

Thursday, 10 august 2006 - morning

08.30-09.30	AULA P. DE SOMER	AULA MAGNA
	P13 Rolf Hilgenfeld (University of Lübeck, Lübeck, Germany) Structural and functional studies on SARS coronavirus - where does antiviral drug discovery stand three years after the (first) outbreak? Chair: Mariusz Jaskolski	P14 Israel Goldberg (Tel Aviv University, Israel) Crystal engineering of porphyrin network materials Chair: Giuseppe Filippini

09.30-10.00	COFFEE BREAK	
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10.00-12.00	MAGRITTE ROOM	DELVAUX ROOM
	<i>MS9: Structural enzymology.</i> Chair: Guy Dodson, Co-chair: Wim Versees	<i>MS18: Crystallography in art and archeological sciences</i> Chair: Jean Louis Hodeau
	10h00 m9.o1 Christopher Schofield (University of Oxford, Oxford, UK) Structures and mechanisms of human oxygenases	10h00 m18.o1 Loïc Bertrand (Heritage and archaeology liaison office, Synchrotron SOLEIL, Saint-Aubin Gif-sur-Yvette, France) Synchrotron X-ray diffraction for art history, archaeology and heritage conservation
	10h30 m9.o2 Bauke W. Dijkstra (University of Groningen, Groningen, The Netherlands) Degradation of halogenated compounds: structures and catalytic mechanisms of dehalogenases	10h30 m18.o2 Salvatore Siano (Institute of Applied Physics "Nello Carrara", National Research Council, Sesto Fiorentino, Italy) The use of time of flight neutron diffraction in bronze archaeometallurgy
	11h00 m9.o3 Victoria A. Money (University of York, York, UK) Substrate distortion by a lichenase highlights the different conformational itineraries harnessed by related glycoside hydrolases	11h00 m18.o3 Peter Paufler (Technische Universität Dresden, Dresden, Germany) Towards an understanding of Damascene blades
	11h20 m9.o4 Andrea Schmidt (European Molecular Biology Laboratory, Hamburg, Germany) Small molecules with big impact: fine static and dynamic detail in the atomic resolution structures of hydroxynitril lyase from <i>Hevea brasiliensis</i> give insight into mechanisms of ligand binding	
	11h40 m9.o5 Anette Henriksen (Biostructure Group, Carlsberg Laboratory, Valby, Denmark) Reaction mechanism of CCH type β -ketoacyl-ACP synthases	

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10.00-12.00	ENSOR ROOM	VAN EYCK ROOM
	<i>MS33: Advances in computational small molecule crystallography</i> Chair: Ton Spek, Co-chair: Gianluca Cascarano	<i>MS36: Crystallography under extreme conditions: state of the art</i> Chair: Alain Polian, Co-chair: Leonid Dubrovinsky
	10h00 m33.o1 Rob W.W. Hooft (Bruker AXS, Delft, The Netherlands) The Bayesian approach to absolute structure determination	10h00 m36.o1 Igor Goncharenko (Laboratoire Léon Brillouin C.E.A.-C.N.R.S., Gif-sur-Yvette, France) Magnetic and crystal structures probed by neutrons in 40 GPa pressure range
	10h30 m33.o2 Horst Puschmann (Durham University, Durham, UK) Automated structure determination	10h30 m36.o2 Mohamed Mezouar (European Synchrotron Radiation Facility, Grenoble France) Development of a new state-of-the-art beamline optimised for single crystal and powder X-ray diffraction under extreme conditions at the ESRF
	11h00 m33.o3 Gábor Oszlányi (Hungarian Academy of Sciences, Budapest, Hungary) How can we cope with negative scattering density?	11h00 m36.o3 Elena Boldyreva (Institute of Solid State Chemistry and Mechanochemistry SB RAS / REC-008, Novosibirsk State University, Novosibirsk, Russia) High-pressure studies of organic molecular crystals
	11h20 m33.o4 A. David Rae (The Australian National University, Canberra, Australia) Prototype structures and structure factor algebra as an aid to the refinement of problem structures	11h20 m36.o4 Gregory Kh. Rozenberg (Tel-Aviv University, Tel Aviv, Israel) Structural features related to pressure-induced electronic/magnetic phenomena in TM compounds
	11h40 m33.o5 Karl F. Fischer (Univ. of Saarbruecken, Germany) Structure determination without Fourier Inversion: a new concept	11h40 m36.o5 Giovanni R. Hearne (University of the Witwatersrand, Johannesburg-Gauteng, South Africa) High pressure response of nanophase materials

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10.00-12.00	BREUGHEL ROOM
	<i>MS42: Structure-property relationships in molecular crystals.</i> Chair: Chick Wilson, Co-chair: Leonard Barbour
	10h00 m42.o1 Luigi R Nassimbeni (University of Cape Town, South Africa) Molecular recognition and selectivity in organic clathrates
	10h30 m42.o2 Joel Bernstein (Ben-Gurion University of the Negev, Beer Sheva, Israel) Polymorphism and structure-property relations in molecular crystals
	11h00 m42.o3 Graeme M. Day (University of Cambridge, UK) Computational investigations of the influence of polymorphism on the lattice dynamics of molecular organic crystals
	11h20 m42.o4 Christophe M.L. Vande Velde (University of Antwerp, Antwerp, Belgium) The packing of methoxy-substituted distyryl-benzenes: questions and answers
	11h40 m42.o5 Dmitry Chernyshov (Swiss-Norwegian Beam Lines at the ESRF, France) A complex spin crossover scenario as seen by synchrotron diffraction and small angle neutron scattering

12.00-13.30	LUNCH BREAK
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Thursday, 10 august 2006 - afternoon

