

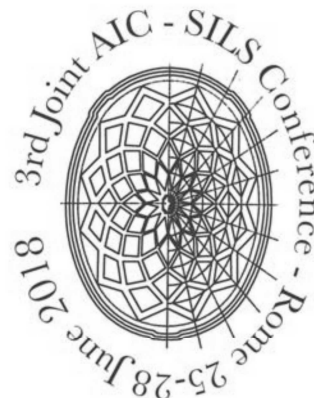
3rd Joint AIC-SILS Conference

Rome 25-28 June 2018



SILS

Programme and Book of Abstracts



Summary

Committees	pag.	3
Sponsor	pag.	4
Conference Schedule	pag.	5
Abstract	pag.	13
Awards	pag.	13
Plenary lectures	pag.	18
MS1-Biocrystallography in Medical and Pharmaceutical Research	pag.	22
MS2-Inorganic & Organic Functional Materials	pag.	28
MS3-Crystal-chemical behaviour in Mineralogy and Materials Science	pag.	34
MS4-Methodological and experimental developments in crystallography and synchrotron techniques, <i>in memory of Davide Viterbo</i>	pag.	40
MS5-Contemporary challenges in Structural Biology: Cryo-EM and Integrative Approaches to understand complex molecular architectures	pag.	46
MS6-Epitaxial Crystal Growth at the Nanoscale	pag.	52
MS7-Workshop SILS: Spectroscopy & Scattering with Synchrotron Radiation and FELs	pag.	59
MS8-Crystallography and Drug Design	pag.	66
MS9-Polycrystalline & Nano Materials	pag.	73
MS10-Crystallography and Cultural heritage: Science and Passion	pag.	79
MS11- <i>In situ</i> and <i>operando</i> investigations on materials synthesis and functional behaviour	pag.	85
Software Fayre	pag.	92
Commercial presentations	pag.	102
Posters	pag	106
Posters (P) and Digital Posters (e-P) Session 1: MS1 – MS4	pag	106
Posters (P) and Digital Posters (e-P) Session 2: MS5 - MS11	pag.	158

COMMITTEES

Organizing Committee

Francesco Capitelli
(CNR-IC)
Adele Di Matteo
(CNR-IBPM)
Giorgio Giardina
(U. Sapienza, Roma)
Annalisa Guerri
(U. Firenze)
Simona Galli
(U. Insubria)
Andrea Ienco
(CNR-ICCOM)
Andrea Ilari
(CNR-IBPM)
Doriano Lamba
(CNR-IC)
Roberta Montanari
(CNR-IC)
Giorgio Pochetti
(CNR-IC)
Carmelinda Savino
(CNR-IBPM)
Beatrice Vallone
(U. Sapienza, Roma)
Giuseppe Zanotti
(AIC past President, U. Padova)

Scientific Committee

Giuliana Aquilanti
(Elettra, Trieste)
Rossella Arletti
(U. Torino)
Gilberto Artioli
(U. Padova)
Federico Boscherini
(U. Bologna)
Michela Brunelli
(ESRF, Grenoble, Fr)
Paola D'Angelo
(U. Sapienza, Roma)
Andrea Di Cicco
(U. Camerino)
Adele Di Matteo
(CNR-IBPM)
Federico Forneris
(U. Pavia)
Cinzia Giannini
(CNR-IC)
Giorgio Giardina
(U. Sapienza, Roma)
Gabriele Giuli
(U. Camerino)
Silvia Gross
(U. Padova)
Andrea Ilari
(CNR-IBPM)
Doriano Lamba
(CNR-IC)
Chiara Massera
(U. Parma)
Adriana Erica Miele
(U. Lione, Fr)
Sabrina Nazzareni
(U. Perugia)
Luca Palin
(U. Piemonte Orientale)
Maurizio Polentarutti (Elettra,
Trieste)
Menico Rizzi
(U. Piemonte Orientale)
Rosanna Rizzi
(CNR-IC)
Stefano Sanguinetti
(U. Milano Bicocca)
Michele Saviano
(CNR-IC)
Carmelinda Savino
(CNR-IBPM)
Paolo Swuec
(U. Milano)
Beatrice Vallone

(U. Sapienza, Roma)

Franco Zanini
(Elettra, Trieste)

Steering Committee

Diego Gatta
(AIC President, U. Milano)
Andrea Di Cicco
(SILS President, U. Camerino)
Giuseppe Zanotti
(U. Padova)
Michele Saviano
(CNR-IC)
Simona Galli
(U. Insubria)
Annalisa Guerri
(U. Firenze)
Andrea Ienco
(CNR-ICCOM)
Gilberto Artioli
(U. Padova)
Norberto Masciocchi
(U. Insubria)
Angela Altomare
(CNR-IC)
Consiglia Tedesco
(U. Salerno)
Michele Zema
(U. Pavia)
Antonietta Guagliardi
(CNR-IC)
Andrea Zappettini
(CNR-IMEM)
Marco Milanesio
(U. Piemonte Orientale)
Massimo Ferrario
(INFN, Frascati)
Beatrice Vallone
(U. Sapienza, Roma)
Cinzia Giannini
(CNR-IC)
Sakura Pascarella
(ESRF, Grenoble, Fr)
Rossella Arletti
(U. Torino)
Silvia Gross
(U. Padova)

