

Programme for High Pressure Crystallography etc. (version June 03, 2009)

Erice, Italy: June 4 (arrival day) to June 14 (departure day), 2009

	June 5, Friday	June 6, Saturday	June 7, Sunday	June 8, Monday	June 9, Tuesday	June 10, Wednesday	June 11, Thursday	June 12, Friday	June 13, Saturday
8.45	Paola Spadon Welcome								
9.00 – 9.45	Przemek Dera Introduction to high pressure science	Tiziana Boffa-Ballaran Compressibility, EOS – applications in geosciences	Florent Occelli Hydrogen and hydrides at very high pressure. New approaches and recent results	Sandro Scandolo First-principles molecular dynamics and applications in planetary science	Moshe Paz-Pasternak Crystallographic Structural Responses to Pressure Induced Electronic-Magnetic Transitions	Andrzej Katrusiak Phase transitions in hydrogen-bonded organic crystal	Elena Boldyreva High-pressure studies of pharmaceuticals & biomimetics. Fundamentals and applications. A general introduction	Roland Winter - Exploring the “Landscape” of Biomolecules under Extreme HP Conditions: From Lipid Membranes to Proteins	Andrea Gauzzi High Pressure & superconductivity: intercalated graphite CaC ₆ as a model system
9.45 – 10.30	Moshe Paz-Pasternak Diamond anvil cell: principles of operation and most modern trends	Robert T. Downs Compression systematics in minerals	Mario Santoro Carbon dioxide at high pressure	Artem Oganov Theoretical prediction of HP structures	Denis Kozlenko Physical phenomena in strongly correlated magnetic oxides: lessons from neutron diffraction at H.P.	Bjorn Winkler Experimental and modelling studies of the role of hydrogen bonding in minerals at high pressure	Francesca Fabbiani New frontiers in physical form discovery: high-pressure recrystallization of pharmaceuticals & other molecular compounds	Roger Fourme HP crystallography of biomolecules. Technical aspects	Vladimir Solozhenko High-pressure synthesis of novel superhard phases in the B-C-N-O system
10.30	Coffee	Coffee	Coffee	Coffee	Coffee	Coffee	Coffee	Coffee	Coffee
11.00 – 11.45	Przemek Dera All different flavors of synchrotron x-ray diffraction at high pressure	Elena Boldyreva Anisotropic compression. What can it teach us about intermolecular interactions?	Alain Polian Boron and Boron-rich solids at high pressures	Piero Macchi Semi-empirical & <i>ab initio</i> quantum chemistry description of solid state phases under HP: Chemical applications	Paul McMillan HP synthesis of advanced materials	Nicola Casati The effect of high pressure on intramolecular geometry	Paulo Freire Pressure-induced phase transitions in crystalline amino acids. Raman spectroscopy and X-ray diffraction	Roger Fourme HP crystallography of biomolecules. Recent achievements	Natalia Dubrovinskaia Structure-properties relationship in novel HP materials
11.45 – 12.30	Mohamed Mezouar Synchrotron high-pressure high/low temperature techniques	Andrzej Katrusiak Structural studies of phases crystallized at HP as a tool of understanding intermolecular interactions	Crystelle Sanloup Amorphous materials at high pressure	Igor Abrikosov First principles simulations of alloy thermodynamics in megabar pressure ranges	Yanbin Wang Elasticity, plasticity and rheology of materials	Fernando Rodriguez Jahn-Teller systems at high pressure	EXC 2	Sebastien Merkel Experimental study of plastic properties of minerals under pressure	Bjorn Winkler Synthesis and structure-property relations of binary metal carbides studied in laser heated diamond anvil cells and with density functional theory calculations
12.30 – 14:00	Lunch on site	Lunch while “watching” Poster Session 1	Lunch on site	Lunch during EXCURSION 1	Lunch while “watching” Poster Session 2	Lunch on site	Lunch during EXCURSION 2	Lunch on site	Lunch on site