13.30-15.30	MAGRITTE ROOM	DELVAUX ROOM
	<i>MS8: Membrane proteins</i> Chair: Savvas Savvides, Co-chair: Piet Gros	<i>MS19: Phase transitions in inorganic and mineralogical materials.</i> Chair: Massimo Nespolo, Co-chair: Ulli Bismayer
	13h30 m8.o1 So Iwata (Imperial College London, UK) Towards structural determination of human membrane proteins	13h30 m19.o1 Ross J. Angel (Virginia Tech, Blacksburg, USA) New ideas about old chestnuts: phase transitions in Perovskites
	14h00 m8.o2 Maria Luisa Rodrigues (Universidade Nova de Lisboa, Oeiras, Portugal) Crystal structure of the membrane-bound complex cytochrome c nitrite reductase	14h00 m19.o2 Michele Catti (Università di Milano Bicocca, Milano, Italy) Ab initio simulations of pressure-driven phase transitions of silver halides
	14h30 m8.o3 Peter Palenčár (University of South Bohemia, Nové Hrad, Czech Republic) Refined structural model of photosystem II from <i>Thermosynechococcus elongatus</i> , structural changes in reaction centre	14h30 m19.o3 Olga Yakubovich (Moscow State Lomonosov University, Moscow, Russia) First row transition metal phosphates: novel structure types, morphotropic and homologous series, topological correlations
	14h50 m8.o4 David Cobessi (ESBS, Illkirch, France) Iron transport and signal transduction in <i>Pseudomonas aeruginosa</i> : crystal structures of the TonB-dependent outer membrane receptors FpvA and FptA	14h50 m19.o4 Yu.M. Smirnov (Tver State University, Russia) Symmetry in the crystal growth processes from the melt
	15h10 m8.o5 Carola Hunte (Max-Planck-Institute of Biophysics, Frankfurt, Germany) Structure of the Na^+/H^+ antiporter NhaA	15h10 m19.o5 Mois Ilia Aroyo (Universidad del Pais Vasco, Bilbao, Spain) Bilbao Crystallographic Server - new databases and computer tools

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13.30-15.30	ENSOR ROOM	VAN EYCK ROOM
	<i>MS34: New crystallographic software.</i> Chair: Rob Hooft, Co-chair: Louis Farrugia	<i>MS41: Structural coordination chemistry</i> Chair: Enrique Gutierrez-Puebla, Co-chair: Marie-Rose Spirelet
	13h30 m34.o1 Artem R. Oganov (ETH Zurich, Switzerland) Prediction of unknown crystal structures with evolutionary algorithms	13h30 m41.o1 Ernesto Carmona (Univesidad de Sevilla y Consejo Superior de Investigaciones Científicas, Sevilla, Spain) The structural diversity of zincocenes: half-sandwich, slipped-sandwich and Dimetallocenes structures
	14h00 m34.o2 Dylan Jayatilaka (University of Western Australia, Nedlands, Australia) CrystalExplorer: A tool for displaying Hirshfeld surfaces and visualising intermolecular interactions in molecular crystals	14h00 m41.o2 Yann Garcia (Université catholique de Louvain, Louvain-la-Neuve, Belgium) Tuning cooperative effects in azole based iron(II) spin crossover coordination polymers
	14h30 m34.o3 Chris Gilmore (University of Glasgow, UK) dSNAP: New software for analysing the results of Cambridge Data Base searches	14h30 m41.o3 Dominik Schaniel (Universität zu Köln, Köln, Germany) Photocrystallography with neutrons - Light-induced structural changes in $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NO}] \cdot 2\text{D}_2\text{O}$
	14h50 m34.o4 James A. Chisholm (Cambridge Crystallographic Data Centre, Cambridge, UK) New software for identifying hydrogen bond motifs	14h50 m41.o4 Richard Welter (Université Louis Pasteur Strasbourg, France / I.P.C.M.S., CNRS-ULP, Groupe des Matériaux Inorganiques, Strasbourg, France) Very strong ferromagnetic interaction in a new asymmetrical binuclear μ -methoxo-bridged Mn(III) complex
	15h10 m34.o5 Xinyi Xian (Utrecht University, Utrecht, the Netherlands) Eval15: accurate data integration by profile prediction	15h10 m41.o5 Ekkehart Tillmanns (Univ. Wien, Vienna, Austria) New compounds of L-Alanine with inorganic materials

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13.30-15.30	BREUGHEL ROOM
	<i>MS45: Communicating and educating crystallography</i> Chair: Paola Spadon, Co-chair: Gervais Chapuis
	13h30 m45.o1 Ivan Orlov (Ecole Polytechnique Federale de Lausanne, Switzerland) Superspace playground: on-line toys for aperiodic crystallographer
	14h00 m45.o2 Marco Milanese (Univ. Piemonte Orientale, Alessandria, Italy) Teaching three-dimensionality and quantum chemistry by a concerted use of structural databases and of computational and molecular graphic tools
	14h30 m45.o3 A. Hunter (Youngstown State University, Youngstown OH, U.S.A.) The STaRBURSTT - CyberInstrumentation Consortium - CyberEnabled Crystallographic Education
	14h50 m45.o4 Gordon Barr (University of Glasgow, UK) Promoting science through art - the Chem-moo-stry Project
	15h10 m45.o5 Simon Coles (University of Southampton, UK) eCrystals: A route for open access to small molecule crystal structure data

17.00-18.00	AULA P. DE SOMER	AULA MAGNA
	P15 Maria Arménia Carrondo (Universidade Nova de Lisboa, Oeiras, Portugal) Structural insights into the RNA degradation mechanism Chair: Martino Bolognesi	P16 Paul Van Houtte (Katholieke Universiteit Leuven, Belgium) Measurement and modelling of residual stresses and texture in aluminium interconnects in micro-electronic devices Chair: Hartmut Fuess