

Tuesday, 8 august 2006 - morning

08.30-09.30	AULA P. DE SOMER	AULA MAGNA
	P5 Gastone Gilli (Chemistry Department and Centre for Structural Diffractometry, University of Ferrara, Ferrara, Italy) Modern hydrogen bonding theory Chair: Roland Boese	P6 Gustaaf Van Tendeloo (University of Antwerp, Belgium) Electron crystallography: who is afraid of dynamical scattering? Chair: Michael Lehmann
09.30-10.00	COFFEE BREAK	
10.00-12.00	MAGRITTE ROOM	DELVAUX ROOM
	<i>MS4: Nucleic acids</i> Chair: Christine Cardin, Co-chair: Philippe Dumas	<i>MS10: New X-ray sources and new possibilities</i> Chair: Edgar Weckert, Co-chair: Christian Riekell
	10h00 m4.o1 Patrick Cramer (Gene Center, University of Munich, Germany) mRNA transcription and its inhibition by RNA	10h00 m10.o1 Ronald Ruth (Lyncean Technologies, Inc, USA) Testing the Compact Light Source: a miniature synchrotron for the home lab
	10h30 m4.o2 Gary Parkinson (Pharmaceutical and Biological Chemistry, BMSG, University of London, UK) Structural aspects of quadruplexes as potential therapeutic targets	10h30 m10.o2 Thomas Tschentscher (Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany) Experiments using ultrashort coherent X-ray radiation at the future European XFEL Facility
	11h00 m4.o3 Matthias Bochtler (International Institute of Molecular and Cell Biology, Warsaw, Poland) A comparison of palindrome and pseudopalindrome cutters	11h00 m10.o3 Shinya Hosokawa (Hiroshima Institute of Technology, Japan) X-ray fluorescence holographic study on a single-crystal thin film of a rewritable optical media
	11h20 m4.o4 Akio Takenaka (Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, Japan) Duplex with non-WC pairings: Crystal structure of d(gcGAGGGAgc)	11h20 m10.o4 Richard Tyrrell (Rigaku Americas Corp., The Woodlands, Texas, USA) Phasing in the home laboratory
	11h40 m4.o5 Koen Robeyns (Department of Chemistry, Katholieke Universiteit Leuven, Leuven, Belgium) Cyclohexene Oligonucleotides: Structure of the L-CeNA sequence GTGTACAC	

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10.00-12.00	ENSOR ROOM	VAN EYCK ROOM
	<i>MS15: Quantified TEM for crystallography</i> Chair: Thomas Weirich, Co-chair: Jon Gjønnes	<i>MS27: Inclusion compounds and solvates</i> Chair: Luigi Nassimbeni, Co-chair: Ingeborg Csoeregh
	10h00 m15.o1 Douglas L. Dorset (ExxonMobil Research and Engineering CoEast, Annandale, New Jersey, USA) The role of electron diffraction in zeolite structure determination	10h00 m27.o1 Carl Henrik Görbitz (Department of Chemistry, University of Oslo, Norway) Crystal structures of hydrophobic dipeptides as hosts for organic solvent molecules
	10h30 m15.o2 Ute Kolb (Institute of Physical Chemistry, Johannes Gutenberg-University, Mainz, Germany) Quantified electron diffraction on pigments	10h30 m27.o2 Mátyás Czugler (Hungarian Academy of Sciences, Chemical Research Center, Hungary) Long distances, weak interactions?
	11h00 m15.o3 Ljubomira Ana Schmitt (Institute for Materials Science, Darmstadt University of Technology, Darmstadt, Germany) Investigation of the domain structure, size and orientation in lead zirconate titanate PZT ceramics by transmission electron microscopy	11h00 m27.o3 Leonard Barbour (Department of Chemistry, University of Stellenbosch, South Africa) Single crystal transformations
	11h20 m15.o4 Khalid Boulahya (Depto. de Química Inorgánica, Madrid, Spain) New one-dimensional phases in the Sr/Ca-Mn/Co-O system	11h20 m27.o4 Katharina Reichenbaecher (Departement of Chemistry and Biochemistry, University of Berne, Berne, Switzerland) Fluorinated phenoxysubstituted triazines as organic zeolites
	11h40 m15.o5 Wolfgang Neumann (Humboldt University of Berlin, Institute of Physics, Berlin, Germany) Computer assisted analysis of diffuse electron diffraction of precipitates in GaAs	11h40 m27.o5 Jacco van de Streek (Cambridge Crystallographic Data Centre, Cambridge, United Kingdom) Searching the Cambridge Structural Database for solvated vs. unsolvated pairs