14:00 – 14.45	Anatoly Balagurov Present day high-intensity and high-resolution neutron diffraction and neutron scattering at high pressure	Vladimir Dmitriev General introduction into the theory of phase transitions	Paul McMillan X-ray diffraction of polyamorphic materials and amyloid fibrils at high pressure	Short boat trip. Extensive walk Mothia Island, Phoenician Archaeology or (free choice) Trapani beach	Jens Kreisel Effect of high-pressure on functional dielectric perovskite-type oxides	Jennifer Jackson Phase transitions in the deep Earth: Relationship with seismic observations	EXC 2 to Selinunte + Segesta, greek archaeology, or (free choice) S Vito lo Capo beach	Leonid Dubrovinsky Effect of spin transitions in iron on structure and properties of Mantle minerals	Alfonso San Miguel Raman spectroscopy at high pressure : carbon nanotubes
14:45 – 15:30	Jennifer Jackson Synchrotron- based spectroscopic techniques: Mossbauer and high-resolution inelastic scattering	Heidrun Sowa Phase transitions in AB systems. Symmetry aspects	15.00:16.30 S Rocco Lecture Hall A round-table discussion (4): Processing diffraction data collected in the DAC Leaders / short presenters: Nicola Casati, Andrzej Katrusiak, Diego Gatta, Przemek Dera, Francesca Fabbiani Any other contributors are welcome!	EXC 1	J.-P. Itie Local aspects of high-pressure transitions in ferroelectrics. X-ray absorption spectroscopy	Olga Degtyareva Simple metals at high pressure	EXC 2	John Loveday Neutron diffraction: Current state of the art and future challenges	Colin Pulham High-pressure studies of energetic materials
15.30 – 16.00	Coffee	Coffee	16.30: 17.00 Coffee at S Rocco Breakfast room	EXC 1	Coffee.	Coffee	EXC 2	Coffee	Coffee
16.00 – 16.45	Leonid Dubrovinsky Measurements of electrical resistivity at high pressures	Yaroslav Filinchuk Light metal hydrides under non-ambient conditions: probing chemistry by diffraction?	17.00: 17.45 S. Rocco Lecture Hall Short presentations of posters for the two Poster Sessions	EXC I	Yanbin Wang Large volume press techniques	Giovanni Hearne Nanomaterials at high pressures. Spectroscopy and diffraction techniques	EXC 2	Diego Gatta Microporous materials at high-pressure: are they really soft?	John Parise Analysis of the total scattering using the quantitative HP pair distribution function: I. Practical considerations
17.00 – 18.00	Introduction into Workshops	Follow-Me Workshop 2: Structure solution from powder diffraction data (S Domenico, 17.00 :18.15)		EXC I	Follow-Me Workshop 5: Quantum-mechanical calculations on molecular solids (S Domenico, 17.00 :18.15)	Workshop 7: Getting the texture information from a 2D dataset; strain analysis Leader: to be announced	EXC 2	Lecture on the effect of Mafia in Sicily	Lars Ehm Analysis of the total scattering using the quantitative HP pair distribution function: II. Case studies (17.00:17.45)
18.00 – 19.00	Follow-Me Workshop 1: DAC handling, HP crystallization (S Domenico)	Follow-Me Workshop 3: EOS calculations (S Domenico, 18.15:19.30)	Poster session 1 in San Francesco Court	Return to Erice at 19 00	Follow-Me Workshop 6: Ab initio crystal structure prediction (S Francesco, 18.30 :19.45)	Poster Session 2 in San Francesco Court	EXC 2	(start at 17.30) Special lecture: W. Grochala The Chemical Imagination at Work in Very Tight Places (MO approach to interpret HP phenomena)	<i>Closing remarks</i>
	Hands-On Supplement to Workshop 2: (Madonna room, 18.15:19.30)	Hands-on Supplement to Workshop 3: (Madonna room, 18.15:19.30)							
20.00	Welcome Buffet Dinner+Folk Show (at S. Francesco)	Dinner	Pasta party (at S. Francesco)	Dinner	Dinner	Pizza party (at S. Francesco)	Dinner in front of the Segesta Temple	Dinner	Good-Bye Buffet Dinner