Program

4th Joint AIC - SILS Conference

TRIESTE, 12-15 SEPTEMBER 2022

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Tuesday 13th September 2022

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - Ground Floor - Main Lecture Hall

Plenary Lecture		**Chair:Simona Galli** - University of Insubria, Como
PL-2 - **Simon Parsons** - University of Edinburgh - UK	08:45 - 09:45	High pressure phase transitions in molecular crystals
Coffee Break - Building C11 - Ground Floor - Atrium	09:45 - 10:15	

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1

MS-01 Modern Integrative Structural Biology		**Chairs:Stefano Mangani** - University of Siena, **Beatrice Vallone** - University of Roma "La Sapienza", Roma
KNL-1 **Marina Mapelli** - European Institute of Oncology, Milano	10:15 - 10:45	Molecular crosstalk between fate determination and orientation in epithelial cell divisions
KNL-2 **Antonio Chaves-Sanjuan** - University of Milano	10:45 - 11:15	Structural characterization of a post-mortem amyloid fibril from a cat kidney
O-1 **Sonia Covaceuszach** - Institute of Crystallography CNR, Trieste	11:15 - 11:30	Insights on the structural determinants of proBDNF V66M variant, a modifier in neuropsychiatric disorders severity
O-2 **Benny Danilo Belviso** - Institute of Crystallography CNR, Bari	11:30 - 11:45	C-terminus of the histone-lysine N-methyltransferase NSD3 characterized by small-angle X-ray scattering
O-3 **Emiliano De Santis** - University of Uppsala - SE	11:45 - 12:00	Directional explosion. A hybrid simulation study
F-1 **Cecilia Pozzi** - University of Siena	12:00 - 12:05	Structural insights into the hYAP-hTEAD4 protein-protein interaction: an emerging target in cancer treatment
F-2 **Roberto Marotta** - Italian Institute of Technology, Genova	12:05 - 12:10	Unravelling the regulation pathway of photosynthetic AB-GAPDH
F-3 **Francesca Paoletti** - National Chemistry Institute, Ljubljana - SLO	12:10 - 12:15	Landscape of the ATP binding to neurotrophins: effects on conformation and dynamic modulation by divalent cations
Commercial Presentations Session I - Building C11 - III Floor - Lecture Hall A1		**Chair:Alberto Cassetta** - Institute of Crystallography CNR, Trieste
S-1 **Andrea Pigozzo** - Alfatest Srl, Roma	12:15 - 12:45	Pushing the boundaries in biomolecular stability and interaction analysis with GCI and MicroCal
S-2 **Max Maletta** - Thermo Fisher Scientific, Eindhoven - NL	12:45 - 13:15	Peeping into the cell with Cryo-Electron Tomography
e-Poster Session I & Commercial Exhibit I - Building C11 - III Floor - Atrium	12:15 - 13-15	
Buffet Lunch - Building C11 - Ground Floor - Atrium	13:15 - 14:15	

University of Trieste - Department of Chemical and Pharmaceutical Sciences - Building C11 - III Floor - Lecture Hall A1

MS-04 Frontiers in Mineralogy and Inorganic Geochemistry		**Chairs:Donato Belmonte** - University of Genova, **Gabriele Giuli** - University of Camerino
KNL-1 **Paolo Lotti** - University of Milano	14:30 - 15:00	Crystal chemistry of natural REE-phosphates and arsenates and their (T,P)-behavior
KNL-2 **Nicola Campomenosi** - University of Hamburg - DE	15:00 - 15:29	Elastic vs. visco-plastic rheology of stressed host-inclusion mineral systems at non-ambient conditions: insights from in situ Raman spectroscopy
O-1 **Mattia La Fortezza** - University of Genova	15:29 - 15:43	Ab initio thermodynamics of $MgSiO_3$ protoenstatite at high temperatures conditions
O-3 **Sabrina Nazzareni** - University of Perugia	15:43 - 15:57	High pressure single-crystal synchrotron XR diffraction of natural pyrochlores
O-2 **Simone Pollastri** - Elettra-Sincrotrone Trieste, Trieste	15:57 - 16:11	Characterization of bottom ashes from incineration process by means of XRF mapping and XANES spectroscopy
O-4 **Sirio Consani** - University of Pisa	16:11 - 16:25	The Cu-Fe-Ni-Co sulphide ore deposits of theMonte Ramazzo-Lagoscuro mines
F-1 **Francesca Menescardi** - University of Genova	16:25 - 16:30	Molecular dynamics strategies to determine the melting curve of CaO
Coffee Break - Building C11 - Ground Floor - Atrium	16:30 - 17:00	
ePoster Session II & Commercial Exhibit II - Building C11 - III Floor - Atrium	17:00 - 18:00	
AIC General Assembly - Building C11 - Ground Floor - Main Lecture Hall	18:00 - 20:00	

