text{tris}(2\text{-picolylamine})\text{Fe}(\text{II})]\text{Cl}_2$  Allyl Solvate

### 4. Solid State Reactions

**P.08.04.1(C317.140)** | S. Seyyidoglu: Solid State Synthesis and Characterization of Some Novel Sodium Rare Earth Phosphates

**P.08.04.2(C317.141)** | I. Rosales: The Systems Li-Ho-P-O and K-Ho-P-O: A Study in Inert Atmosphere

## P.08.04.3(C317.142) | S.-M. Chen:

Studies of Spin Crossover Complexes via Solvo-thermal Syntheses and their Thermal Relaxation of Light Excited Kinetic Phenomena

## P.08.04.4(C317.143) | M. J. Diánez:

Study of the Mechanism of Cu-Zn Mechanical Alloying by X-ray Powder Diffraction

**P.08.04.5(C318.144)** | J. Cai: Studies on the Solid State Structures and Properties of Metal Arenedisulfonates

**P.08.04.6(C318.145)** | Y. Ohashi: Structure Analysis of the Excited Molecules in the Equilibrium State

**P.08.04.7(C318.146)** | F. Camus: X-ray Induced Changes in Organic and Biological Crystalline Materials

## 6. Phase Transitions

**P.08.06.13(C321.147)** | Y. Ueda: Metal-Insulator Transition in Hollandite Vanadate,  $\text{K}_2\text{V}_8\text{O}_{16}$

## 09 CRYSTAL ENGINEERING

### 5. Intermolecular Interactions: Exploitation

**P.09.05.1(C360.148)** | M. G. Haywood: Highly Symmetrical Hydrogen-bonded Networks

**P.09.05.2(C360.149)** | T. C. W. Mak: Supramolecular Approach to Generation and Stabilization of Labile Organic Anions

**P.09.05.3(C361.150)** | A. M. E. Griffin: Synthesis of 2D and 3D Nets Using Biimidazole Complexes

**P.09.05.4(C361.151)** | A. Vij: Bio-mimicking Self Assembly in Materials: Role of Hydrogen and Halogen

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

## Bonding

**P.09.05.5(C361.152)** | M. Hodorowicz: Benzylidimethylalkylammonium Haloplumbates: Organic/Inorganic Composite Materials

**P.09.05.6(C361.153)** | T. N. Sokolov: Crystalline Supramolecular Ladders *via* Co-Crystals

**P.09.05.7(C362.154)** | F. Zordan: M-X···X'–C Halogen Bonds as Efficient and Reliable Supramolecular Synths in Organic-Inorganic Crystals

**P.09.05.8(C362.155)** | G. Minguez: Halogen Bonds in Inorganic Crystal Design

**P.09.05.9(C362.156)** | T. Friscic: Control of Reactivity in the Solid State through Principles of Supramolecular Chemistry

**P.09.05.10(C362.157)** | P. Metrangolo: Halogen Bonding in Crystal Engineering

**P.09.05.11(C362.158)** | R. M. Claramunt: A Non-Symmetric Disordered Tetramer: The Unusual Structure of 3(5)-Ethyl-5(3)-phenyl-1H-pyrazole in the Solid State

**P.09.05.12(C363.159)** | T. Pilati: Topologic Features of Three Structures Based on I-Base Halogen Bonding

**P.09.05.13(C363.160)** | A. Neels: Inter- and Intra-solid Reactions Studied by X-ray Powder Diffraction

**P.09.05.14(C363.161)** | E. Bosetti: Anion-Dependent Switch between Sheets and Diamondoid Assembly for  $Zn(LOH)_2X_2$

**P.09.05.15(C363.162)** | D. Gonzalez Mantero: 2-D and 3-

## D Metal-Organic Frameworks: A Crystal Engineering Approach

**P.09.05.16(C364.163)** | D. C. Levendis: The Interplay between N-H···O Hydrogen Bonding and Cl···Cl Interactions in Arylformamides

## 12 SURFACES, INTERFACES, LIQUIDS AND THIN FILMS

### 2. Surfaces and Catalysis

**P.12.02.1(C410.164)** | T. F. Diaz Becerril: Chemical preparation of GaAs (100), (110), (111) and (112) substrates with HF:H<sub>2</sub>O<sub>2</sub>:Citric acid:H<sub>2</sub>O

### 6. Recent Liquid Structure Determination

**P.12.06.1(C411.165)** | K. Kurihara: Hydrogen-Bonded Structure of Alcohols Adsorbed on Silica Surface in Cyclohexane

## 12. Magnetic and Conducting Properties of Thin Films

**P.12.12.1(C416.166)** | E. Tamanis: The Influence of Thermal Annealing on Magnetostatic Properties of Thin Fe and Ni Films

## 14 CHARGE, SPIN AND MOMENTUM DENSITY

### 1. Multipole and other Modelling Methods

**P.14.01.1(C419.167)** | D. Foerster: Comparative Charge Density Studies on Tripeptides of the Ala-Xxx-Ala-type

**P.14.01.2(C419.168)** | S. Mebs: Charge Density of Amino Acids with Strong Hydrogen Bonds: A Comparative Study

**P.14.01.3(C419.169)** | T. Koritsanszky: Experimental

## Charge Density Study on Vitamin B12

**P.14.01.4(C419.170)** | M. J. Turner: Determination of 'Experimental' Wavefunctions from X-ray Diffraction Data

**P.14.01.5(C419.171)** | S. Scheins: Comparing Charge Densities of Opioids: Morphine, Codeine and Dextromethorphan

**P.14.01.6(C420.172)** | C. B. Huebschle: Thymidin Invariom Transfer and Multipole Refinement of a 20 K Data Set: A Comparison

**P.14.01.7(C420.173)** | K. Poomani: Experimental Electron Density and Topological Analysis of D- and DL-Camphoric Anhydride

**P.14.01.8(C420.174)** | D. Mannix: Light on Phase IV in Ce<sub>0.7</sub>La0.3B<sub>6</sub>

**P.14.01.9(C420.175)** | B. Dittrich: Anisotropic Displacement Parameters (ADPs) of Hydrogen Atoms. Can Invariom Modeling Contribute?

### 2. Software Developments

**P.14.02.1(C421.176)** | C. Jelsch: Advances in Charge Density and Electrostatic Interaction Analyses

### 3. Applications of Synchrotron Data

**P.14.03.1(C421.177)** | U. Pietsch: Bond-dependent Crystal Response on Electric Field: Synchrotron Diffraction Study

**P.14.03.2(C421.178)** | T. Leisegang: Electron Density Analysis of Borocarbides

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

P.14.03.3(C421.179) | L.-J. Hsu: Chemical Bonding and Electronic Configuration of Nitrosyl Iron Complexes

P.14.03.4(C421.180) | Y. Wang: Pump and Probe the Structure and Electronic Configuration of LIESST State

## 4. Maximum Entropy Applications

P.14.04.1(C422.181) | M. Sakata: Structure Refinements of Protein-ligand Complex by the Maximum Entropy Method

P.14.04.2(C422.182) | M. Tada: Maximum-entropy and Fourier Study on Electron Density of MnO, LaCoO<sub>3</sub> and MgSiO<sub>3</sub>

## 5. Experimental Methods and Techniques

P.14.05.1(C422.183) | W. Jauch: Electron Density in Cubic SrTiO<sub>3</sub> from  $\gamma$ -ray Diffraction

P.14.05.2(C422.184) | M. Itou: High-resolution Magnetic Compton Profile of Iron

P.14.05.3(C423.185) | N. Ishizawa: The Effect of Fourier Series Truncation Errors on the Electron Density Distribution of LiMn<sub>2</sub>O<sub>4</sub>

P.14.05.4(C423.186) | M. Chruszcz: Ultra-high Resolution Data for Charge Densities Studies

P.14.05.5(C423.187) | E. Molins: Electron Density and Electrostatic Potential Study of an Organic Phosphate

P.14.05.6(C423.188) | A. A. Pinkerton: Accurate Charge Densities in under a Day with a Home X-ray Source

## 6. Topological Analyses

P.14.06.1(C423.189) | P. Munshi: Topological Analysis of Charge Densities in Polymorphs of 3-Acetylcoumarin

P.14.06.2(C424.190) | C. Evans: Experimental and Theoretical Charge Densities of Fe(CO)<sub>3</sub>(η<sup>4</sup>-C<sub>4</sub>H<sub>6</sub>)

P.14.06.3(C424.191) | R. Bianchi: Multipole-Refined Charge Density Study of Diopside

P.14.06.4(C424.192) | C.-R. Lee: Topological Analysis of Bio-molecules

P.14.06.5(C424.193) | J. Zaleski: Charge Density and Topological Properties of Chosen Aromatic Nitramines

P.14.06.6(C425.194) | D. Parrish: Rapid Charge Density Data Collection

## 8. Magnetisation and Spin Densities

P.14.08.1(C429.195) | P. Gusin: On the Conditions Leading to the Gaussian Distribution of the Magnetic Moments in a Spin-glass State

P.14.08.2(C429.196) | N. Tsuji: Spin Density and Ordered Orbital of YTiO<sub>3</sub> Observed by X-ray Magnetic Diffraction

## 10. No Sub-Theme

P.14.10.1(C430.197) | M. Fronc: Charge Density Study of Cu<sub>3</sub>(en)<sub>2</sub>(CN)<sub>4</sub>•H<sub>2</sub>O

## 15 DIFFRACTION PHYSICS AND OPTICS

### 8. Dynamical Diffraction

P.15.08.6(C434.198) | A. Goodwin: Dynamics from

## Diffraction

### 17 CHARACTERIZATION OF DEFECTS, MICROSTRUCTURES AND TEXTURES 2. Electron Microscopy

P.17.02.1(C447.199) | P. Franklyn: Mixed Metal Oxide Nanoparticles – Synthesis and Characterisation

P.17.02.2(C447.200) | S. I. Son: Fivefold Twinning of Diamond

### 5. STM and AFM Microscopy

P.17.05.1(C452.201) | D. Passeri: Local Elastic Measurement in Nanostructured Materials via Atomic Force Acoustic Microscopy Technique

### 6. Other Techniques Including Polarised Light and Infrared Studies

P.17.06.1(C453.202) | A. E. Cordero-Borboa: Spatial Maps of Eu-aggregates in NaCl:Eu<sup>2+</sup> and KCl:KBr:Eu<sup>2+</sup> Single-crystals

## 19 ELECTRON DIFFRACTION

### 1. New Techniques and New Instrumentation

P.19.01.1(C457.203) | C. Hebeisen: Generation and Characterization of Ultrashort Electron Pulses

P.19.01.2(C457.204) | J. Dwyer: Ultrafast Melting in Metals Probed with Femtosecond Electron Diffraction

## 24 DATABASES

### 1. Creation and Exploitation

# MONDAY, AUGUST 29, 2005 – POSTER SESSION

P.24.01.1(C481.205) | A. Le Bail: COD (Crystallography Open Database) and PCOD (Predicted)

P.24.01.2(C481.206) | R. Kuroki: Hydrogen and Hydration DataBase for Bio-Macromolecules (HHDB)

P.24.01.3(C481.207) | R. Harrington: Four Years of the EPSRC SRS Service

## 2. Coping with Rapid Expansions of Data. The Next Generation of Databases

P.24.02.1(C481.208) | P. Murray-Rust: The Crystallographic Semantic Web

P.24.02.2(C481.209) | M. Hursthouse: ECRYSTALS(.CHEM.SOTON.AC.UK): Open Archive Publication of Crystal Structure Data

## 3. Research Applications of the CSD

P.24.03.1(C482.210) | S. Motherwell: Hydrogen Bond Capacity of Organic Functional Groups: a CSD derived Database

## 4. Research Applications of the PDB/NADB

P.24.04.1(C482.211) | L. Esposito: Unveiling the omega/psi Correlation in High Resolution Protein Structures

P.24.04.2(C482.212) | D. M. Standley: Beyond Text-based Queries at the Protein Data Bank, Japan

## 6. Research Applications of the PDF

P.24.06.1(C482.213) | S. Kabekkodu: Implementation of

Calculated Patterns Quality Marks in The Powder Diffraction File

P.24.06.2(C483.214) | J. Faber: The New PDF-4+ 2005: A Relational Database (RDB) with Atomic Structure Information and On-the-fly Total Pattern Analysis Capability

## 7. Data Mining and Knowledge Generation

P.24.07.1(C483.215) | H. A. Sparkes: Carbonyl-Carbonyl Interactions in First-row Transition Metal Complexes

P.24.07.2(C483.216) | J. M. M. Smits: ISOBASEmm: Isostructurality in the Protein Data Bank

P.24.07.3(C483.217) | B. Toby: Powder Diffraction CIFs: Preparation and Review.

P.24.07.4(C483.218) | G. Barr: Automating the Identification of Packing Motifs; dSNAP

P.24.07.5(C484.219) | P. Vinson: Description of Software for the Planning, Execution, and Refinement of Crystallography Experiments

## 8. Bio-informatics: The Future

P.24.08.1(C484.220) | V. Cody: Covariance Correlations from Genome-Wide Homology Sequence Analysis of DHFR

P.24.08.2(C484.221) | H. J. Bernstein: The PDB Format in the 21st Century, a Modest Proposal

## 10. No sub theme

**TUESDAY, AUGUST 30 2005 - KEYNOTE LECTURES****MORNING SESSION 8.30-9.30**

Michelangelo (*KN 33*)

**KN33.30(C8) | Ahmed Zewail:**  
Ultrafast Electron Crystallography

*Chair: Xiadong Zou*

**AFTERNOON SESSION 17.30-18.30**

Michelangelo (*KN 34*)

**KN34.30(C8) | David Eisenberg:**  
Structural Studies of Amyloid

*Chair: Maria Armenia Carrondo*

Cimabue (*KN 35*)

**KN35.30(C8) | Salvador Ferrer:**  
The Surface Structure of Model Catalyst in Action  
Investigated by X-ray Diffraction

*Chair: Mikhail Koval'chuk*

Botticelli (*KN 36*)

