

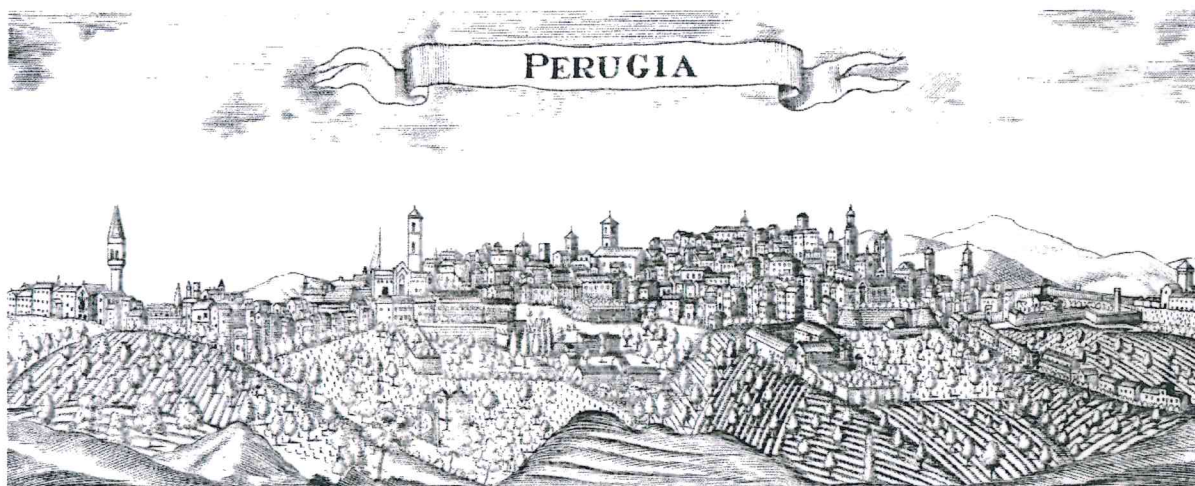
Abstracts and Programme Book



**Italian
Crystallographic
Association**

XLVI Annual Meeting

**Perugia, Palazzo Murena
June 26-29, 2017**



1967 - 2017

WELCOME

The Italian Crystallographic Association (AIC) is pleased to welcome you to the XLVI annual meeting in Perugia, hosted by the Università degli Studi of Perugia. The conference is located in Palazzo Murena, venue of the University, located in the historic center of Perugia.

AIC is celebrating its 50th anniversary shortly after hundred years from the discovery of X-ray diffraction by crystals by Laue and the Bragg's.

In 1967 the foundation assembly of the Italian Crystallographic Association, held in Roma and attended by 108 crystallographers, approved the statute and elected the first Executive Council.

The first Congress and general Assembly of AIC were held from 11 to 13 January 1968 in Perugia and the venue was Palazzo Murena

The meeting is organized with a multidisciplinary approach, covering a wide range of subjects from biocrystallography to mineralogy, from crystal growth to materials science and crystallographic methods; the program encourages the discussion on emerging methods in crystallography, opening new fields for the investigation of the condensed matter world.

We gratefully acknowledge the many ideas in continuous efforts provided by all colleagues of the committees. Finally, we express our gratitude to all institutions and companies who financially supported the meeting.

Giuseppe Zanotti - AIC President

Maria Cristina Burla - Chair of the Organizing Committee

Organized by:

Department of Physics and Geology

Department of Pharmaceutical Sciences

Department of Chemistry, Biology and Biotechnology

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9 P6: The natural borate colemanite at non-ambient conditions: behavior at low temperature and high pressure

Paolo Lotti,^{a,b} G. Diego Gatta,^a Nicola Demitri^b, Davide Comboni^a, Marco Merlini^a,
Silvia Rizzato^c

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

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

^c*Dipartimento di Chimica, Università degli Studi di Milano, Milano, Italy*

paolo.lotti@unimi.it

Colemanite, $\text{CaB}_3\text{O}_4(\text{OH})_3 \cdot \text{H}_2\text{O}$, is a common mineral in borate sedimentary deposits in saline lakes, related to hydrothermal volcanic activity, and it is one of the main mineral commodities for the extraction of boron. Due to its relative abundance, in particular at the mine dumps, several recent works were devoted to explore its potential technological and industrial applications (see e.g. [1] for a list of references). Despite this interest, very few was known on the behavior of the colemanite crystal structure at non-ambient conditions of temperature and pressure. This contribution reports the results obtained from in situ low-temperature ($T \leq 293$ K) and high-pressure experiments.

A displacive phase transition from the centrosymmetric $P2_1/a$ colemanite to a ferroelectric polymorph with $P2_1$ symmetry was long time known to occur in the T -range between 273 and 263 K (e.g. [2]). Thermal analysis and in situ single-crystal X-ray diffraction data confirmed the transition, which was found to occur between 265 and 260 K. A thorough chemical analysis, performed by a combination of techniques, revealed the relative pureness of the natural sample of colemanite investigated, supporting the hypothesis that the absence of impurities reduces the T of transition to the ferroelectric state (i.e. it reduces the stability field of the ferroelectric polymorph) [3]. Single crystal X-ray and neutron diffraction data (down to 104 and 20 K, respectively) showed that the transition has limited effects on the crystal structure of colemanite. On the other hand, in situ high-pressure single-crystal X-ray diffraction experiments disclosed a much more complex scenario, with a first-order reconstructive phase transition occurring between 13.95 and 14.91 GPa, toward a denser polymorph with $\mathbf{a} = 3 \cdot \mathbf{a}_{\text{COL}}$, $\mathbf{b} = \mathbf{b}_{\text{COL}}$ and $\mathbf{c} = 2 \cdot \mathbf{c}_{\text{COL}}$. Despite reconstructive, the transition is single crystal-to-single crystal and involves an increase in the average coordination number of both the Ca and B sites. The tripling of the \mathbf{a} -axis and the doubling of the \mathbf{c} -axis imply the split of every independent atomic site of colemanite in six new independent positions in the high- P polymorph. In particular, three of the six new sites, generated from the parent triangularly coordinated B, increase their coordination number from three to four, gaining a bond with a H_2O oxygen. The elastic behavior of colemanite and of the high- P polymorph have been described by means of III- and II-order Birch-Murnaghan equations of state, respectively, yielding the following bulk moduli: 67(4) GPa (colemanite, $K_V' = 5.5(7)$) and 50(8) GPa (high- P colemanite).

[1] P. Lotti, G.D. Gatta, D. Comboni, G. Guastella, M. Merlini, A. Guastoni, H-P. Liermann *J. Am. Cer. Soc.* **2017**, in press, DOI: 10.1111/jace.14730.

[2] F.N. Hainsworth, H.E. Petch *Can. J. Phys.* **1966**, *44*, 3083.

[3] H.H. Wieder, A.R. Clawson, C.R. Perkerson *J. Appl. Phys.* **1962**, *33*, 1720.