Crystal Chemistry of Natural REE-Phosphates and Arsenates and their (*T*,*P*)-Behavior

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Rare Earth Elements (REE, i.e. lanthanides, Y and Sc) are nowadays fundamental components in many technological applications. For their strategic importance and supply risk, REE have been included in the EU list of the so-called "critical raw materials" [1]. This has recently fostered the study of REE minerals, aiming at a deeper understanding of their crystal chemistry, formation and accumulation processes. This contribution focusses on the crystal-chemical features and (*T*,*P*)-behavior of REE phosphates and arsenates from Mt. Cervandone (Western Alps, Italy), where REE minerals are common constituents of Alpine quartz-bearing hydrothermal veins, cross-cutting pegmatitic dykes intruded in leucocratic gneisses of the metamorphic basement.

The mineral species under study are the isostructural monazite-(Ce) (ideally $CePO_4$) and gasparite-(Ce) ($CeAsO_4$), Sp. Gr. $P2_1/n$, hosting the larger Light REE, and the isostructural xenotime-(Y) (YPO_4) and chernovite-(Y) ($YAsO_4$), Sp. Gr. $I4_1/amd$, hosting the larger Heavy REE. They define two solid solutions characterized by the monoclinic monazite-type and the tetragonal zircon-type structures, respectively. Chemical data obatined by WDS electron microprobe analysis show that an almost complete solid solution occurs along the xenotime-chernovite tetragonal series, with Y being the dominant cation in the 8-coordinated A site followed by the HREE, whereas a strong depletion in LREE is observed. The latters populate the 9-coordinated A site in the monoclinic structure of monazite and gasparite, for which an apparent miscibility gap is observed among the end members, differently to what observed in samples from other localities [2]. Single-crystal XRD analyses on samples with different crystal chemistry pointed out the prevailing control exerted by the composition of the tetrahedra (P *vs*. As) on the size and disortion of the structural units and, in turn, of the unit cell volume, independently from the REE composion of the A site. *In situ* single-crystal and powder synchrotron XRD esperiments have been performed at high-*T* (Elettra, Trieste), high-*P* (ESRF, Grenoble; PETRA-III, Hamburg) and combined H*PH*T (PETRA). The interplay among the crystal chemical and structural features control the bulk response of the investigated $REETO_4$ phases to external thermal and compressional stimuli. The results showed that the monazite-type structure is more compressibile and expandable than the tetragonal zircon-type, whereas, among the zircon-type minerals, chernovite is more compressibile than xenotime, but at high temperature xenotime shows the higher thermal expansion coefficient. *In situ* H*PH*T XRD experiments have been performed for the first time on monazite and chernovite: monazite was found to be stable within the investigated range (T < 500 °C and P < 20 GPa), whereas chernovite, which at ambient-*T* undergoes a phase transition to a scheelite-type polymorph at P > 8-12 GPa, at $250 \leq T$ (°C) ≤ 500 preserves the zircon-type tetragonal structure at P < 20 GPa, even though with signs of structural destabilization above 12-15 GPa. A comparison with the thermo-elastic parameters reported in the literature for synthetic end members (see e.g. [2,3]) suggests that further studies on complex multi-component natural solid solutions are needed for a thorough comprehension of the structure-related properties in these minerals.

[1] G.A. Blengini, F. Mathieux, L. Mancini, M. Nyberg, H.M. Viegas *Study on the EU's list of Critical Raw Materials. Executive Summary.* Publication Office of the European Commission, Luxembourg, **2020**.
[2] F. Pagliaro, P. Lotti, A. Guastoni, N. Rotiroti, T. Battiston, G.D. Gatta, *Mineral. Mag.* **2022**, *86*, 150.
[3] D. Errandonea *Phys. Status Solidi B.* **2017**, *254*, 1700016.