**KN36.30(C8) | Lia Addadi:**  
Strategies and Design Principles in Biominerilization

*Chair: Leslie Leiserowitz*

# TUESDAY, AUGUST 30 2005 – MORNING - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 85</b> )	Botticelli ( <b>MS 86</b> )	Giotto ( <b>MS 87</b> )
10.00-10.05 Opening Remarks	<b>BIOLOGICAL MOLECULES AS TARGETS FOR DRUG DESIGN</b> <i>Chairs:</i> S. Di Marco, W. Stallings	<b>PROGRAMMING ROBUST CIF AND XML INTO CRYSTALLOGRAPHIC SOFTWARE</b> <i>Chairs:</i> H. J. Bernstein, B. McMahon	<b>REACTIONS IN MOLECULAR SOLIDS</b> <i>Chairs:</i> L. R. MacGillivray, F. Toda <b>Talks of 25 min. each</b>
10.05-10.35	<b>MS85.30.1(C108)</b>   T. K. Sixma: AChBP Structures for Understanding Ligand Binding in Nicotinic Receptors	<b>MS86.30.1(C109)</b>   P. Murray-Rust: CIF2CML - Automatic Processing of Chemical Crystallography in XML/CML	<b>MS87.30.1(C110)</b>   F. Grepioni: Mechanically Induced Reactivity of Molecular Crystals: Chemistry (Almost) without Solvents
10.35-11.05	<b>MS85.30.2(C108)</b>   J. Becker: Classical and Non-Classical Structure-Based Drug Design	<b>MS86.30.2(C109)</b>   S. Hall: The Role of Data Ontologies in CIF Deposition and Access	<b>MS87.30.2(C110)</b>   L. R. Nassimbeni: Solid-Solid Reactions of Xanthenols with Unsaturated Hydrocarbons
11.05-11.35	<b>MS85.30.3(C108)</b>   C. Phillips: Structure based Drug Design of novel Inhibitors of cGMP Phosphodiesterase, PDE5	<b>MS86.30.3(C109)</b>   K. Z. Mitev: CIFFOLD: Managing Long Lines in CIF	<b>MS87.30.6(C111)</b>   R. G. Kostyanovsky: Homo- and Heterochirality in Crystal
11.35-12.05	<b>MS85.30.4(C108)</b>   S. K. Burley: Structure-guided Drug Discovery for Protein Kinases using Fragment-based Lead Identification/Lead Optimization	<b>MS86.30.4(C110)</b>   J. Kaercher: A Relational Database Approach to Report Generation	<b>MS87.30.3(C110)</b>   A. Nangia: Structural and Thermochemical Studies of Lattice Inclusion Hosts
12.05-12.35	<b>MS85.30.5(C109)</b>   M. Miyano: Structural Basis of Multi-functional Lipocalin-type Prostaglandin D <sub>2</sub> Synthase	<b>MS86.30.5(C110)</b>   G. J. Swaminathan: Structure Integration with Function, Taxonomy and Sequences (SIFTS)	<b>MS87.30.4(C111)</b>   T. Lavy: Photochemical Reactions in Inclusion Compounds
			<b>MS87.30.5(C111)</b>   P. Sozzani: Confinement of Gases and Polymers in van der Waals Crystals

# TUESDAY, AUGUST 30 2005 - MORNING - MICROSYMPOSIA

<b>Donatello (MS 88)</b>	<b>Leonardo da Vinci (MS 89)</b>	<b>Cimabue (MS 90)</b>	<b>Brunelleschi (MS 91)</b>
<b>ELECTRONIC EXCITATIONS</b> <i>Chairs: J. J. Rehr, K. Hamalainen</i>	<b>STRUCTURAL CHARACTERIZATION OF CONTROLLED SOLID-LIQUID INTERFACES</b> <i>Chairs: J. Martín-Gago, G. Fragneto</i>	<b>APPLYING NON-CRYSTALLOGRAPHIC ALGORITHMS TO CRYSTALLOGRAPHY</b> <i>Chairs: R. W. Grosse-Kunstleve, M. Tremayne</i>	<b>ELECTRON CRYSTALLOGRAPHY ON INORGANIC CRYSTALS</b> <i>Chairs: J. Jansen, V. Kletschkovskaya</i>
<b>MS88.30.1(C111)</b>   <u>W. Schuelke</u> : Electronic Excitations: What Inelastic X-ray Scattering Can Reveal	<b>MS89.30.1(C113)</b>   <u>R. K. Thomas</u> : Neutron Reflection from Complex Layers Adsorbed at the Solid/Aqueous Interface	<b>MS90.30.1(C114)</b>   <u>G. Barr</u> : Cluster Analysis in Crystallography	<b>MS91.30.1(C115)</b>   <u>T.E. Weirich</u> : Present Status of Electron Crystallography on Inorganic Materials
<b>MS88.30.2(C112)</b>   <u>J. A. Soininen</u> : Theory and Calculations of Inelastic X-Ray Scattering	<b>MS89.30.2(C113)</b>   <u>R. C. Salvarezza</u> : Self Assembled Thiols Monolayers on Au(C111) Surfaces: Structure Defects and Dynamics	<b>MS90.30.2(C114)</b>   <u>E. Cheung</u> : Crystal Structures from Powder X-ray Diffraction using Genetic Algorithms	<b>MS91.30.2(C115)</b>   <u>K. Tsuda</u> : Structural and Charge-density Studies of Transition Metal Oxides Using Convergent-beam Electron Diffraction
<b>MS88.30.3(C112)</b>   <u>J. Hill</u> : Across the Mott Gap: Electronic Excitations in Transition Metal Oxides	<b>MS89.30.3(C113)</b>   <u>T. Charitat</u> : Fluctuations of a Single Floating Lipid Bilayer: a Specular and Off-specular Reflectivity Study	<b>MS90.30.3(C114)</b>   <u>C. Seaton</u> : Powders, Prediction and Epitaxy: Applications of Differential Evolution	<b>MS91.30.3(C115)</b>   <u>F. Li</u> : Incommensurate Modulated Structure Determination by Combining HREM and ED
<b>MS88.30.4(C112)</b>   <u>P. A. Montano</u> : Magnetic Inelastic X-ray Scattering as a Probe of Electronic Excitations in Correlated Electron Materials	<b>MS89.30.4(C113)</b>   <u>M. Ito</u> : The New Distributions of Water Molecules at Ni(C111)-2x2-O and Cu(C111) Electrode Interfaces	<b>MS90.30.4(C114)</b>   <u>M. Chapman</u> : Refinement when Amplitudes aren't Enough: Real-space, H-bonding & Electrostatics	<b>MS91.30.4(C116)</b>   <u>S. Dudarev</u> : Electron Dynamical Diffraction Imaging and Diffuse Scattering by Small Dislocation Loops
<b>MS88.30.5(C112)</b>   <u>T. A. Colson</u> : Correlations in Inelastic Scattering and Plasmon Filtered Imaging	<b>MS89.30.5(C113)</b>   <u>J. W. Andreassen</u> : Structural Dynamics of the Competing Forces of Light and Matter	<b>MS90.30.5(C115)</b>   <u>K. Suhre</u> : <i>elNémo</i> : Using normal mode analysis in molecular replacement	<b>MS91.30.5(C116)</b>   <u>E. Suvorova</u> : Characterization of Nanophases in HRTEM: Fourier Transform and Simulation

# TUESDAY, AUGUST 30 2005 – AFTERNOON - MICROSYMPOSIA

TIME	Michelangelo ( <b>MS 92</b> )	Donatello( <b>MS 93</b> )	Botticelli( <b>MS 94</b> )
14.45-14.50 Opening Remarks	<b>EMERGING TECHNOLOGIES FOR STRUCTURAL BIOLOGY</b> <i>Chairs: S. Larsen, M. Becker</i>	<b>CRYSTALLOGRAPHY AND ENVIRONMENTAL SCIENCE</b> <i>Chairs: M. Mellini, M. Posfai</i>	<b>CRYSTALLOGRAPHIC KNOWLEDGE IN DRUG DESIGN STRATEGIES</b> <i>Chairs: F. Leveiller, M. Saviano</i>
14.50-15.20	<b>MS92.30.1(CI16)</b>   <u>J. C. Spence</u> : Diffraction from a Laser-aligned Beam of Hydrated Proteins	<b>MS93.30.1(CI17)</b>   <u>A. Gualtieri</u> : Application of Natural Zeolites: Understanding the Properties at a Molecular Scale	<b>MS94.30.1(CI18)</b>   <u>A. Yonath</u> : Can Structures lead to better Drugs? Lessons from Ribosomal Antibiotics
15.20-15.50	<b>MS92.30.2(CI16)</b>   <u>D. van der Spoel</u> : Protein Structures without Crystals	<b>MS93.30.2(CI17)</b>   <u>F. Guyot</u> : A Structural View of Carbonate Biomineralization by Bacteria	<b>MS94.30.2(CI19)</b>   <u>M. Groll</u> : Inhibitors of the Eukaryotic 20S Proteasome Core Particle: a Structural Approach
16.50-16.20	<b>MS92.30.3(CI16)</b>   <u>T. Kigawa</u> : Structural Proteomics Using NMR in RIKEN Structural Genomics/Proteomics Initiative	<b>MS93.30.3(CI18)</b>   <u>G. Jordan</u> : Nano-scale Studies of Processes on Crystal Surfaces in Aqueous Solutions	<b>MS94.30.3(CI19)</b>   <u>F. Fanelli</u> : Computational Modeling of GPCRS: Insight into the Function of the Most Privileged Drug Targets
16.20-16.50	<b>MS92.30.4(CI17)</b>   <u>M.-T. Tang</u> : X-ray Microscopy Project at NSRRC	<b>MS93.30.4(CI18)</b>   <u>A. K. Subramani</u> : Hydrothermal Preparation of TiO <sub>2</sub> : AC Composite Crystalline Particulates	<b>MS94.30.4(CI19)</b>   <u>K. Das</u> : Structure-Based Design of New AIDS Drugs: Overcoming Drug Resistance
16.50-17.20	<b>MS92.30.5(CI17)</b>   <u>E. Garman</u> : Analysis of Liquid and Crystalline Proteins by Particle Induced X-ray Emission (PIXE)	<b>MS93.30.5(CI18)</b>   <u>K. Mori</u> : Crystalline Structure of Biodegradable Polyhydroxybutyrate Thin Films	<b>MS94.30.5(CI19)</b>   <u>N. Hirayama</u> : Evaluation of Docking Results by Diffraction-component Precision Index (DPI)

# TUESDAY, AUGUST 30 2005 – AFTERNOON - MICROSYMPOSIA

<b>Leonardo da Vinci (MS 95)</b>	<b>Giotto (MS 96)</b>	<b>Cimabue (MS 97)</b>	<b>Brunelleschi (MS 98)</b>
<b>ADVANCED FUNCTIONAL MATERIALS (INCLUDING MOLECULAR BIOLOGICAL FUEL CELL BATTERY)</b> <b>Chairs:</b> M. Catti, D. Argyriou	<b>CRYSTALLOGRAPHIC TEACHING</b> <b>Chairs:</b> Å. Oskarsson, R. Read	<b>BIO-INORGANICS IN BIOLOGICAL MACROMOLECULES</b> <b>Chairs:</b> A. Bigi, E. Rizzarelli	<b>ANALYSIS OF ANISOTROPIC MATERIALS</b> <b>Chairs:</b> Y. Amemiya, I. Torriani
<b>MS95.30.1(CI20)</b>   <u>Y. Andreev</u> : New Approach to Structure Determination of Crystalline Polymer Electrolytes	<b>MS96.30.1(CI21)</b>   <u>J. W. Pflugrath</u> : Crystallography Boot Camp at Cold Spring Harbor Laboratory	<b>MS97.30.1(CI22)</b>   <u>K. Piontek</u> : Structural Biology of Ligninolytic Enzymes: Laccases and Heme Peroxidases	<b>MS98.30.1(CI23)</b>   <u>C. Riekel</u> : Polymer and Biopolymer Microstructure Analysis by Scanning SAXS/WAXS
<b>MS95.30.2(CI20)</b>   <u>T. Kimura</u> : Magnetic Control of Electric Polarization in Magnetic Oxides with Nonprintable areaon-collinear Magnetic Structures	<b>MS96.30.2(CI21)</b>   <u>S. Parsons</u> : Introducing Twinning	<b>MS97.30.2(CI22)</b>   <u>A. D. Podjarny</u> : Inhibitor Binding to Aldose Reductase Studied at Subatomic Resolution	<b>MS98.30.2(CI23)</b>   <u>H. Takeji</u> : Small-Angle X-ray Scattering Analysis of Anisotropic Block Copolymer Microdomains
<b>MS95.30.3(CI20)</b>   <u>D. Pelloquin</u> : Crystal Structure and Magneto-transport Properties of new Cobalt based Layered Oxides	<b>MS96.30.3(CI21)</b>   <u>M. Jaskolski</u> : Real versus Virtual Aids in Teaching Crystallography	<b>MS97.30.3(CI23)</b>   <u>P. Matias</u> : The Activation Process of D.desulfuricans ATCC 27774 [NiFe] Hydrogenase	<b>MS98.30.3(CI24)</b>   <u>P. Thiagarajan</u> : Supramolecular Structures via Self-Assembly of A-beta Congeners
<b>MS95.30.4(CI20)</b>   <u>M. Mitsumi</u> : Single-Component Molecular Conductor Formed by Electron Transfer between d and $\delta$ Orbitals	<b>MS96.30.4(CI21)</b>   <u>G. Chapuis</u> : Towards a Web-based Interactive Environment for the Teaching of Crystallography	<b>MS97.30.4(CI23)</b>   <u>P. Fratzl</u> : Time- and Position-resolved X-ray Scattering of Bone and Cartilage	<b>MS98.30.4(CI24)</b>   <u>Y. Shinohara</u> : Real-Time Observation of Anisotropic Structure of Aggregates in Stretched Rubber by 2D-USAXS
<b>MS95.30.5(CI21)</b>   <u>N. Aliouane</u> : In field Incommensurate-Commensurate Phase Transition in the Multiferroic TbMnO <sub>3</sub>	<b>MS96.30.5(CI22)</b>   <u>P. Dumas</u> : Teaching Crystallography with a LASER, Two Lens and Einstein's Tongue	<b>MS97.30.5(CI23)</b>   <u>G. Croce</u> : A Mesoporous Pattern Created by Nature in Siliceous Spicules from Marine Sponges	<b>MS98.30.5(CI24)</b>   <u>J. Benedict</u> : Spherulites for Polar Dye Organization

## **TUESDAY, AUGUST 30 2005 – OTHER ACTIVITIES**

**COMPUTER FAYRE** Ghirlandaio

(11.00-12.00)      S. Ramsden, V. Robins, S.

Hungerford, S. Hyde:

EPINET (Euclidean Patterns in Non-Euclidean Tilings)

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(14.00-16.00)      C. Gilmore, G. Barr, A. Parkin, C.