MS3 – e-P8: High-pressure and high-temperature behaviors of intermediate scapolite by in situ synchrotron X-ray diffraction

Paolo Lotti,^a Davide Comboni^a, Lara Gigli^b, Marco Merlini^a, G. Diego Gatta^a, Hannes Krüger^c

^a*Dipartimento di Scienze della Terra, Università degli Studi di Milano, Milano, Italy*

^b*Elettra Sincrotrone Trieste S.c.P.A., Basovizza, Trieste, Italy.*

^c*Institut für Mineralogie und Petrographie, Universität Innsbruck, Innsbruck, Austria
paolo.lotti@unimi.it*

Scapolites represent a complex solid solution of volatiles-bearing aluminosilicate minerals common in metamorphic environments, from the hydrothermal to the granulite facies conditions. The three end members of the solid solution are: marialite ($\text{Na}_4\text{Al}_3\text{Si}_9\text{O}_{24}\text{Cl}$), meionite ($\text{Ca}_4\text{Al}_6\text{Si}_6\text{O}_{24}\text{CO}_3$) and silvialite ($\text{Ca}_4\text{Al}_6\text{Si}_6\text{O}_{24}\text{SO}_4$). Scapolites usually form for the reaction of plagioclase with salts-bearing metamorphic fluids at non-ambient pressure and temperature and, therefore, may act as reservoirs for volatiles down to the lower crust [1], or induce fluids release if destabilized [2]. To understand and predict the relative stability of a scapolite of a given crystal chemistry in a mineral assemblage at metamorphic conditions, it is crucial to determine the thermo-elastic constants across the solid-solution members, as well as the crystal structure response to varying pressure and temperature. In this light, we have investigated the high- P (at ambient- T) and high- T (at ambient- P) behaviors of a natural sample of scapolite, chemical formula $(\text{Na}_{1.86}\text{Ca}_{1.86}\text{K}_{0.23}\text{Fe}_{0.01})(\text{Al}_{4.36}\text{Si}_{7.64})\text{O}_{24}[\text{Cl}_{0.48}(\text{CO}_3)_{0.48}(\text{SO}_4)_{0.01}]$ intermediate between the end members marialite and meionite, by means of in situ single-crystal and powder X-ray diffraction, using both conventional and synchrotron X-ray sources.

At high pressure, the investigated scapolite undergoes a phase transition, between 9.23 and 9.87 GPa, from the tetragonal $I4/m$ space group (stable at room conditions) toward a triclinic polymorph, characterized by a highly distorted tetrahedral framework. The elastic behavior of the tetragonal scapolite has been described by fitting the experimental V - P data to a III-order Birch-Murnaghan equation of state, which provided a refined $K_{V0} = 70(2)$ GPa ($\beta_{V0} = 0.0143(4)$ GPa⁻¹) and $K_{V'} = 4.8(7)$. A comparison with the refined bulk moduli reported in the literature for three further members belonging to the marialite-meionite joint [3,4], allows to define, at a first approximation, a chemical dependence of the scapolite bulk modulus: K_{V0} (GPa) = 53(2) + 0.45(4)*(%Me), where %Me = 100*[M²⁺/(M⁺ + M²⁺)], M = Na⁺, Ca²⁺, K⁺... An anomalous compressibility along the [001] axis and a change in the structure deformation mechanisms at the atomic scale suggest a destabilization at $P > 3$ GPa (at ambient- T).

Preliminary analysis of the high- T experimental data revealed a dramatic anisotropy of the thermal expansion, which is only accommodated within the ($hk0$) plane, whereas for the c unit-cell parameter no T -induced deviations from the ambient value are observed within the experimental uncertainty, in agreement with what previously reported for other scapolite solid solution members [5,6].

[1] J. Hammerli, A.I.S. Kemp, N. Barrett, B.A. Wing, M. Roberts, R.J. Arculus, P. Boivin, P.M. Nade, K. Rankenburg *Chem. Geol.* **2017**, 454, 54-66.

[2] J.K. Porter, H. Austrheim *Terra Nova* **2017**, 29, 29-35.

[3] R.M. Hazen, Z.D. Sharp *Am. Mineral.* **1988**, 73, 1120-1122.

[4] P. Comodi, M. Mellini, P.F. Zanazzi *Eur. J. Mineral.* **1990**, 2, 195-202.

[5] G. Graziani, S. Lucchesi *Am. Mineral.* **1982**, 67, 1229-1241.

[6] J. Baker *Am. Mineral.* **1994**, 79, 878-884.