https://doi.org/10.3301/ABSGI.2022.02

Torino 19-21 September 2022



a cura della Società Geologica Italiana



GEOSCIENCES FOR A SUSTAINABLE FUTURE







ThermoFisher





PRESIDENTS OF THE CONGRESS

Rodolfo Carosi and Daniele Castelli.

SCIENTIFIC COMMITTEE

Germana Barone, Fabrizio Berra, Matteo Berti, Fernando Camara, Piergulio Cappelletti, Claudio Chiarabba, Rita Chirico, Renato Colucci, Chiara D'Ambrogi, Rosanna De Rosa, Laura De Santis, Daniela Ducci, Patrizia Fumagalli, Biagio Giaccio, Fausto Guzzetti, Giulia Innamorati, Ilaria Mazzini, Mimmo Palano, Claudia Piromallo, Mario Soldati, Stefania Venturi, Andrea Zanchi.

ORGANISING COMMITTEE

Donato Belmonte, Sabrina Bonetto, Bernardo Carmina, Francesco Dela Pierre, Evdokia Tema, Lorenza Fascio, Salvatore Iaccarino, Andrea Maffeis, Nadia Malaspina, Chiara Montomoli, Marcello Natalicchio, Alessandro Petroccia, Fabio Massimo Petti, Fabrizio Piana, Franco Rolfo, Licia Santoro, Mario Tribaudino, Alessandro Zuccari.

ABSTRACT BOOK EDITORS

Bernardo Carmina, Lorenza Fascio, Giulia Innamorati, Marco Pasero & Fabio Massimo Petti.

COVER IMAGE:

Aerial cityscape image of Turin during sunset.

Papers, data, figures, maps and any other material published are covered by the copyright own by the **Società Geologica** Italiana.

DISCLAIMER: The Società Geologica Italiana, the Editors are not responsible for the ideas, opinions, and contents of the papers published; the authors of each paper are responsible for the ideas opinions and contents published.

La Società Geologica Italiana, i curatori scientifici non sono responsabili delle opinioni espresse e delle affermazioni pubblicate negli articoli: l'autore/i è/sono il/i solo/i responsabile/i.

Effect of the crystal chemistry on the structural and thermo-elastic properties of natural REE-arsenates and phosphates

Pagliaro F.*1, Lotti P.1, Comboni D.2, Fumagalli P.1, Battiston T.1, Guastoni A.3, Rotiroti N.1 & Gatta G.D.1

¹ Dipartimento di Scienze della Terra "A. Desio", Università di Milano. ² ESRF, Grenoble (France). ³ Dipartimento di Geoscienze, Università di Padova.

Corresponding author e-mail: francesco.pagliaro@unimi.it

Keywords: REE, XRD, synchrotron.

The wide group of ATO_4 minerals (A = Sc, Y, Ln, U and Th, whereas T stands for tetrahedrally-coordinated cations as P, As and minor Si), includes the important REE-bearing minerals xenotime-(Y) (nominally YPO₄) and monazite-(Ce) (nominally CePO₄), as well as the rare REE-arsenates chernovite-(Y) (nominally YASO₄) and gasparite-(Ce) (nominally CeAsO₄). The Y- and HREE-rich chernovite-(Y) and xenotime-(Y) share the same zircon-type structure (space group $I4_1/amd$), while gasparite-(Ce) and monazite-(Ce) represent the LREE-rich ATO_4 minerals, crystallizing in the monoclinic monazite-type structure (space group $P2_1/n$). The renowned REE-bearing site of Mount Cervandone (Lepontine Alps, Italy), has been chosen as a case-study: all the above-mentioned minerals occur in hydrothermal quartz veins crosscutting previously metamorphosed pegmatitic dykes. The present study focuses on 1) the chemical composition of the selected minerals, 2) the role played by crystal chemistry on the structural and thermo-elastic features, and 3) the structural response to T and P stimuli, including the occurrence of phase transitions.

A chemical and structural characterization has been performed via EPMA-WDS, Raman spectroscopy and single-crystal X-ray diffraction analysis. Chemical data showed that the zircon-structured minerals chernovite-(Y) and xenotime-(Y) are characterized by a very similar (Y,HREE) composition and the same conclusion can be drawn for the LREE content of the two monazite-type minerals. An almost complete solid solution has been found between xenotime-(Y) and chernovite-(Y), while a wide miscibility gap has been observed within the monazite series minerals of Mt. Cervandone. Despite strong similarities in the composition of the REE-site within the zircon- and monazite-type series, respectively, isostructural phosphate and arsenate differ in some structural features. In particular, both the unit-cell and the REE-coordination polyhedron volumes are strongly controlled by the cationic population at the T-site: an increase in As not only expands the volume of the TO₄ tetrahedron, but even that of the REE-polyhedron, irrespective of the A-site population. A comparative analysis of the thermo-elastic behavior of selected minerals has been conducted, by in situ high-P, high-T and combined HPHT X-ray diffraction experiments using conventional and synchrotron facilities. The non-ambient data confirm the central role played by the T-site in controlling the structural deformation and, consequently, the bulk thermal expansion and compressibility. In conclusion, zircon-type structure has been found to be always less compressible than monazite-type counterparts, while, within each structural type, phosphates are systematically less compressible than arsenates. The occurrence of P-induced phase transitions in both chernovite-(Y) and xenotime-(Y) leads to a larger HP stability field of phosphates if compared to arsenates with a zircon-type structure.