Wilson:

dSNAP: Software for Analysing Hits from the Cambridge  
Structural Database Using Cluster Analysis

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# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

## 01 INSTRUMENTATION AND EXPERIMENTAL TECHNIQUES

### 12. Cryo-Crystallography: Techniques and Instrumentation

P.01.12.1(CI48.1) | M. R. Probert: A Design for a New State-of-the-Art Diffraction Facility

### 13. Fast (pico-second) Crystallography

P.01.13.1(CI48.2) | Y. Tanaka: Picosecond Lattice Dynamics Probed by Time- and Angle-resolved X-ray Diffraction

P.01.13.2(CI48.3) | R. Pahl: Time-resolved Studies with Pulsed X-rays at BioCARS: Present Capabilities and Future Directions

### 15. No sub theme

P.01.15.1(CI48.4) | J. J. Lovelace: Analyzing Mosaic Domain Changes Induced by Cryo-Cooling with Digital Topography

P.01.15.2(CI49.5) | T. Ida: Symmetrisation of Powder Diffraction Peak Profiles by a Fourier Method

P.01.15.3(CI49.6) | S. Coles: The role of e-Science in Service Crystallography: The UK National Crystallography Service on the Grid

P.01.15.4(CI49.7) | A. Mulichak: Automated Data Collection at the IMCA-CAT Advanced Photon Source User Facility

P.01.15.5(CI49.8) | M. Gembicky: An Ultra-fast Mechanical Shutter for Sub-microsecond Time-resolved Experiments

P.01.15.6(CI49.9) | M. Hiraki: High-throughput Protein Crystallization

P.01.15.7(CI50.10) | E. Abola: Miniaturization in Structural Biology Pipelines

P.01.15.8(CI50.11) | L. Daniels: High-resolution Data Using Short Wavelength Confocal Optics and a Cylindrical IP

## 02 METHODS FOR STRUCTURE DETERMINATION

### 16. Rietveld Refinement Methods

P.02.16.1(CI59.12) | S. Mondal: Ab-initio Structure Determination of a Metal Complex from Laboratory X-ray Powder Data

P.02.16.2(CI60.13) | H. M. Park: Crystal Structure Refinement of Sr(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>

P.02.16.3(CI60.14) | U. Amann: Improvement of Automated Phase Analysis by Scaling on Standard

### 17. No sub theme

P.02.17.1(CI60.15) | P. Afonine: A Robust Bulk Solvent Correction and Anisotropic Scaling Procedure in the CCTBX

P.02.17.2(CI60.16) | D. J. Rodi: Monitoring Molecular Metamorphosis Using Wide-angle Solution Scattering Data

P.02.17.3(CI60.17) | T. Proffen: Total Scattering: the Key to the Local and Medium Range Structure of Complex Materials

P.02.17.4(CI61.18) | K. Bethanis: Structure Determination

from a Quantum Mechanical Formulation in Momentum Space

P.02.17.5(CI61.19) | K. Suhre: Molecular Replacement Via Normal Mode Analysis and Homology Modelling on the Web

P.02.17.6(CI61.20) | D. M. Toebbens: HUNTER: A Package of Small Tools to Manipulate FOX

P.02.17.7(CI61.21) | M. Yoshimura: Monte Carlo Search with Many CPUs: Application to 6 dim. Molecular Replacement

P.02.17.8(CI62.22) | A. Hanson: Optimization of Genetic Algorithm Techniques for Powder Structure Solution

P.02.17.9(CI62.23) | S. Ciccarello: Removal of the Phase Problem by the Atomicity Assumption

## 03 COMPUTERS IN ANALYSIS, MOLECULAR MODELLING AND MOLECULAR DESIGN

### 4. Rational Drug Design

P.03.04.1(CI65.24) | T. Peat: AFITT- Working with Good Chemistry

P.03.04.2(CI65.25) | A. S. Araujo: Molecular Dynamics Simulations of Tetramethylketone p-tert-butyl Calix[4]arene

P.03.04.3(CI66.26) | S. Godinho: Structural Properties of Pt-based Anti-cancer Drugs; Computational Studies

04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

### 2. Enzymes and Enzyme Catalysis

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

P.04.02.1(C180.27)   N. K. Lokanath: Crystal Structure of the NADP-dependent 3-hydroxyisobutyrate Dehydrogenase	Loop Movement and Cooperativity	Catalysis
P.04.02.2(C180.28)   E. Tocheva: Visualization of the Forward and Reverse Reactions Catalyzed by Nitrite Reductase	P.04.02.14(C183.39)   A. Nakamura: Crystal Structure of a Glu-Trnagln Amidotransferase at 2.7 Å	P.04.02.26(C186.50)   S. Ravaud: Structural Studies of the Sucrose Isomerase MutB from <i>Pseudomonas mesoacidiphila</i>
P.04.02.3(C180.29)   J. T. Maynes: The Structural Basis for Ser/Thr Protein Phosphatase Inhibition	P.04.02.15(C183.40)   S. Fermani: The 1.4 Å Structure of Dianthin 30 Indicates a Role of Surface Potential at the Active Site of Type 1 Ribosome Inactivating Proteins	P.04.02.27(C186.51)   M. Y. W. Tsai: Recovery of Argininosuccinate Lyase Activity in Duck δ1 Crystallin
P.04.02.4(C181.30)   M. Marsh: Active Site Structure of Actinorhodin Polyketide (actII) Reductase	P.04.02.16(C184.41)   S. Aich: Structure of Monomeric NADP-isocitrate Dehydrogenase: an Open Conformation	P.04.02.28(C186.52)   K. Yang: Crystal Structure of a Native Chitinase from the Fungal Pathogen <i>Aspergillus fumigatus</i> YJ-407 (afCHI)
P.04.02.5(C181.31)   Y. Yamagata: The MutT Crystal Retains the Ability to Hydrolyze 8-oxo-dGTP	P.04.02.17(C184.42)   S. D. Kernaghan: Study of Structural Change in SCOT upon Binding CoA	P.04.02.29(C187.53)   D. Li: Crystal Structures of Two <i>Bacillus subtilis</i> Protein YjcG and YflL
P.04.02.6(C181.32)   Z.-X. Xia: Crystal Structure of Recombinant Human Cyclophilin J and its Complex	P.04.02.18(C184.43)   J. Cotelesage: The Structure of Anaerobiospirillum succiniciproducens PEPCK Reveals an Important Loop	P.04.02.30(C187.54)   B. F. Anderson: Crystal Structures of DAH7PS Synthase from <i>Pyrococcus furiosus</i>
P.04.02.7(C181.33)   M. Korczynska: Structural Studies of an Antibiotic Resistance Factor	P.04.02.19(C184.44)   A. E. A. Openshaw: Structural Analysis of Listeria Neutral Sphingomyelinase (SmCL)	P.04.02.31(C187.55)   E. Broströmer: Crystal Structure of the <i>Bacillus subtilis</i> YwIE Protein
P.04.02.8(C182.34)   M. Kosmopoulou: Crystallographic Studies on Acyl Ureas, a New Class of Inhibitors of Glycogen Phosphorylase	P.04.02.20(C185.45)   K. Banaszak: The Refinement of the Yeast Phosphofructokinase-1 Atomic Model	P.04.02.32(C187.56)   V. Carbone: Structure of Aldehyde Reductase Complex: Implications for Inhibitor Specificity
P.04.02.9(C182.35)   T. Dela Mora: X-ray Structures of Methylamine Dehydrogenase Reaction Intermediates	P.04.02.22(C185.46)   S. Hirotsuo-Fujimoto: Comparison between Crystal Structures of cMDH in Apo and NAD/NADH Binding Form	P.04.02.33(C188.57)   Y. Sakamoto: Crystal Structure of the Catalytic Fragment of 2',3'-Cyclic nucleotide 3'-Phosphodiesterase from Human Brain
P.04.02.10(C182.36)   R. Kanai: Crystallographic Analysis of Maltohexaose-producing Amylase	P.04.02.23(C185.47)   E. Johansson: Deamination and Dephosphorylation of dCTP – Two Reactions Catalysed by a Family of Enzymes	P.04.02.34(C188.58)   A. Buschiarizzo: Crystal Structure and Catalytic Mechanism of Proline Racemase
P.04.02.11(C182.37)   A. Castell: M. Tuberculosis Rv0216; Unknown, Now Known?	P.04.02.24(C185.48)   A. Merlini: Structural and Dynamic Studies of Onconase Mutants	P.04.02.35(C188.59)   L. Miallau: Crystal Structure of an Enzyme Involved in the Biosynthesis of Isoprenoids: 4-diphosphocytidyl-2-C-methyl-D-erythritol Kinase from <i>E. coli</i> , a Potential Drug Target
P.04.02.13(C183.38)   M. Lee: <i>E. coli</i> Dihydroorotase:	P.04.02.25(C186.49)   J. D. Dombraukas: Structural Basis for Tumor Pyruvate Kinase M2 Allosteric Regulation and	P.04.02.36(C188.60)   B. Bagautdinov: Crystal Structure

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

of the Biotin Protein Ligase from *Pyrococcus horikoshii* OT3: Insights into the Mechanism of Biotin Activation.

**P.04.02.37(C188.61)** | H. Kishida: Structure and Mechanism of 2-C-methyl-D-erythritol 2,4-cyclodiphosphate Synthase

**P.04.02.38(C189.62)** | R. Natsume: Crystal Structure of the  $\beta$ -subunit of Acetyl-CoA Carboxylase in *C. glutamicum*

**P.04.02.39(C189.63)** | N. Ishiyama: Structural Studies of FlaA1, a UDP-GlcNAc 4,6-dehydratase

**P.04.02.40(C189.64)** | J. Zhang: The Crystal Structure of Murine 11 $\beta$ -hydroxysteroid Dehydrogenase 1: an Important Therapeutic Target for Diabetes

**P.04.02.41(C189.65)** | T. Nakai: Crystal Structure of P-protein of the Glycine Cleavage System

**P.04.02.42(C190.66)** | Y. Hata: Structure and Inhibition Mode of Protein F' in Complex with Carboxypeptidase Y

## 4. Muscle and Motor Proteins

**P.04.04.1(C217.67)** | N. Pinotsis: Molecular Basis of the Myomesin Dimerisation: Implications for the Sarcomeric Assembly of the M-band

**P.04.04.2(C217.68)** | S. Mueller: Structural Studies on Titin and Titin Kinase's Downstream Signaling Pathway

**P.04.04.3(C218.69)** | W. Blankenfeldt: Carving a Beanstalk: the Structure of  $\Delta S2$  from Human Myosin II

## 10. Cryo-Crystallography: Applications to Macromolecules

**P.04.10.1(C228.70)** | R. Davies: The Effects Of Temperature And Radiation On Holo and Apo Ferritin Crystals

**P.04.10.2(C229.71)** | U. Chinte: Mitigation of Radiation Damage to Protein Crystals Using a Helium Cryostream

**P.04.10.3(C229.72)** | C. U. Kim: High Pressure Cooling of Protein Crystals without Cryoprotectants

## 07 CRYSTALLOGRAPHY OF ORGANOMETALLIC, COORDINATION AND MAIN GROUP COMPOUNDS

### 5. Main Group Chemistry

**P.07.05.1(C309.73)** | V. N. Khrustalev: New Stable Ge(II) and Sn(II) Organic Derivatives: an X-Ray Diffraction Study

**P.07.05.2(C309.74)** | F. Belaj: Gentle Hydrolysis of a Trichlorophosphazeno-1,3,5,2 $\lambda^5$ -triazaphosphorine

**P.07.05.4(C310.75)** | H. Miyamae: Structural Variation of 1,1 Adducts of Lead(II) Chloride and Bromide with *N,N'*-Dimethylethylenediamine from 123K to 303K

**P.07.05.5(C310.76)** | M. R. J. Elsegood: Structural Studies of Boracalixarenes

**P.07.05.6(C310.77)** | A. S. F. Au Yeung: Flux Synthesis of New Organo-borate Hybrids

### 6. Cage and Metallo-Cage Structures

**P.07.06.1(C310.78)** | L. Glukhov: The Role of Inter- and Intramolecular H-H Contacts in the Crystals of Carboranes

**P.07.06.2(C311.79)** | A. Guehring-Laidoudi: Polynuclear

Coordination Polymer with Glutarate Ligand:  $\text{Sr}(\text{C}_5\text{H}_7\text{O}_4)_2(\text{H}_2\text{O})_2$

**P.07.06.3(C311.80)** | M. Kawano: Direct Observation of Photochemical Reactions by X-ray Crystallography – Supramolecular Approach

## 7. Bio-inorganic Structures

**P.07.07.1(C311.81)** | N. Bouhmaida: Metal-Ligand and Metal-Metal Bonding Characterization from X-ray Diffraction

**P.07.07.2(C311.82)** | W. Wagermaier: Scanning Texture Analysis of Lamellar Bone using Microbeam Synchrotron Radiation

**P.07.07.4(C312.83)** | S. Furlan: Modelling Copper-Protein Backbone Binding

## 8. Bio-mineralization and Modifications

**P.07.08.1(C312.84)** | U. Bismayer: Oscillatory Biomineralization in Mollusc Shells

**P.07.08.2(C312.85)** | A. Preisinger: The Biomineralization of Iron Sulfides under Anoxic Conditions

## 10. Molecular Magnets

**P.07.10.1(C312.86)** | M. Hernandez Molina: Design of New Mn Precursors for Single-molecule Magnet

## 11. No sub theme

**P.07.11.1(C313.87)** | S. Bouacida: Synthesis and Characterization by Diffraction of X-rays of a new Hybrid Compound based on Tin

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

**P.07.11.3(C313.88)** | G. I. Kociok-Kohn: C-H-X  
Intermolecular Interaction in Crystals of  
Triazacyclohexane Complexes

**P.07.11.4(C313.89)** | A. Sekine: Chirality Inversion  
Process in Cobaloxime Complex Crystals by  
Photoirradiation

## 08 STRUCTURE/PROPERTY RELATIONSHIP

### 1. Molecular Recognition

**P.08.01.1(C315.90)** | F. Bachechi: Chiral Recognition of  
Derivatives Based on the Ergot Alkaloid Terguride

**P.08.01.2(C315.91)** | O. Büyüktüngör: Spectroscopic  
Investigation of Some Azo-azomethine Compounds

**P.08.01.3(C315.92)** | M. Safro: Electrostatic Potential of  
AaRS Navigates tRNA on its Pathway to the Binding Site

**P.08.01.4(C315.93)** | M. Saviano: Structural  
Characterization of Functionalized  $\beta$ -Cyclodestrins

**P.08.01.5(C316.94)** | S. Takamizawa: Transformable  
Single-Crystal Adsorbent Based on 1-D Coordination  
Polymer Skeletons

### 10. Polymorphism and Isomorphism: Identification and Characterisation

**P.08.10.1(C335.95)** | I. V. Chernyshev: Yellow and Violet  
Polymorphs of (2Z)-2-(Nitromethylene)-2H-1,4-  
benzothiazine-3(4H)-one

**P.08.10.2(C335.96)** | P. Bombicz: Isostructurality of  
Analogues Triarylsilanol and -Methanol Inclusion  
Compounds

**P.08.10.4(C336.97)** | A. Nangia: Polymorphs of 4,4'-  
Diphenyl-2,5-cyclohexadienone

**P.08.10.5(C336.98)** | S. Matsumoto: A Series of  
Polymorphs with Different Colours in  
Diaminodicyanopyrazine Dyes

**P.08.10.6(C336.99)** | G. Righini: A New Crystallographic  
Form of the layered Weak-Ferromagnet  
 $\text{Fe}[(\text{CH}_3\text{PO}_3)(\text{H}_2\text{O})]$

**P.08.10.7(C337.100)** | A. Johnston: Robotic Adventures in  
Crystallisation Space

**P.08.10.8(C337.101)** | H. Novoa de Armas: Crystal  
Structure of a Polymorph of Carnidazole from Synchrotron  
X-ray Powder Diffraction

### 11. Polymorphism: Applications

**P.08.11.1(C337.102)** | E. Dova: High-throughput  
Polymorph Screen of Cimetidine and Clarification of its  
Nomenclature