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10.00-12.00	BREUGHEL ROOM	RUBENS ROOM
	<i>MS31: Advances in powder diffraction: microstructural aspects</i> Chair: Paolo Scardi, Co-chair: Nathalie Audebrand	<i>MS39: Natural and synthetic organic-inorganic systems.</i> Chair: Heinz Amenitsch, Co-chair: Riccardo Vivani
	10h00 m31.o1 Gábor Ribárik (Eötvös University Budapest, Budapest, Hungary) Microstructure of crystalline materials determined by whole powder pattern X-ray line profile analysis	10h00 m39.o1 Bruno Bujoli (Laboratoire de Synthèse Organique - University of Nantes, Nantes, France) Phosphonate-based hybrids: from structural aspects to biological applications
	10h30 m31.o2 Antonietta Guagliardi (Istituto di Cristallografia, IC - CNR, Bari, Italy) Whole Powder Pattern Methods for Nanoparticles characterization	10h30 m39.o2 Oskar Paris (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany) Plant tissues as hierarchical templates for inorganic nanomaterials
	11h00 m31.o3 Kristin Alice Schoenau (Institute for Materials Science, Darmstadt University of Technology, Darmstadt, Germany) Response of the ferroelectric domain structure of morphotropic PZT to the application of an electric field - in-situ Synchrotron X-ray diffraction	11h00 m39.o3 Gerald.A. Zickler (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany) Physisorbed films in periodic mesoporous silica studied by in-situ synchrotron small-angle diffraction
	11h20 m31.o4 Radomir Kužel (Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic) X-ray scattering study of crystallization of magnetron sputtered TiO ₂ thin films	11h20 m39.o4 Sergey V. Krivovichev (St.Petersburg State University, St.Petersburg, Russia) Charge density matching in organic-inorganic uranyl compounds
		11h40 m39.o5 Leonardo Marchese (Università del Piemonte Orientale, Alessandria, Italy) A combined single crystal X-ray diffraction and FTIR study of CAL-1 a novel microporous silico-aluminophosphate
12.00-13.30	LUNCH BREAK	

Tuesday, 8 august 2006 - afternoon

13.30-15.30	MAGRITTE ROOM	DELVAUX ROOM
	<i>MS3: Pipelining in macromolecular crystallography.</i> Chair: Colin Nave, Co-chair: Klaas Decanniere	<i>MS11: Molecular recognition in biomolecular systems.</i> Chair: Carl. H. Gorbitz, Co-chair: Stefano Mangani
	13h30 m3.o1 Robert M. Esnouf (Oxford Protein Production Facility and Division of Structural Biology, University of Oxford, Oxford, UK) An overview of informatics developments for managing target selection to x-ray data collection	13h30 m11.o1 Monika Mazik (Institut für Organische Chemie der Technischen Universität Braunschweig, Germany) Molecular recognition of carbohydrates with artificial receptors
	14h00 m3.o2 Santosh Panjikar (European Molecular Biology Laboratory, Hamburg, Germany) Auto-Rickshaw: An automated crystal structure determination pipeline as an efficient tool for fast validation of an X-ray diffraction experiment	14h00 m11.o2 Gunter Schneider (Karolinska Institutet, Stockholm, Sweden) Promiscuity in biosynthetic enzymes: structural basis for antibiotic diversity
	14h30 m3.o3 Martyn D. Winn (Computer Science and Engineering Department, CCLRC Daresbury Laboratory, UK) "MrBUMP: automated search model discovery and preparation for structure solution by molecular replacement"	14h30 m11.o3 Humberto Fernandes (Center for Biocrystallographic Research, Inst. of Bioorg. Chem., Pol. Acad. Sci., Poznan, Poland) Pathogenesis-related plant protein in complex with multiple hormone molecules
	14h50 m3.o4 Jawahar Swaminathan (European Bioinformatics Institute, Hinxton, United Kingdom) AutoDep 4.0: A web-based deposition and archival system	14h50 m11.o4 Petra Verdino (Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, USA) Antibodies: specificity and promiscuity of ligand recognition
	15h10 m3.o5 Judit É. Debreczeni (University of Oxford, Structural Genomics Consortium, Botnar Research Centre, Oxford, UK) Structural genomics on human kinases at SGC Oxford	15h10 m11.o5 Loes M.J. Kroon-Batenburg (Bijvoet Center for Biomolecular Research, Utrecht University, The Netherlands) Formation of amyloid fibres followed by X-ray diffraction in real time. Implications for the identity of bio-active species in conformational diseases like Alzheimer's disease