**P.08.11.2(C337.103)** | M. Caetano: *In situ* X-ray  
Diffraction, DSC and Raman Spectroscopy Thermal  
Investigation of Chlorpropamide

**P.08.11.3(C337.104)** | O. Grassmann: Quantification of  
(Pseudo)polymorphic Mixtures using Full Pattern Analysis  
of X-ray Powder Diffraction Data

**P.08.11.4(C338.105)** | J. M. Kellaher: Effect on Additive  
Structure on Crystal Nucleation: Sulfathiazole

**P.08.11.5(C338.106)** | H. Uekusa: Polymorphism  
Dependent Crystalline Photochromism of

Salicylideneanilines

## 09 CRYSTAL ENGINEERING

### 3. Inorganic Compounds

**P.09.03.1(C355.107)** | C. Hu: Single-Crystal to Single-  
Crystal Reactions

**P.09.03.2(C355.108)** | L. J. Moitsheki: Crystal  
Engineering of Metal-Organic Frameworks using 4,4'-  
Dipyridyl-N,N'-Dioxide

**P.09.03.3(C355.109)** | S. A. Bourne: MOFs of  
Phenylamine and Pyridine Derivatives: Structure and  
Thermal Analysis

**P.09.03.4(C356.110)** | M. B. Duriska: Crystal Engineering  
with Scorpionate Ligands

**P.09.03.5(C356.111)** | R. Gheorghe: Impact of Linkers on  
the Structural Diversity of 3d-4f Coordination Polymers

**P.09.03.6(C356.112)** | J. M. Tanski: Covalent Aryloxide  
Metal-Organic Network Materials

**P.09.03.8(C357.113)** | C. Paraschiv: Synthesis and  
Characterization of New Cyano-Bridged Oligonuclear  
Complexes

**P.09.03.9(C357.114)** | H. Kara: Pyridine Boronic acids as  
Building Blocks in Crystal Engineering

**P.09.03.10(C357.115)** | D. G. Billing: Structural Diversity  
in Lead-halide Based Organic-Inorganic Hybrids

**P.09.03.11(C357.116)** | G. Marin: High-Dimensional  
Structures Constructed from Alkoxo-Bridged Complexes  
as Nodes

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

P.09.03.12(C358.117) | R. Rodriguez-Mijangos:

Characterization of a Novel Quaternary Dielectric Crystallographic Family

P.09.03.13(C358.118) | E. M. Bauer: Co(II) *n*-alkyl Phosphonates: Examples of Hybrid Organic-Inorganic Compounds

## 4. Organometallic Complexes

P.09.04.1(C358.119) | Ó. Fabelo: Crystal packing in Co(II) Pyromellitate Complexes Tuning the Water Aggregation

P.09.04.2(C358.120) | F. S. Delgado: Alkali-Templated Malonate Copper(II) Complexes

P.09.04.3(C358.121) | L. Cañadillas-Delgado: (4,4)-Metal Organic Framework Templated by 1,2,3,4-Butanetetracarboxylic Acid

P.09.04.4(C359.122) | J.-P. Zhang: Supramolecular Isomerism of Three dimensional 3-Connected Coordination Polymers

P.09.04.5(C359.123) | A. Bacchi: Novel Organometallic Molecular Building Blocks for Crystal Engineering

P.09.04.6(C359.124) | A. van der Lee: Constitutional Dynamic Self-Amplification in Double-Helix Imine Systems

P.09.04.8(C360.125) | G. Romanenko: Polynuclear Core [Mn<sub>6</sub>(O)<sub>2</sub>Piv<sub>10</sub>] in the Molecular Magnets Design

P.09.04.9(C360.126) | S. Quintal: Crystal Structures of Mo(II) Complexes with 2,2'-Dipyridylamine

## 10 INORGANIC CRYSTALLOGRAPHY AND GEOSCIENCES

### 2. Systematics of Inorganic Compounds

P.10.02.1(C367.127) | E. L. Belokoneva: Borophosphate: Crystal Chemistry, Systematic and Synthesis

P.10.02.2(C367.128) | M. V. Peskov: Crystallochemical Analysis of Halogenides and Chalcogenides of *d*-Metals

P.10.02.3(C367.129) | A. Larrañaga: Crystal Structure of Two Related Selenites

P.10.02.4(C367.130) | O. Romaniv: Partial substitution by Y, Pb or Bi in Sr<sub>8</sub>Ca<sub>6</sub>Cu<sub>2</sub>O<sub>41</sub>

P.10.02.5(C368.131) | S. Pukas: Influence of Al, Ga and In on the Crystal Structure of ErGe<sub>2±x</sub>

P.10.02.6(C368.132) | N. Lyaskovska: Solid solutions in the PrNi<sub>2</sub>-PrAl<sub>2</sub>-PrGe<sub>2</sub> system

P.10.02.7(C368.133) | E. N. Silva: Low Temperature Stability of Fluoride Pyrochlores Investigated by Neutron Powder Diffraction and Raman Spectroscopy

P.10.02.8(C368.134) | F. Merlo: The Pseudo-Ternary Intermetallic System CaAg<sub>2</sub>-CaZn<sub>2</sub>-CaAl<sub>2</sub>

P.10.02.9(C369.135) | M. L. Fornasini: Ternary Phases in the Yb-Zn-Al System

P.10.02.10(C369.136) | E. Makovicky: An Unconventional Look at Sulfides and Selenides: Anion-centred Polyhedra

P.10.02.11(C369.137) | N. L. Smirnova: The Term Systematics

P.10.02.12(C369.138) | V. Kahlenberg: Alkaline Earth

Aluminates / Gallates and Perovskites: Two Sides of the Same Coin

P.10.02.14(C370.139) | A. Speghini: Iron Substituted Hydroxyapatite by Two Powder Preparation Method: A Comparison

P.10.02.16(C370.140) | W. Depmeier: Systematic Violation of Loewenstein's Rule Established

P.10.02.18(C371.141) | M. Wörle: Synthesis and Crystal Structure of the New Zintl Phase Eu<sub>3</sub>Mg<sub>2</sub>Ge<sub>6</sub>

P.10.02.17(C370.142) | G. Salviulo: Iron Substituted Ca-Sr-Ba Apatites: Preliminary Results

P.10.02.19(C371.143) | M. Debbabi: Metallic Clusters Interactions: Structures of Co(H<sub>2</sub>O)<sub>6</sub>K<sub>2</sub>M<sub>2</sub>W<sub>4</sub>O<sub>19</sub>.xH<sub>2</sub>O (M = V, Nb)

P.10.02.20(C371.144) | H. Effenberger: Hydrogen Bonds in Triclinic MH(XO<sub>4</sub>) Compounds

P.10.02.21(C371.145) | H. Yamada: Structural and Electron Density Studies of Stuffed Tridymite

P.10.02.22(C372.146) | Y. Galadzhun: RE<sub>6</sub>Ni<sub>2</sub>In (RE = Gd, Tb, Dy, Ho, Lu) – The New Representatives of Ho<sub>6</sub>Co<sub>2</sub>Ga Structure Type

## 11 CRYSTALLOGRAPHY IN MATERIAL SCIENCE

### 8. Polymers

P.11.08.1(C391.147) | G. Maier: Scanning X-ray Scattering Study on Structural Changes at Crack Tips in PVDF

P.11.08.2(C391.148) | T. Lord: An Investigation into the

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

Effects of Temperature and Crystallization Conditions on the Lattice Parameters of Ultra Long n-alkane Crystals

P.11.08.4(C391.149) | M. Bortolotti: Crystal Structure and Texture Refinement of Polymers from Diffraction Images

## 9. Liquid Crystals

P.11.09.1(C392.150) | M. Nishikawa: Novel Structure of 1,1'-Disubstituted Ferrocene Derivative

P.11.09.2(C392.151) | A. Ohishi: Crystal Structure of 1,24-Dibromotetacosane

P.11.09.3(C392.152) | N. Nakamura: Crystal Structure of Monosubstituted Ferrocene Derivatives

P.11.09.4(C392.153) | K. Nakazaki: Crystal Structure of a Liquid Crystalline Ferrocene Derivative

P.11.09.5(C392.154) | A. Iida: Layer and Molecular Orientation in Electroclinic Liquid Crystals: Dynamic  $\mu$ -diffraction

## 12 SURFACES, INTERFACES, LIQUIDS AND THIN FILMS

### 1. Surface and Interface Crystallography by X-ray and Neutron Diffraction

P.12.01.1(C409.155) | B. He: Phase and Stress Analysis of Porous Titania Layer with Two-dimensional XRD

P.12.01.2(C409.156) | H.-H. Wu: Three-Beam Diffraction Anomalous Fine Structure Of Thin Films

P.12.01.3(C409.157) | A. Alexeyev: X-ray Study of Titanium Coatings Made in Shaped Charge Jet Condition

P.12.01.4(C409.158) | K. Orlinska: X-ray Investigation of

## Hydrogen Implanted GaAs

P.12.01.5(C409.159) | M. Koivisto: Grazing Incidence X-Ray Diffraction Studies of Pharmaceutical Tablets

P.12.01.6(C410.160) | C.-H. Hsu: Structural and Compositional Investigation of Semiconductor Quantum Materials

P.12.01.7(C410.161) | Y. Fujii: Structure Analysis of Crystal Grain Nearby Surface using X-ray Scattering at Small Glancing Angle of Incidence

P.12.01.8(C410.162) | W.-C. Sun: Probing Interface Strain With X-ray Bragg-Surface Diffraction

## 15 DIFFRACTION PHYSICS AND OPTICS

### 1. Interferometry

P.15.01.1(C431.163) | S.-L. Chang: Direct Observation of Resonance Fringes in X-ray Cavity: A Diffraction Experiment

### 4. X-ray Optics: Lenses, Guides and Focusing

P.15.04.1(C431.164) | W. Gibson: The Convergent Beam Method for X-Ray and Neutron Microbeam Diffraction Applications

P.15.04.2(C431.165) | J. Wiesmann: State-of-the-art X-ray Optics for In-house Crystallography and Synchrotrons

P.15.04.3(C431.166) | C. Michaelsen: Multilayer Optics for Mo Radiation Based X-ray Crystallography

P.15.04.4(C432.167) | R. Gabrielyan: A Three-block X-ray Monolite Resonator

### 6. Anisotropic Resonant Scattering

P.15.06.1(C432.168) | K. Ishida: ATS Scattering from Isomorphic and Polymorphic Crystals

P.15.06.2(C432.169) | J. Kokubun: Anisotropic Resonant X-ray Scattering from Antiferromagnet Hematite,  $Fe_2O_3$

P.15.06.3(C432.170) | E. Ovchinnikova: Near-Edge Forbidden Reflections in Resonant Diffraction by Modulated Crystals

P.15.06.4(C432.171) | V. E. Dmitrienko: Thermal-Motion-Induced Forbidden Resonant Scattering: Experiment vs Theory

P.15.06.5(C433.172) | V. Tchijikov: MATHEMATICA Software for Anisotropic Resonant Scattering

### 7. Polarisation: Generation and Explication

P.15.07.1(C433.173) | Y. Uejii: Universal X-ray Ellipsometer and X-ray Depolarizer

### 8. Dynamical Diffraction

P.15.08.1(C433.174) | T. Nakajima: An Alternative Formation Theory of Beat Applied to the Pendelloesung Beat

P.15.08.2(C433.175) | M. Shevchenko: Fine Structure of Bragg's Peak as Dynamical Effect Specifying Nano-Clusters

P.15.08.3(C434.176) | O. Pobydaylo: Application of Particular X-ray Standing Wave for Accurate Determination of Electron Density

# TUESDAY, AUGUST 30, 2005 – POSTER SESSION

P.15.08.4(C434.177) | A. Movsisyan: Some Features of X-ray Diffraction in Monocrystals in Presence of the Temperature Gradient

P.15.08.5(C434.178) | T. Takahashi: Parametric Down Conversion of X-rays Under the Dynamical Diffraction Condition

## 11. Grazing Angle Incidence

P.15.11.1(C435.179) | S. E. Bezirganyan: Space Shift between Relaxed Si and Strain-compensated SiGeC Epitaxial Layers

P.15.11.2(C435.180) | G. Khachaturyan: Crystal Relief Investigation under the X-ray Diffraction on Surface Acoustic Wave in Bragg-Laue Grazing Geometry

P.15.11.3(C435.181) | V. Kocharyan: X-ray Diffraction Image under the Grazing Angles of Incidence on a Surface Acoustic Wave

## 12. No sub theme

P.15.12.1(C435.182) | A. H. Mkrtchyan: New Method of Solid State Structural and Composition Analysis

## 17 CHARACTERIZATION OF DEFECTS, MICROSTRUCTURES AND TEXTURES

### 1. Techniques, Theory and Instrumentation

P.17.01.1(C447.183) | F. Loglio: *In-situ* X-Ray Analysis under Controlled Potential Conditions: an Innovative Setup and its Application to the Investigation of Ultrathin Films Electrodeposited on Ag(111)

### 3. X-ray Topography

P.17.03.1(C447.184) | T. Mukaide: 3D-visualization for Structure of Large CaF<sub>2</sub> by Step-scanning Section Topography

P.17.03.2(C447.185) | R. Negishi: X-ray Topography by using Resonant Scattering

P.17.03.3(C448.186) | K. Kojima: Characterization of Dislocations in Protein Crystals using Synchrotron White-beam Topography

## 23 CRYSTALLOGRAPHY TOPOLOGY

### 3. Quasicrystals

P.23.03.1(C479.187) | S. I. Ben-Abraham: Quasiperiodic Structures Constructed by Projection in Two Stages

### 4. Networks

P.23.04.1(C479.188) | N. Benali-Cherif: Hydrogen Bonding in New Hybrid Compounds

P.23.04.3(C479.189) | J. L. Jorda: Ring Topology and Strain in Pure Silica Zeolites

### 5. Critical points

P.23.05.1(C480.190) | L. Torre: Topological Properties from Conventional Fourier Maps

## LATE CONTRIBUTION

### 04 CRYSTALLOGRAPHY OF BIOLOGICAL MACROMOLECULES

#### 2 Enzymes and Enzyme Catalysis

P.04.02.43(N.A.-191) | N.M. Cerqueira: Enzyme Ribonucleotide Reductase: The paradigm of enzyme inhibition by furanone derivatives

# PRESENTING AUTHOR INDEX

Aakeröy, C. B.	B13	Andreev, Y.	B89	Baburin, I.	B20	Becker, J.	B86	Billing, D. G.	B94
Abola, E.	B91	Andruh, M.	B72	Bacchi, A.	B95	Becker, M.	B79	Billinge, S.	B20
Adam, M.	B13	Angel, J.	B25	Bachechi, F.	B94	Becker, P. J.	B39	Billinge, S. J. L.	B5
Adams, A.	B22	Antipin, M. Y.	B18	Bader, R. F. W.	B59	Belaj, F.	B93	Bilokapic, S.	B22
Adams, D.	B69	Aoki, K.	B64	Bagaudinov, B.	B92	Belokoneva, E. L.	B95	Bindi, L.	B5
Addadi, L.	B85	Aoyagi, S.	B68	Baggio, R.	B80	Ben-Abraham, S. I.	B97	Bismayer, U.	B93
Adir, N.	B78	Aoyama, H.	B4	Baisch, U.	B81	Benali-Cherif, N.	B14, B97	Bjernemose, J.	B69
Afonine, P.	B91	Arakcheeva, A.	B31	Baker, E. N.	B6, B10	Bénard-Rocherullé, P.	B26	Blagden, N.	B40
Aggarwal, A. K.	B44	Aranda, M. A. G.	B47	Baker, H. M.	B79	Bendeif, E.	B39	Blakeley, M. P.	B58
Ahmed, H. U.	B64	Araujo, A. S.	B91	Balagurov, A.	B54	Benedict, J.	B89	Blankenfeldt, W.	B93
Aich, S.	B92	Archer, M.	B23	Balan, A.	B38	Benguedouar, L.	B23	Blatov, V. A.	B60
Akashi, H.	B24	Aree, T.	B12	Balegroune, F.	B80	Benito, J. M.	B26	Blatova, O. A.	B53
Akiba, T.	B79	Argyriou, D. N.	B74	Ballirano, P.	B67	Benmore, C.	B61	Boanini, E.	B39
Akimitsu, J.	B25	Arita, K.	B50	Balzani, V.	B30	Bennett, M. D.	B66	Boeyens, J.	B35
Akita, F.	B51	Arjunan, P.	B8	Balzar, D.	B27	Benning, M. M.	B50	Bogdanova, A. N.	B25
Akyol, E.	B40	Arletti, R.	B58	Ban, N.	B57	Bényai, A. C.	B11	Bogdanovic, G.	B39
Albinati, A.	B58	Armstrong, A.	B38	Banaszak, K.	B92	Berglund, J.	B8	Boldyreva, E.	B10
Albov, D. V.	B26	Armstrong, N.	B27, B59	Barabas, O.	B22	Berisio, R.	B23	Boller, H.	B53
Alekseeva, O.	B52	Arndt, J.	B79	Baram, D.	B74	Berman, H.	B49	Bolognesi, M.	B1
Alemi, A.	B26	Arnold, E.	B32, B49	Barannikova, S. A.	B52	Berman, H. M.	B30	Bombardi, A.	B36
Alexeyev, A.	B96	Arod, F.	B53	Baratta, W.	B74	Berman, L. E.	B36	Bombicz, P.	B94
Aliouane, N.	B89	Aroyo, M. I.	B28	Barbosa, J.	B8	Bernstein, H. J.	B84	Bond, M. R.	B80
Alkire, R.	B36	Artioli, G.	B61	Barbour, L.	B44	Bernstein, J.	B2	Bonifácio, C.	B78
Allan, D.	B45	Artizzu, F.	B53	Barnett, S. A.	B7	Bescrovny, D.	B11	Booth, M.	B78
Allen, A. J.	B14	Ashcroft, N.	B48	Baron, A. O. R.	B36	Besnard, C.	B13	Borca, E.	B55
Allen, F. H.	B16, B34	Asherie, N.	B37	Barr, G.	B84, B87, B90	Bethanis, K.	B91	Bordallo, H. N.	B53
Allmann, R.	B48	Askhabov, A.	B41	Bartoszak-Adamska, E.	B13	Betti, M. C.	B67	Bordet, P.	B33
Almeida Paz, F. A.	B56	Aslantas, M.	B65	Bataille, T.	B30	Beukes, J. A.	B12	Bordo, D.	B8
Alshahateet, S. F.	B13	Atwood, J. L.	B30	Báthori, N.	B11	Bevitt, J. J.	B56	Borek, D.	B63
Alterio, V.	B78	Au Yeung, A. S. F.	B93	Batten, S.	B60	Bezirganyan, H.	B27	Borgstahl, G.	B17
Alvarez, E.	B10	Au, S. W.	B9	Battistutta, R.	B64	Bezirganyan, S. E.	B97	Borowiak, T.	B11
Amann, U.	B25, B91	Au-Alvarez, O.	B12	Bau, R.	B58	Bezrodna, T.	B52	Borrmann, H.	B69
Anand, R.	B8	Audebrand, N.	B27	Bauer, E. M.	B95	Bhat, H. L.	B54	Bortolotti, M.	B96
Anderson, B. F.	B92	Authier, A.	B48	Bayarjargal, L.	B55	Biadene, M.	B79	Boschetto, D.	B47
Anderson, W. F.	B18	Avancı, L. H.	B41	Bayesen, F.	B7	Bialonska, B.	B11	Bosetti, E.	B82
Andjelkovic, K.	B80	Awaleh, M. O.	B24	Bazzicalupi, C.	B13	Bianchet, M. A.	B66	Bostrom, M.	B67
Andreasen, J. W.	B87	Baba, D.	B21	Beaucage, G.	B61	Bianchi, R.	B83	Botoshansky, M.	B11

# PRESENTING AUTHOR INDEX

Bouacida, S.	B93	Cai, J.	B81	Cerny, R.	B75	Choi, J. M.	B66	Courcot, B.	B39
Bouchouit, K.	B11	Cai, Y.	B13	Cerdeira, M.N.	B97	Choi, S. Y.	B26	Covaceuszach, S.	B79
Boudet, N.	B50	Cakir, O.	B25	Chabriere, E.	B65	Chong, S.	B5	Craievich, A. F.	B25
Bouhmaida, N.	B93	Calamini, B.	B64	Chainok, K.	B24	Chopra, D.	B11	Creze, C.	B22
Bourne, C.	B52	Calderone, V.	B78	Chakraborty, S.	B27	Choudhury, A. R.	B41	Criado, A.	B14
Bourne, P.	B49	Caliandro, R.	B60	Chaminade, J. P.	B25	Chruszcz, M.	B83	Criado, J. M.	B25
Bourne, S. A.	B94	Callear, S.	B41	Chan, C.	B79	Chu, H.-M.	B50	Crichton, W. A.	B68
Bovormratanarakts, T.	B68	Callow, P.	B47	Chang, S.-L.	B96	Chu, Y.	B44	Criswell, A.	B9
Boytssov, O.	B27	Cameron, S.	B39	Chapman, K. W.	B61	Chuang, Y.-C.	B39	Croce, G.	B89
Braden, M.	B3	Campana, C.	B50	Chapman, M.	B87	Chupas, P.	B61	Cuesta-Seijo, J. A.	B22
Brammer, L.	B14	Campbell, B.	B5, B35	Chapuis, G.	B89	Ciccarello, S.	B91	Cuocci, C.	B77
Brandt, A.-M.	B38	Camus, F.	B81	Charitat, T.	B87	Cirera, J.	B81	Curfs, C.	B47
Braun, W.	B44	Cañadillas-Delgado, L.	B95	Charkin, D. O.	B5	Cisarova, I.	B41	Curmí, P.	B65
Breger, J.	B47	Cao, Z.	B50	Chatterjee, S. K.	B42	Civalleri, B.	B13	Curry, S.	B32
Brisse, F.	B24	Capelli, S. C.	B25	Chatterji, T. K.	B3	Claramunt, R. M.	B82	Da Silva, J. I.	B67
Brock, C. P.	B6, B39	Capillas, C.	B25	Chattopadhyay, S.	B23	Clearfield, A.	B29	Dabkowska, H. A.	B40
Broder, C. K.	B25	Capitani, G.	B54	Chatziefthimiou, S.	B13	Cleasby, A.	B64	Dacunha, B.	B20
Broennimann, C.	B5	Capitelli, F.	B55	Chaudhary, S. K.	B40	Clegg, W.	B6, B37	Dalconi, M. C.	B53
Brokmeier, H.-G.	B33	Capsoni, D.	B53	Chayen, N. E.	B40	Coddington, P. W.	B12	Dale, S. H.	B30
Broströmer, E.	B92	Caracelli, I.	B77	Chen, C.-J.	B79	Cody, V.	B84	Danchuk, V. D.	B12
Brown, I. D.	B48	Carbone, V.	B92	Chen, C.-Y.	B22	Coetzee, A.	B50	Daniels, L.	B91
Brüning, J.	B10	Cargnoni, F.	B53	Chen, S.-M.	B81	Cogdell, R.	B58	Daran, J.-C.	B26
Brunzelle, J.	B9	Cario, L.	B5	Chen, X.	B53	Coles, S.	B62, B91	Das, K.	B88
Buchwald, G.	B63	Carradò, A.	B56	Chen, X.-M.	B46	Colligan, M.	B68	Dasgupta, P.	B56
Bucio, L.	B55	Carrell, C.	B39	Chen, Z.	B65	Collins, A.	B28	Datchi, F.	B59
Budarina, N.	B27	Carrozzini, B.	B37	Cheng, C.-Y.	B67	Collins, B. M.	B32	Dattagupta, J. K.	B22
Budzianowski, A.	B68	Carton, A.	B52	Chernyshev, I. V.	B94	Colson, T. A.	B87	Davey, R.	B32
Bull, C. L.	B66	Casati, N.	B69	Chernyshev, V. V.	B19	Comba, P.	B4	Davidson, A.	B68
Burger, C.	B75	Casini, A.	B64	Chernyshov, D.	B26	Comotti, A.	B32	Davies, R.	B93
Burghammer, M.	B36	Castell, A.	B92	Cheung, E.	B87	Conti, E.	B32	Dawson, A.	B64
Burley, S. K.	B86	Castellano, E. E.	B24	Chiari, G.	B58	Cook, A.	B32	Day, G. M.	B73
Burton, N.	B78	Cate, J.	B74	Chida, H.	B78	Coppens, P.	B4	Daymond, M.	B17
Buschiazzo, A.	B92	Catti, M.	B33	Chimsook, P.	B23	Cordero-Borboa, A. E.	B83	De Boissieu, M.	B19
Büyükgünör, O.	B94	Cavalcanti, L. P.	B10	Chinte, U.	B93	Corin, K. C.	B23	De Ranter, C.	B51
Byrappa, K.	B67	Cedola, A.	B45	Chisholm, J.	B11	Costa, M. M. R.	B26	De Simone, G.	B8
Cabo, A.	B63	Celik, O.	B23	Chiti, F.	B2	Costamagna, J.	B80	Deb, A. K.	B27
Caetano, M.	B94	Cenedese, S.	B53	Chiu, W.	B28	Cotelesage, J.	B92	Debbabi, M.	B95

# PRESENTING AUTHOR INDEX

Debler, E.	B38	Dombrauckas, J. D.	B92	Eisenberg, D.	B85	Ferguson, G.	B6	Fransen, M.	B50
Debreczeni, J. E.	B64	Domoroshchina, E.	B53	Ejsmont, K.	B11	Fermani, S.	B92	Fratzl, P.	B89
Degen, T.	B20	Dooryhee, E.	B58, B67	Elerman, Y.	B54	Fernandes, P.	B19	Frazao, C.	B65
Degtyareva, O.	B45, B69	Doudna, J. A.	B44	Elsegood, M. R. J.	B93	Fernandez, D.	B52	Fredrickson, D.	B17
Degtyareva, V. F.	B61	Dova, E.	B94	Elsliger, M.	B9	Ferraris, C.	B3	Frenkel, Y.	B14
Dela Mora, T.	B92	Dovesi, R.	B7, B29	Emsley, J.	B45	Ferraris, G.	B5, B28	Fridman, N.	B23
Delgado, F. S.	B95	Dragomir-Cernatescu, I.	B42	Eneqvist, T.	B72	Ferraroni, M.	B77	Frisch, G.	B67
Delgado, J. M.	B19	Draskovic, B. M.	B80	Enright, G. D.	B23	Ferreira, J. G.	B24	Friscic, T.	B82
Deloudi, D.	B41	Du Plessis, H. E.	B68	Erdönmez, A.	B12	Ferrer, S.	B85	Fronc, M.	B83
Demitri, N.	B64	Du, C.	B25	Eriksson, T.	B36	Ferretti, V.	B10	Fronczek, F. R.	B23
Deniz, N. G.	B11	Duarte, M. T.	B52	Esposito, L.	B84	Ficner, R.	B44	Fu, L.	B77
Depero, L. E.	B69	Duax, W. L.	B16	Esterhuysen, C.	B13	Finet, S.	B31	Fu, S.-J.	B13
Depmeier, W.	B14, B95	Dubrovinsky, L.	B59	Estrada, M. D.	B10	Fioravanti, E.	B65	Fu, Z.	B50
Dera, P.	B59, B76	Duc, F.	B54	Evans, C.	B83	Fioretto, D.	B16	Fuess, H.	B48, B55
Deschamps, J. R.	B10	Dudarev, S.	B27, B87	Evans, I. R.	B69	Fiori, A.	B41	Fujihashi, M.	B51
Dessanti, P.	B8	Duffy, T. S.	B47	Evans, J.	B17	Fiquet, G.	B16	Fujii, Y.	B96
Dewaele, A.	B47	Duke, E.	B36	Fabbiani, F.	B68	Firley, D.	B23	Fujimoto, Z.	B50
Dharmaprakash, S. M.	B40	Dumas, P.	B89	Fabelo, Ó.	B95	Fischetti, R.	B36	Fujisawa, T.	B31
Di Fiore, A.	B78	Dunstone, M.	B72	Faber, J.	B84	Fischetti, R. F.	B46	Fuksa, J.	B67
Di Marco, S.	B64	Duriska, M. B.	B94	Fabian, L.	B25	Fitch, A.	B20	Fukuda, K.	B27
Di Vaira, M.	B80	Durst, R.	B19	Fabra-Caro, M. J.	B81	Fitzpatrick, M.	B17	Fukumura, E.	B65
Diacomo, M.	B79	Dusek, M.	B75	Fabregas, I. O.	B7	Fitzpatrick, R. W.	B3	Fukuyama, K.	B51
Diáñez, M. J.	B81	Duskova, J.	B12	Falconi, S.	B61	Flack, H. D.	B24	Funakoshi, K.	B66
Diaz Becerril, T. F.	B82	Dwyer, J.	B83	Falini, G.	B46	Flaig, R.	B39	Furey, W.	B3
Diaz de Delgado, G.	B24	Dyachenko, O.	B54	Fan, H.	B7	Florencie, A.	B11	Furey, W.	B49
Diederich, F.	B16	Dziubek, K.	B18	Fan, H.-f.	B76	Forster, D.	B82	Furlan, S.	B93
Dincer, M.	B12	Ebihara, A.	B9	Fanelli, F.	B88	Fonso, L.	B38	Gabelli, S. B.	B51
Dines, M.	B63	Echigo, T.	B53	Fantini, M. C. A.	B56	Fontana, L.	B68	Gabrielyan, R.	B96
Ding, J.	B51	Edstrom, K.	B47	Farrugia, L. J.	B76	Fornasini, M. L.	B95	Gaffney, K.	B5
Dinnebier, R.	B30	Edwards, A.	B16	Fass, D.	B29	Forni, A.	B55	Gagor, A.	B25
Dinnebier, R. E.	B20	Edwards, A. J.	B11	Favre-Nicolin, V.	B19, B42,	Forrester, J. S.	B55	Gainsford, G.	B74
Dittrich, B.	B82	Edwards, L.	B33	B62	Francois, M.	B36	Gajda, R.	B68	
Dix, I.	B50	Effenberger, H.	B95	Fedorov, A.	B9	Frank, J.	B46	Galadzhun, Y.	B95
Dmitrienko, V. E.	B96	Egami, T.	B73	Fedorov, R.	B22	Frank, M.	B37	Galindo, A.	B24, B74
Dmitriev, V.	B26	Egli, M.	B16	Feidenhans'l, R.	B73	Frank, R.	B58	Gallois-Montbrun, D.	B23
Dogan, Ö.	B40	Einspahr, H.	B6, B35	Felts, R.	B50	Frankel, D.	B40	Garin, J. L.	B27
Dohnalek, J.	B63	Eisebitt, S.	B18	Feng, Z.	B34	Franklyn, P.	B83	Garman, E.	B88