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13.30-15.30	ENSOR ROOM	VAN EYCK ROOM
	<i>MS14: Structure determination of modulated and aperiodic crystals.</i> Chair: Artem Abakumov, Co-chair: Michel Evain	<i>MS21: XAS: EXAFS and XANES</i> Chair: Caterina Rinaudo, Co-chair: Rik van Deun
	13h30 m14.o1 Ray L. Withers (Research School of Chemistry, Australian National University, Canberra, Australia) The use of electron diffraction for the structural characterization of modulated and aperiodic structures	13h30 m21.o1 Christoph Hennig (Forschungszentrum Rossendorf, Institute of Radiochemistry, Dresden, Germany) Structure analysis of actinide compounds in solution by X-ray absorption spectroscopy
	14h00 m14.o2 Sven Lidin (Stockholm University, Stockholm, Sweden) Modulations and order in Sb-Zn and related systems	14h00 m21.o2 Annibale Mottana (Università degli Studi Tre, Roma, Italy) Short- and long-range structure of crystals by XAFS spectroscopy
	14h30 m14.o3 Joke Hadermann (University of Antwerp, Belgium) Manganese oxide tunnel structures determined with TEM	14h30 m21.o3 Victor Ilyasov (Don State Technical University, Rostov-on-Don, Russia) Structural change wide-gap semiconductor in reconstructive phase transitions: AlN, BN and $B_xAl_{1-x}N$ solid solutions
	14h45 m14.o4 Thomas Richard Welberry , (Research School of Chemistry, Australian National University, Canberra, Australia) Deformed penrose tilings,	14h50 m21.o4 Alain Polian (Université P. et M. Curie, Paris, France) High pressure x-ray absorption study of $BaTiO_3$ and $SrTiO_3$ at the Ti K edge
	15h00 m14.o5 Michal Dusek (Institute of Physics, Praha, Czech Republic) Introduction to JANA2006	15h10 m21.o5 Juliana Manica (Universidade Federal do Paraná, Brazil) O 1s X-ray absorption spectra of Sr_2RuO_4 and $SrRuO_3$
	15h15 m14.o6 Alla Arakcheeva (Université de Lausanne, Institut de minéralogie et géochimie, Lausanne, Switzerland) Superspace embedding of sheelite-like structures	

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13.30-15.30	BREUGHEL ROOM	RUBENS ROOM
	<i>MS40: Battery and fuel cell materials</i> Chairs: Helmut Ehrenberg, Co-chair: Olivier Diat	<i>MS44: Neutron diffraction in structural chemistry</i> Chair: Alan Hewat, Co-chair: Paul Raithby
	13h30 m40.o1 Elena Arroyo y de Dompablo (Universidad Complutense, Madrid, Spain) High pressure materials as electrodes for lithium batteries: a computational and experimental approach	13h30 m44.o1 Trevor Forsyth (Institut Laue Langevin, Grenoble, France/ Keele University, UK) Neutron diffraction facilities for structural studies of crystals and fibres
	14h00 m40.o2 James A. Elliott (University of Cambridge, Cambridge, UK) Morphological insights into polymer electrolyte membranes from SAXS and maximum entropy	14h00 m44.o2 Juan Rodríguez-Carvajal (Institut Laue-Langevin, Grenoble, France) New opportunities for neutron diffraction in structural science
	14h30 m40.o3 Michele Catti (Università di Milano Bicocca, Milano, Italy) Lithium Ion Conducting $\text{Li}_{0.3}\text{La}_{0.567}\text{TiO}_3$ Perovskite: neutron diffraction study of the quenched form	14h30 m44.o3 Thomas F. Koetzle (Argonne National Laboratory, Argonne, IL USA) Topaz: A single-crystal diffractometer for the Spallation Neutron Source
	14h50 m40.o4 Natalia Bramnik (Darmstadt University of Technology, Darmstadt, Germany) Mechanism of lithium insertion-extraction in metallophosphates with olivine-like structure	14h50 m44.o4 Richard Welter (DECOMET lab., Université Louis Pasteur, Strasbourg, France) Incommensurate magnetic structure of PrPd_2Ge_2 from powder neutron diffraction
	15h10 m40.o5 Denis Pasero (The University of Sheffield, UK) Oxygen deficiency in lithium ion materials	15h10 m44.o5 Anatoliy Senyshyn (Institute of Material Science, Darmstadt University of Technology, Germany/Semiconductor Electronics Department, Lviv Polytechnic National University, Ukraine) Thermal expansion and atomic vibrations in CaWO_4 studied by neutron and synchrotron powder diffraction
17.00-18.00	AULA P. DE SOMER	AULA MAGNA
	P7 Dmitri Puschcharovsky (Moscow State University, Moscow, Russia) Elegant and Mysterious Structures of Minerals Chair: Massimo Nespolo	P8 Lee Brammer (University of Sheffield, Sheffield, UK) Halogen-mediated supramolecular chemistry in the solid state Chair: André Roodt