# PRESENTING AUTHOR INDEX

Garrett, T.	B39	Glukhov, I.	B93	Groll, M.	B88	Hahn, T.	B49	Heine, A.	B20
Gatta, G. D.	B45	Gobechiya, E.	B52	Gronenborn, A.	B2	Haines, J.	B52	Hejny, C.	B69, B76
Gatti, C.	B31	Godinho, S.	B91	Gros, P.	B72	Halavaty, A.	B78	Helliwell, J. R.	B6, B73
Gavan, P.	B13	Godzik, A.	B30	Grosse-Kunstleve, R.	B34,	Hall, G. A.	B64	Helliwell, M.	B53
Gavrilenko, P.	B67	Goldstone, D.	B65		B59	Hall, S.	B86	Hendrix, J.	B19
Gebauer, B.	B19	Golshan, M.	B17	Grossie, D.	B56	Hall, S. R.	B49	Henrick, K.	B34, B49
Gee, C. L.	B64	Golubev, Y. A.	B53	Grove, H.	B26	Haller, K.	B10	Henriksen, A.	B8
Geiger, C. A.	B3	Gomes Guimaraes, B.	B22	Gruetter, M. G.	B2	Haluska, M.	B69	Henry, P. F.	B63
Geiger, S.	B54	Goncalves Hönnicke, M.	B37	Grunwaldt, J.-D.	B4	Hamadène, M.	B39	Heo, Y.-S.	B60
Gelbrich, T.	B11	Goncalves, S. G.	B38	Grygar, T.	B54	Hamilton, T. D.	B24	Herbst-Irmer, R.	B31
Gembicky, M.	B91	Goncharenko, I.	B76	Grzeta, B.	B55	Han, D.	B79	Herdweck, E.	B80
Geremia, S.	B66	Gonnade, R.	B10	Grzywa, M.	B77	Hansen, T.	B75	Hernandez Molina, M.	B93
Germaneau, E.	B20	Gonzalez Mantero, D.	B82	Gu, Q.	B41	Hansen, V.	B56	Herrero-Gómez, E.	B26
Gervais, C.	B44	Gonzalez, A.	B42	Guagliardi, A.	B20	Hanson, A.	B91	Hersleth, H.-P.	B78
Gervasio, G.	B40	Gonzalez-Platas, J.	B20	Gualtieri, A.	B88	Hansson, S.	B23	Herzberg, O.	B16
Gesing, T. M.	B14	González-Ramírez, L. A.	B38	Guehreria-Laidoudi, A.	B93	Hara, S.	B55	Hester, J.	B50
Ghammamy, S.	B80	Goodwin, A.	B83	Guérin, D. M. A.	B63	Harata, K.	B5	Hibi, T.	B51
Gheorghe, R.	B94	Görbitz, C. H.	B32	Guerri, A.	B10	Harrington, R.	B84	Higuchi, Y.	B78
Ghisletti, D.	B36	Gordon, R.	B79	Guevarra, J.	B67	Harris, P.	B65	Hill, C.	B60
Giacovazzo, C.	B17	Goto, M.	B7	Guille, K.	B80	Harte, S.	B10	Hill, J.	B87
Giannellini, V.	B42	Gouet, P.	B30	Guillot, B.	B45	Hasegawa, K.	B50	Himmel, D. M.	B65
Giannini, C.	B68	Gowda, K. V. A.	B12	Guinebretiere, R.	B61	Hasek, J.	B64	Hinrichsen, B.	B20
Giannini, E.	B54	Gozzo, F.	B36	Guo, R.-T.	B50	Hashimoto, H.	B22	Hiraki, M.	B91
Gibson, W.	B96	Graber, T. J.	B36	Gusin, P.	B83	Hashizume, D.	B39	Hirano, S.	B38
Gies, H.	B74	Gradzielski, M.	B61	Gustafsson, J. C. M.	B55	Haskell, D.	B4	Hirano, Y.	B39
Giglio, M.	B61	Gramm, F.	B56	Gustchina, A.	B50	Hassdenteufel, K. H.	B42	Hirata, K.	B79
Gillet, J.-M.	B59	Grassmann, O.	B94	Guthrie, M.	B73, B76	Hassell, A.	B2	Hirayama, N.	B88
Gilli, G.	B13	Gravereau, P.	B25	Gutmann, M.	B20	Hata, Y.	B93	Hirotsuo-Fujimoto, S.	B92
Gilli, P.	B4	Grazzi, F.	B63	Guyot, F.	B88	Hatch, D. M.	B25	Hisano, T.	B50
Gillon, A. L.	B44	Greenhough, T. J.	B38	Guzei, I. A.	B53	Hauback, B. C.	B47	Hodeau, J.-L.	B17
Gillon, B.	B18	Grenzer, J.	B75	Haake, A.	B28	Hau-Riege, S.	B18	Hodorowicz, M.	B82
Gilmore, C.	B33, B90	Grepioni, F.	B86	Hackert, M.	B9	Haussuhl, E.	B25	Hoeft, R.	B77
Giordano, V.	B68	Griesser, U. J.	B23	Haddow, M. F.	B26	Haywood, M. G.	B81	Hoell, A.	B47
Girard, E.	B31	Griffin, A. M. E.	B81	Hadermann, J.	B41	He, B.	B96	Hoffmann, C.	B63
Gladyshevskii, R. E.	B53	Grimmer, H.	B41	Hagelüken, G.	B78	He, Y.	B37	Hoffmann, K.	B38
Glass, C. W.	B47	Grobety, B.	B19	Hagiwara, Y.	B51	Hebeisen, C.	B83	Hoffmann, R.	B1
Glowka, M. L.	B10	Grochulski, P.	B78	Hagiya, K.	B66	Heijnen, W.	B3	Hol, W.	B72

# PRESENTING AUTHOR INDEX

Holm, P.	B61	Ice, G.	B45	Jauch, W.	B83	Kahn, R.	B7	Kemp, M.	B31
Holub-Krappe, E.	B27	Ida, K.	B50	Jayatilak, D.	B31	Kahraman, A.	B7	Kerfeld, C.	B72
Holý, V.	B75	Ida, T.	B91	Jelsch, C.	B82	Kaiser-Bischoff, I.	B5	Kernaghan, S. D.	B92
Holyoak, T.	B8	Ienco, A.	B24	Jeng, U-S.	B14	Kakuta, Y.	B8	Kezuka, Y.	B50
Homeida, H.	B52	Igarashi, N.	B37	Jenko Kokalj, S.	B65	Kalinowska-Tlusck, J. M.	B23	Khachaturyan, G.	B97
Honisich, U.	B56	Igura, M.	B52	Jenner, L.	B23	Kalmam, A.	B11	Kharchenko, A.	B44
Hooley, E.	B22	Iida, A.	B96	Jensen, A. F.	B12	Kamashev, D.	B54	Kharitonova, E.	B55
Hori, T.	B64	Ilyasov, V.	B52	Jeong, II-K.	B73	Kaminsky, W.	B2	Khor, K.	B56
Horigome, D.	B66	Imamoto, T.	B74	Jetti, R. K. R.	B11	Kamiyama, T.	B73	Khosavithkul, N.	B24
Horjales, E.	B79	Imasaki, T.	B22	Jevtovic, V. S.	B80	Kanagawa, M.	B23	Khrustalev, V. N.	B93
Hosokawa, S.	B16, B54	Imayoshi, N.	B42	Jeyaraman, J.	B65	Kanai, R.	B92	Kia, R.	B80
Hosoya, T.	B37	Immirzi, A.	B68	Jinek, M.	B79	Kanbayashi, K.	B8	Kigawa, T.	B88
Hosseini, M. W.	B32	Imura, H.	B56	Joachimiak, A.	B10	Kanechisa, N.	B81	Kikuchi, A.	B65
Hostettler, M.	B27	In, Y.	B10	Johansson, E.	B92	Kang, H. J.	B50	Kim, C. U.	B31, B93
Hountas, A.	B24	Inaka, K.	B84	Johnson, B.	B77	Kapor, A.	B81	Kim, J.-G.	B28
Howard, C. J.	B3, B25	Inami, T.	B69	Johnson, C.	B31	Kara, H.	B94	Kim, M.	B9
Hrdá, J.	B36	Irifune, T.	B45	Johnson, L. N.	B43	Karamertzanis, P.	B73	Kim, Y.	B40
Hrdy, J.	B36	Ishida, K.	B96	Johnston, A.	B94	Karen, P.	B67	Kimura, T.	B89
Hsiao, C.-D.	B22	Ishigaki, T.	B42, B78	Jokiah, R.	B51	Karlberg, T.	B78	Kinoshita, T.	B64
Hsu, C.-H.	B52, B96	Ishikawa, M.	B46	Jones, E. Y.	B60	Kasatani, H.	B55	Kirpichnikova, L.	B25
Hsu, I.-J.	B83	Ishiyama, N.	B93	Jorda, J. L.	B97	Kashii, M.	B66	Kiseleva, E. A.	B80
Hu, C.	B94	Ishizawa, N.	B83	Jordan, G.	B88	Kasper, C.	B79	Kishida, H.	B93
Hu, H.-C.	B63	Ito, M.	B87	Joseph, J.	B16	Kassimova, R. I.	B54	Kisi, E. H.	B55
Huang, D.	B39	Itou, H.	B9	Juan, E. C. M.	B44	Kastrup, J. S.	B79	Kita, A.	B63
Huebschle, C. B.	B82	Itou, M.	B83	Juarez Santiesteban, H.	B27	Kaszkur, Z.	B73	Kitadokoro, K.	B38
Huelsken, G. S.	B19	Ivanova, A.	B66	Juhas, P.	B30	Kato, K.	B69	Kitagawa, Y.	B77
Huether, R.	B22	Ivashevskaya, S.	B68	Jung, D. Y.	B97	Katsura, T.	B76	Kitago, Y.	B7
Huldt, G.	B18	Ivleva, L.	B40	Jurek, Z.	B18	Kaur, P.	B64	Kitano, A.	B42
Hungerford, S.	B90	Iwasaki, W.	B50	Kabekkodu, S.	B84	Kavanagh, K.	B64	Kitano, K.	B79
Hursthouse, M.	B84	Izaola, Z.	B75	Kaci, S.	B40	Kawaguchi, A.	B61	Klebe, G.	B71
Husheer, S. L. G.	B36	Izard, T.	B45	Kado, Y.	B53	Kawano, M.	B93	Klechkovskaya, V.	B27
Hyacinth, M. A.	B13	Izotova, L. Y.	B23	Kaduk, J.	B74	Kawano, Y.	B77	Klein, H.	B56
Hybler, J.	B5	Izumi, A.	B37	Kadziola, A.	B8	Kawasaki, M.	B38	Klein, H.-J.	B70
Hyde, S.	B60, B90	Jacobs, A.	B24	Kaercher, J.	B86	Kazak, C.	B80	Klooster, W.	B63
Ibberson, R.	B75	James, M.	B32	Kaganer, V.	B27	Kazheva, O.	B52	Koch, E.	B60
Ibers, J. A.	B43	Jaskolski, M.	B89	Kagoshima, Y.	B45	Kellaher, J. M.	B94	Koch, M.	B38
Ibragimov, B. T.	B23	Jauch, R.	B51	Kahlenberg, V.	B95	Keller, L.	B63	Kocharyan, V.	B97

# PRESENTING AUTHOR INDEX

Kocher, L.	B30	Kozisek, J.	B39	Lacorre, P.	B47	Lesci, I. G.	B53	Lu, X.	B24
Kochetkov, S.	B40	Krachodnok, S.	B24	Lah, N.	B80	Leusen, F. J. J.	B3	Lubambo, A.	B38
Kociok-Kohn, G. I.	B93	Kranold, R.	B75	Lamas, D.	B42	Levendis, D. C.	B82	Luchinat, C.	B46
Kodess, B. N.	B50	Krastanova, I.	B9	Lamberti, C.	B19	Levy, C.	B8	Luger, P.	B59
Kodess, P.	B42	Krauss, G.	B19	Langs, D. A.	B37	Lewis, G.	B42	Lund Jensen, A.-M.	B37
Koerner, C.	B37	Krishnaiah, M.	B11	Laponogov, I.	B38	Lewis, H.	B79	Lundgaard, L. F.	B59
Koetzele, T. F.	B63	Krissinel, E.	B63	Larrañaga, A.	B95	Leynaud, O.	B69	Lundell, A.	B45
Kogan, V.	B42	Krivovichev, S.	B3	Larsen, S.	B9	Li, D.	B92	Lundqvist, J.	B8
Koganezawa, T.	B36	Kroeker, M.	B20	Lasocha, W.	B20	Li, F.	B87	Luo, S. N.	B47
Kohara, S.	B61	Kroto, H.	B43	Lau, J. P.	B80	Li, J.	B4, B46	Luthi Nyffeler, T.	B12
Kohda, D.	B32	Kryazhev, A.	B14	Laundy, D.	B19	Li, X.-D.	B4	Lutterotti, L.	B77
Koivisto, M.	B96	Ksenofontov, D.	B41	Lavina, B.	B54	Li, Y.	B63	Lyaskovska, N.	B95
Koizumi, H.	B13	Ku, S.-Y.	B64	Lavy, T.	B86	Liang, C.	B19	Lykke, L.	B7
Kojic-Prodic, B.	B30	Kubicki, M.	B44	Lawrence, M.	B78	Liang, Y.	B9	Lysiuk, A.	B66
Kojima, K.	B97	Kubota, Y.	B56	Lazzari, R.	B14	Liddington, R. C.	B45	Lyuttsau, A.	B42
Kokh, K.	B40	Kudrenko, E.	B67	Le Bail, A.	B73, B84	Lifshitz, R.	B41	Mac Gillivray, L. R.	B44
Kokubun, J.	B96	Kugler, W.	B3	Le Bas, G.	B10	Lin, T.	B23	Madsen, A. Ø.	B59
Konarev, P.	B14	Kulicka, B.	B25	Lea, S.	B45	Lin, Y.-C.	B52	Maeda, Y.	B51
Kondo, J.	B22	Kulkarni, K.	B65	Leban, I.	B53	Linden, A.	B42	Maier, G.	B95
Kondrashkina, E.	B61	Kunz, M.	B66	Lebedev, O. I.	B17	Lippmann, T.	B45	Mak, T. C. W.	B81
Kong, G. K.-W.	B77	Kuramitsu, S.	B16	Lebioda, L.	B46	Lisovytksiy, D.	B25	Makarova, O.	B69
Kongshaug, K. O.	B56	Kurihara, K.	B82	Lee, C.-H.	B53	Litvin, D. B.	B28, B48	Makino, M.	B78
Konno, M.	B22	Kurnosov, A.	B69	Lee, C.-R.	B83	Liu, C.-T.	B68	Makovicky, E.	B48, B95
Kopf, J.	B49	Kuroki, R.	B84	Lee, J.-J.	B66	Liu, P.	B42	Malashkevich, V.	B77
Kopsky, V.	B25	Kusakabe, Y.	B64	Lee, M.	B92	Liu, S.-X.	B24	Male, L.	B68
Korczynska, M.	B92	Kusakari, Y.	B8	Lee, P.	B33	Liziero, F.	B54	Maltsev, V.	B40
Koritsanszky, T.	B82	Kusunoki, M.	B78	Lee, T.-W.	B51	Lloyd, G. O.	B26	Mangani, S.	B9
Korlyukov, A.	B59	Kuta Smatanova, I.	B38	Lehane, K. N.	B14	Loehlin, J.	B42	Mannix, D.	B82
Korolkov, I.	B66	Kuty, M.	B77	Lehtiö, L.	B8	Loglio, F.	B97	Manomenova, V.	B40
Korsunsky, A.	B50	Kuzel, R.	B27, B59	Leisegang, T.	B82	Lokanath, N. K.	B92	Manuel, S. M.-C.	B68
Kosinska, U.	B65	Kuzin, A. P.	B12	Lemieux, M. J.	B7	Lolli, G.	B38	Mao, W.	B45
Kosmopoulou, M.	B92	Kuz'micheva, G.	B52	Lemus-Fuentes, E.	B14	Lord, T.	B95	Marabello, D.	B40
Kostorz, G.	B6	Kuznetsov, A.	B27	Lengeler, B.	B5	Lorenzo, J. E.	B54	Marcaida, M. J.	B72
Kostyanovsky, R. G.	B86	Kvick, Å.	B75	Lennie, A.	B68	Louprias, G.	B39	Marchesini, S.	B5
Kotryl, M.	B28	Kyono, A.	B54	Lennon, J.	B12	Loveday, J. S.	B69	Marchini, N.	B12
Kovaleva, O.	B54	Kyunggon, K.	B38	Leomi, M.	B59	Lovelace, J. J.	B91	Marchio', L.	B81
Kozak, M.	B65	Labesse, G.	B65	Leoni, S.	B3	Lozano-Casal, P.	B23	Marfo-Owusu, E.	B14

# PRESENTING AUTHOR INDEX

Margiolas, I.	B33	Mc Mahon, B.	B34	Millican, J. N.	B53	MoraesFerreira, F.	B66	Naoe, C.	B8
Margulies, L.	B57	Mc Mahon, M.	B43, B69	Mills, D.	B6	Morar, M.	B8	Naoe, Y.	B51
Marin, G.	B94	Mebs, S.	B82	Minguez, G.	B82	Moreno, A.	B38	Napolitano, H. B.	B11
Marinoni, G.	B80	Mechaly, A.	B36	Minor, W.	B18	Mori, K.	B88	Nardini, M.	B77
Mario, S.	B51	Medakovic, V. B.	B13	Mironova, E.	B23	Morikawa, K.	B74	Nassimbeni, L. R.	B86
Markiewicz, M.	B10	Meden, A.	B55	Misaki, S.	B42	Morris, R. E.	B58	Natsume, R.	B93
Marler, B.	B17	Medrish, I. V.	B80	Misture, S.	B67	Mossakowska, I. A.	B7	Navarra, G.	B55
Marmeggi, J.-C.	B25	Meekes, H.	B41	Mitchell, E.	B79	Motherwell, S.	B84	Navasardyan, M.	B36
Marques, L.	B11	Meents, A.	B38	Mitev, K. Z.	B86	Moutran, A.	B77	Navasardyan, M. A.	B73
Marsh, M.	B92	Meneghetti, F.	B22	Mitsumi, M.	B89	Movsisyan, A.	B97	Nazarenko, A.	B25
Martin-Albina, M. L.	B81	Meramveliotaki, C.	B22	Mittl, P.	B38	Mueller, S.	B93	Nazzareni, S.	B66
Martinez, J.	B55	Merlino, A.	B92	Miura, K.	B42	Mueller, U.	B48	Neder, R.	B35
Martin-Gago, J. A.	B27	Merlino, S.	B48	Miyahara, I.	B51	Mukaide, T.	B97	Neder, R. B.	B73
Martins, D. M. S.	B7	Merlo, F.	B95	Miyamae, H.	B93	Muktha, B.	B52	Neels, A.	B82
Martins, R. V.	B56	Merritt, E. A.	B34	Miyano, M.	B86	Mulichak, A.	B91	Negishi, R.	B97
Martin-Zarza, P.	B80	Meshi, L.	B37	Miyata, T.	B27	Muñoz, I.	B78	Nelmes, R.	B68
Martonak, R.	B61	Mesto, E.	B54	Miyatake, H.	B7	Munshi, P.	B83	Nespolo, M.	B31
Marvaud, V.	B72	Metrangolo, P.	B2, B82	Miyazono, K.	B66	Muraoka, S.	B78	Ness, S.	B33
Mascarenhas, Y. P.	B55	Meven, M.	B63	Mizutani, K.	B38	Murphy, M.	B71	Neumann, M. A.	B73
Massera, C.	B24	Meyer, E.	B31	Mkrtychyan, A. H.	B97	Murray-Rust, J.	B22	Nichol, G. S.	B25
Matias, P.	B89	Mezey, P. G.	B31	Mo, F.	B55	Murray-Rust, P.	B84, B86	Nickolsky, M.	B56
Matijasic, I.	B24	Mezouar, M.	B76	Moffat, K.	B47	Muzzolini, L.	B28	Nii, H.	B51
Matsugaki, N.	B36	Mezzetti, A.	B74	Moggach, S. A.	B68	Nagata, A.	B78	Niimura, N.	B73
Matsuji, M.	B48	Miallau, L.	B92	Moitsheki, L. J.	B94	Nagata, K.	B63	Nishi, F.	B54
Matsumoto, S.	B94	Michaelsen, C.	B96	Molcanov, K.	B26	Nakagawa, A.	B63	Nishibori, E.	B20
Matsunami, H.	B63	Michel, F. M.	B53	Molenbroek, A.	B42	Nakai, T.	B93	Nishikawa, M.	B96
Matsushita, M.	B65	Michiue, Y.	B17	Molins, E.	B83	Nakajima, K.	B67	Nishio, K.	B50
Matsushita, Y.	B19	Mihajlovi, T.	B67	Moliterni, A. G.	B30	Nakajima, T.	B96	Noda, Y.	B55
Matsuura, T.	B8	Miida, R.	B52	Momma, M.	B65	Nakamoto, Y.	B68	Nollert, P.	B41
Maurin, J. K.	B10	Mikami, B.	B50	Monari, M.	B81	Nakamura, A.	B92	Nomura, K.	B68
Mavridis, I. M.	B51	Mikhin, O.	B37	Mondal, S.	B91	Nakamura, H.	B34, B49	Nonaka, T.	B50
Mayerová, Z.	B67	Mikula, P.	B63	Money, V. A.	B9	Nakamura, N.	B96	Norrman, M.	B66
Maynes, J. T.	B92	Milanesio, M.	B69	Montano, P. A.	B87	Nakamura, T.	B51, B65	Novakovic, S.	B39
Mazumder, S.	B53	Milani, M.	B78	Montejo Bernardo, J.	B12	Nakashima, P.	B28	Novoade Armas, H.	B94
Mc Auley, K.	B8	Milcic, M. K.	B13	Montilla, F.	B26	Nakazaki, K.	B96	Novotny, J.	B40
Mc Cusker, L.	B15	Miles, S.	B22	Montoya, G.	B63	Nan, J.	B20	Noyan, I. C.	B33
Mc Grath, R.	B19	Miller, R. J. D.	B47	Moore, M.	B19	Nangia, A.	B86, B94	Nozue, Y.	B55

# PRESENTING AUTHOR INDEX

Numoto, N.	B63	Orlow, A.	B23	Pasán, J.	B46	Pilia, L.	B55	Pruzan, P.	B68
Nyilas, K.	B27	Orpen, A. G.	B29	Pasaoglu, H.	B80	Pimenta Jr., A. A.	B12	Puchkovska, G.	B25
Oakley, S. H.	B77	Oswald, I.	B69	Pasquato, N.	B39	Pinkerton, A. A.	B83	Pukas, S.	B95
Oberhauser, W.	B26	Oszlanyi, G.	B17	Passeri, D.	B83	Pinotsis, N.	B93	Pulham, C.	B3
Oberti, R.	B54	Otwinowski, Z.	B34, B77	Pasternak, O.	B63	Pinto Camargo, J. L.	B23	Punte, G.	B56
Ochrombel, R.	B55	Ovchinnikova, E.	B96	Patel, S. B.	B64	Pinto, D.	B31	Puntharod, R.	B23
Ochsenbein, P.	B10	Owen, R.	B65	Paterson, N.	B65	Piontek, K.	B89	Purhonen, P.	B61
Oeckler, O.	B66	Ozawa, Y.	B18	Paufler, P.	B67	Piro, O. E.	B24	Puschmann, H.	B20
Oganov, A.	B33	Ozcan, Y.	B24	Paulmann, C.	B36	Pischetola, V.	B68	Pushcharovsky, D.	B48
Ogawa, K.	B13	Ozek, A.	B12	Pauly, T.	B64	Piskarov, V.	B20	Pustovalov, V. V.	B67
Ogawa, T.	B8	Ozkok, F.	B12	Pavlovic, G.	B11	Piskunova, N.	B40	Pyetan, E.	B64
Ogitsu, T.	B33, B69	Pacek, P.	B55	Pearson, A.	B51	Pitak, M.	B39	Pytel, P. D.	B22
Ohachi, T.	B41	Padyana, A. K.	B79	Peat, T.	B91	Plachinda, P. A.	B26	Qiu, X.	B38
Ohashi, Y.	B81	Pahl, R.	B91	Pecharsky, V.	B69	Pletnev, S.	B9	Quartieri, S.	B4
Ohishi, A.	B96	Pähler, A.	B20	Pechik, I.	B63	Pletnev, V.	B77	Quintal, S.	B95
Ohishi, Y.	B66	Pai, C.-H.	B22	Pedersen, B. L.	B26	Pobdaylo, O.	B96	Radaelli, P. G.	B73
Ohno, T.	B56	Pai, R.	B20	Pedersen, J. S.	B75	Podjarny, A. D.	B89	Rademeyer, M.	B13
Ohsato, H.	B53	Pajdzik, L. A.	B67	Pelloquin, D.	B67, B89	Podobnik, M.	B77	Rae, A. D.	B28
Ohtsuki, T.	B65	Palatinus, L.	B75	Perez, C. S.	B32	Podsiadlo, M.	B12	Rafilovich, M.	B12
Ohwada, K.	B25	Pandey, D.	B3	Perez-Mato, J. M.	B17, B25	Podust, L. M.	B79	Raiteri, P.	B73
Ojala, W. H.	B12	Panina, N.	B41	Pérez-Prieto, M.	B67	Pompidor, G.	B7	Ramakumar, S.	B10
Okada, K.	B17	Pantos, S.	B20	Persoons, A.	B2	Poomani, K.	B82	Ramon, G.	B11
O'Keefe, M.	B60	Paoletti, F.	B79	Pesaresi, A.	B8	Popa, N.	B59	Ramos Parente, C. B.	B63
Okube, M.	B66	Papadopoulos, Z.	B19	Peskov, M. V.	B95	Popovic, J.	B55	Ramos Silva, M.	B80
Okuchi, T.	B69	Papadopoulos, B.	B54	Petoukhov, M.	B75	Popovic, S.	B25	Ramsden, S.	B90
Olesen, C.	B4	Papinutto, E.	B51	Petricek, V.	B15	Pósfai, M.	B54	Ramsland, P. A.	B38
Oleynikov, P.	B42	Paraschiv, C.	B94	Petrova, S.	B69	Poulsen, J.-C. N.	B38	Randaccio, L.	B11
Oliva, G.	B38	Paris, O.	B45	Petrova, T.	B7	Poulsen, R. D.	B39	Rao, Z.	B32
Olvera, J.	B41	Park, H.	B56	Petrakhina, M. A.	B24	Powell, H.	B35	Rathore, R.	B77
Omi, R.	B8	Park, H. M.	B66, B91	Pflugrath, J. W.	B89	Pozzi, C. G.	B55	Ratia, K.	B51
Ondracek, J.	B20	Park, Y.-J.	B10	Philippsen, A.	B61	Prabu-Jeyabalan, M.	B51	Ravaud, S.	B92
Onoda, M.	B41	Parker, L.	B64	Phillips, C.	B86	Preisinger, A.	B93	Ravy, S.	B26
Ooga, T.	B26	Parker, M.	B43	Phillips, G.	B38	Pretto, L.	B13	Rawiso, M.	B47
Openshaw, A. E. A.	B92	Parkin, A.	B90	Pidcock, E.	B14	Probert, M. R.	B91	Read, R.	B59
Orlando, R.	B31	Parrish, D.	B83	Pietraszko, A.	B55	Proffen, T.	B35, B91	Reimers, W.	B1
Orlinska, K.	B96	Parsons, S.	B89	Pietsch, U.	B82	Proietti, M. G.	B4	Reutzel-Edens, S. M.	B3
Orlov, I.	B75	Parvez, M.	B80	Pilati, T.	B82	Prugovecki, S.	B33	Rhee, S.	B38

# PRESENTING AUTHOR INDEX

Richmond, T.	B74	Rotiroti, N.	B67	Sato, K.	B3	Schuck, G.	B54	Shinohara, Y.	B89
Riekel, C.	B89	Rousse, G.	B68	Sato, M.	B40	Schuelke, W.	B87	Shiono, M.	B23
Rife, C.	B9	Rovira, C.	B72	Sato, Y.	B50	Schulze, J.	B79	Shiozawa, K.	B65
Righini, G.	B94	Rudiñío-Piñera, E.	B60	Satoh, T.	B38	Schvezov, C.	B41	Shirakawa, M.	B22
Rigolet, P.	B79	Rudolph, M.	B46	Sauvage, E.	B79	Schwalbe, C. H.	B53	Shiroishi, M.	B38
Riley, D. P.	B68	Rueff, J.-P.	B76	Savarese, T. L.	B69	Schwarz, K.	B4, B39	Shishkin, O. V.	B11
Rinaldi, F.	B37	Ruf, A.	B64	Saviano, M.	B94	Schwarzenbach, D.	B6	Shmueli, U.	B49
Risal, D.	B77	Ruiz-Pérez, C.	B32	Sawa, H.	B75	Sciortino, N. F.	B56	Shrive, A. K.	B72
Rius, J.	B54	Rupp, B.	B2	Sayil, C. M.	B11	Seal, A.	B77	Shuvalova, L.	B9
Roberts, K. J.	B27	Rüscher, C. H.	B14	Sayre, D.	B15	Seaton, C.	B87	Sica, F.	B63
Robeyns, K.	B22	Rush, C.	B36	Sazaki, G.	B44	Seijbel, L.	B36	Siliqi, D.	B7
Robins, V.	B90	Russi, S.	B22	Scandolo, S.	B33	Sekiguchi, T.	B23	Silva, A. M.	B51
Robu, I. N.	B55	Russo, L.	B24	Scarlett, N.	B75	Sekine, A.	B94	Silva, E. N.	B95
Robu, L.	B67	Ruth, R.	B36	Schall, C.	B2	Sekulic, N.	B51	Simone, S.	B38
Roces, L.	B38	Rypniewski, W.	B46	Schattschneider, D.	B31	Selvanayagam, S.	B37	Simonov, S.	B52
Rocha, J.	B17	Safro, M.	B94	Schauerle, C.	B12	Semmingsen, D.	B13	Simova, V.	B58
Rodi, D. J.	B91	Sage, J. T.	B16	Schefer, J.	B52	Senda, M.	B51	Sippl, M. J.	B30
Rodrigues, B.	B39	Sainz-Diaz, I.	B13	Scheins, S.	B82	Senda, T.	B51	Sixma, T. K.	B86
Rodriguez, M. S.	B41	Saitoh, K.	B56	Schenk, H.	B10, B14	Sergeev, D. S.	B53	Skalova, T.	B64
Rodríguez-Carvajal, J.	B5	Saitoh, T.	B77	Scherer, W.	B58	Serpé, A.	B26	Skubak, P.	B59
Rodríguez-Mijangos, R.	B95	Sakamoto, Y.	B92	Schierbeek, B.	B7	Sevvana, M.	B79	Sleator, O.	B78
Rodríguez-Navarro, A.	B27	Sakata, M.	B83	Schierholz, R.	B55	Seyyidoglu, S.	B81	Smirnova, N. L.	B95
Roe, M.	B22	Sakurai, Y.	B45	Schlitz, M.	B59	Shahar, A.	B37	Smith, A. B.	B37
Roessli, B.	B61	Saldin, D.	B73	Schirwitz, K.	B9	Shalimov, A.	B27	Smith, A. E.	B14
Röhr, Å. K.	B77	Sali, A.	B29	Schmid, M.	B46	Shan, N.	B41	Smith, J. L.	B71
Röhr, C.	B67	Salvarezza, R. C.	B87	Schmid, S.	B56	Shankland, K.	B19	Smits, J. M. M.	B84
Romanenko, G.	B95	Salviulo, G.	B95	Schmid-Rausch, K.	B67	Shapiro, D.	B18	Sobolev, A. N.	B11
Romaniv, O.	B95	Samoilovith, M.	B28	Schmidt, A.	B16	Shepard, W.	B16	Soininen, J. A.	B87
Romão, M. J.	B64	San Miguel, A.	B4	Schmidt, M. U.	B72	Sheu, C.-F.	B68	Sokolov, T. N.	B82
Rosair, G. M.	B14	Sanchez, I.	B64	Schnabel, S.	B67	Sheu, H.-S.	B20	Sokolova, A.	B14
Rosales, I.	B81	Sanjoh, A.	B40	Schnablegger, H.	B36	Shevchenko, M.	B96	Solans, X.	B42
Rose, J.	B18	Santillana, E.	B37	Schneider, S.	B52	Shi, D.	B50	Somphon, W.	B25
Rosendo, E.	B27	Santoro, M.	B68	Schoenborn, B.	B66	Shibata, N.	B79	Son, S. I.	B83
Rossi, M.	B23, B42	Santos, I. C.	B53	Schoenleber, A.	B69	Shiina, M.	B53	Soriano, E.	B79
Rossmann, M. G.	B58	Santos-Silva, T.	B78	Schreiner, P.	B38	Shimizu, N.	B79	Sortais-Soulard, C.	B25
Roszak, A. W.	B65	Sasaki, K.	B23	Schroder, M.	B46	Shimizu, T.	B22	Soshnikov, A.	B54
Rotella, F. J.	B36	Sasaki, S.	B37	Schroer, C.	B45	Shinashi, K.	B11	Sourek, Z.	B26

# PRESENTING AUTHOR INDEX

Sozzani, P.	B86	Sugimoto, K.	B50	Tang, M.-T.	B88	Tokuoka, K.	B8	Uhrikova, D.	B47
Spackman, M. A.	B57	Sugishima, M.	B78	Tanski, J. M.	B94	Tomchick, D.	B58	Umeda, T.	B7
Spagna, R.	B80	Suh, M. P.	B71	Tashkhodjaev, B.	B11	Tomcova, I.	B10	Umena, Y.	B51
Spano-Budayova, M.	B38	Suhre, K.	B87, B91	Tastan Bishop, A. O.	B78	Tomoo, K.	B38	Ungar, T.	B59
Spanswick, C. K.	B13	Sun, W.-C.	B96	Tatar Yildirim, L.	B81	Toms, A.	B8	Unno, H.	B65
Sparkes, H. A.	B84	Sun, Y.-J.	B50	Tauelle, F.	B19	Tom-Yew, S.	B77	Uodome, A.	B69
Speghini, A.	B95	Sung, H. H.-Y.	B26	Tazaki, R.	B54	Tondi, D.	B65	Urzhumtsev, A.	B79
Spence, J. C.	B88	Suryanarayanan, R.	B61	Tchijikov, V.	B96	Toriumi, K.	B26	Vachette, P.	B75
Spodine, E.	B52	Suvorova, E.	B87	Te Nijenhuis, J.	B27	Törnroos, K. W.	B81	Vachieri, S.	B53
Sprauel, J.-M.	B17	Suzuki, K.	B23, B42	Tedesco, C.	B11	Torre, L.	B97	Vagovic, P.	B27
Srajer, G.	B75	Suzuki, M.	B53	Teh, A. H.	B8	Torriani, I. L.	B14	Van der Lee, A.	B95
Srajer, V.	B9	Suzuki, N.	B65	Teichert, C.	B75	Toudic, B.	B42	Van der Maele Uriá, J. F.	B80
Staker, B. L.	B64	Svensson, O.	B36	Tellgren, R.	B67	Toyoshima, C.	B1	Van der Spoel, D.	B88
Stalke, D.	B45	Svergun, D.	B57	Temperini, C.	B14	Tozzo, É.	B24	Van Hecke, K.	B22
Stammers, D.	B32	Svoboda, I.	B12	Telyakov, A.	B9	Trapani, S.	B60	Van Smaalen, S.	B75
Standley, D. M.	B84	Swain, D.	B55	Terada, Y.	B3	Troyanov, S.	B4	Van Tri, N.	B52
Stangl, J.	B73	Swaminathan, G. J.	B86	Terradot, L.	B63	Tsai, M. Y. W.	B92	Vande Velde, C. M.	B40
Steed, J. W.	B30	Swenson, D.	B81	Terwilliger, T.	B33, B34	Tse, J.	B29	Vandeputte-Rutten, L.	B4
Steiner, C.	B14	Sztucki, M.	B14	Teslenko, P.	B67	Tsirelson, V.	B39	Vangdal, B.	B81
Stepanov, S.	B42	Tada, M.	B83	Thackeray, M.	B43	Tsoucaris, G.	B31	Vass, S.	B14
Stephens, P.	B15, B66	Tada, S. F. S.	B36	Thalal, A.	B55	Tsuchiya, Y.	B20	Vaughan, G.	B5
Stergiou, C.	B54	Taibi, K.	B55	Thiyagarajan, P.	B63, B89	Tsuda, K.	B87	Vegas, A.	B3
Stevens, R.	B15	Takahashi, T.	B97	Thomas, E. L.	B53	Tsuge, H.	B51	Vekhter, Y.	B66
Stoeckli-Evans, H.	B14	Takahashi, Y.	B8	Thomas, R. K.	B87	Tsuji, N.	B83	Velasco, P.	B26
Stojanoff, V.	B2	Takakura, H.	B41	Thompson, A.	B70	Tsunoda, M.	B22	Vella-Zarb, L.	B7
Stokes, H. T.	B25, B35	Takamizawa, S.	B94	Tilley, S.	B2	Tsusaka, Y.	B27	Vendier, L.	B81
Straver, L.	B41	Takata, M.	B79	Tillmanns, E.	B66	Tucker, M.	B73	Venegas-Yazigi, D.	B52
Strelkov, S. V.	B58	Takeji, H.	B89	Timmins, J.	B21	Tulk, C. A.	B73	Venter, A.	B69
Streltsov, V.	B72	Takemura, K.	B68	Timofeeva, T.	B7	Turgunov, K.	B10	Vidal, K.	B74
Strickland, P.	B20	Tamanis, E.	B82	Tinant, B.	B80	Turk, D.	B77	Viitanen, L.	B7
Strohmaier, K. G.	B17	Tamu, D. V.	B79	Ting, V. P.	B74	Turner, M. J.	B82	Vij, A.	B81
Struble, E.	B22	Tamura, H.	B9	Tkalcec, E.	B55	Tyunina, E.	B52	Vijayan, M.	B78
Strumpel, M. K.	B2	Tanaka, H.	B40	Toby, B.	B84	Uchida, A.	B12	Vinson, P.	B84
Su, X.-D.	B9	Tanaka, K.	B50	Tocheva, E.	B92	Uchida, Y.	B25	Viola, J.-P.	B42
Subramani, A. K.	B88	Tanaka, M.	B20, B71	Tochowicz, A.	B78	Ueda, Y.	B81	Violot, S.	B52
Suck, D.	B41	Tanaka, N.	B64	Toebbens, D. M.	B91	Ueji, Y.	B96	Višnjevac, A.	B14
Sugimoto, H.	B78	Tanaka, Y.	B42	Tokareva, A. O.	B26	Uekusa, H.	B94	Visser, D.	B58

# PRESENTING AUTHOR INDEX

Vitagliano, L.	B78	Wentzcovitch, R.M.M.	B33	Wu, B.	B37	Yoneda, S.	B81	Zordan, F.	B82
Viti, C.	B31	Werckmann, j.	B26	Wu, H.-H.	B96	Yoon, H.-J.	B64	Zorina, L.	B52
Vlieg, E.	B44	Weyer, H. J.	B42	Wu, L.-C.	B52	Yoshikawa, N.	B81	Zou, X.	B67
Vogel, A.	B65	Whisstock, J.	B2	Wu, W.-S.	B80	Yoshimura, M.	B91	Zouev, I.	B23
Volkova, E.	B41	White, F.	B20	Xia, Z.-X.	B92	Yoshimura, Y.	B25	Zubkova, N.	B3
Vologzhanina, A. V.	B52	White, T.	B71	Xi-Rui, Z.	B80	Yoshiteru, S.	B21	Zukerman-Schpector, J.	B24
Von Dreele, R.	B33	Whitten, A. E.	B39	Xu, H.	B59	Young, V.	B36	Zuo, J.-M.	B45
Vonk, V.	B41	Wierzchowski, W.	B27	Yabashi, M.	B5	Yuan, H. S.	B60		
Vonrhein, C.	B65	Wiesmann, C.	B78	Yadani, T.	B8	Yuan, Z.	B56		
Vorontsov, D.	B40	Wiesmann, J.	B96	Yaghi, O.	B46	Yucel, A.	B69		
Vujovic, D.	B24	Wieteska, K.	B27	Yagi, N.	B50	Yufit, D.	B69		
Wagermaier, W.	B93	Wigley, D.	B60	Yagi, T.	B47	Yushkin, N. P.	B66		
Wagner, A.	B66	Wignall, G.	B47	Yakhvarov, D.	B81	Zadesenets, A.	B66		
Wahl, M. C.	B74	Williams, A.	B30	Yamada, H.	B95	Zagari, A.	B23		
Wakatsuki, S.	B72	Williams, P. A.	B46	Yamada, Y.	B36	Zaghis, F.	B28		
Waksman, G.	B45	Wills, A.	B5	Yamagata, T.	B81	Zakrassov, A.	B12		
Walsh, M. A.	B18	Wilmann, P.	B37	Yamagata, Y.	B92	Zaleski, J.	B83		
Wang, B.-C.	B36	Wilson, C.	B18, B90	Yamaguchi, H.	B8	Zanotti, G.	B9		
Wang, J.	B9	Wilson, C. C.	B13	Yamamoto, A.	B15	Zaug, J. M.	B66		
Wang, W.-C.	B13	Wilson, I. A.	B72	Yamamoto, M.	B33	Zavartsev, F.	B40		
Wang, X.	B47	Wilson, K. S.	B18	Yamamura, S.	B26	Zavorotko, M.	B3		
Wang, Y.	B83	Winter, R.	B31	Yamanaka, M.	B40	Zehnder, M.	B20		
Warczewski, J. Z.	B28	Withers, R.	B17	Yamanaka, T.	B69	Zein, F.	B66		
Warkentin, E.	B66	Wlodawer, A.	B60	Yang, C.	B7	Zewail, A.	B85		
Watanabe, S.	B50	Wojciechowski, J.	B10	Yang, H.	B9, B64	Zhang, B.	B72		
Watanuki, T.	B59	Wolf, G.	B33	Yang, K.	B92	Zhang, J.	B93		
Watermeyer, J.	B64	Wolfova, J.	B37	Yao, D.	B7	Zhang, J.-P.	B95		
Watkin, D. J.	B17	Wolska, I.	B13	Yao, J.	B37	Zhang, P.	B78		
Webb, C. T.	B63	Wolstenholme, D.	B39	Yao, M.	B22	Zhang, R.	B9		
Weber, T.	B5	Wondergem, H.	B54	Yarovsky, I.	B7	Zhang, Y.	B8		
Weckert, E.	B36	Wong, J.	B16	Yasuda, N.	B36	Zhao, L.	B80		
Weeks, C.	B37, B49	Wong, W.-T.	B80	Yeates, T.	B60	Zhao, Q.	B22		
Wehenkel, A.	B78	Wong-Ng, W.	B54	Yilmaz, S.	B54	Zheng, H.	B34		
Weichenberger, C.	B28	Wood, P. A.	B69	Yin, J.	B8	Zhou, Y.	B20		
Weierstall, U.	B61	Wörle, M.	B95	Yin, W.	B44	Zhu, Y.	B56		
Weirich, T. E.	B87	Wosylus, A.	B68	Yokoyama, T.	B77	Zimmerman, M.	B38		
Welberry, T. R.	B5, B12	Wright, J.	B33	Yonath, A.	B88	Zolotoyabko, E.	B17		