



IV MISCA

Meeting of the
Italian and Spanish
Crystallographic Association

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21st-25th June
Tenerife - SPAIN



Real
Sociedad
Española de
Física



WELCOME

After three successful Meetings (MISCA 2007, Copanello di Staletti; MISCA 2010, Oviedo and MISSCA 2013, Como), these joint congresses of the Italian and the Spanish Crystallographic Associations have become customary, and now, three years after the last meeting, we announce MISCA 2016.

The IV MISCA is organized in the city of Puerto de la Cruz in the beautiful Island of Tenerife, Canary Islands, in the middle of the Atlantic Ocean, the most distant place of Spain from Italy. In some way, supporting the idea that Crystallography has no barriers and it is everywhere.

This MISCA meeting continues to be the place to reinforce the strong bonds between the Italian and Spanish crystallographic communities, and it is also the opportunity to award the MISCA Medal, a tradition to honour our excellent crystallographers. This IV MISCA is organized around seven microsymbiosia covering the state-of-the-art in the many fields the crystallography plays a central role, but there will be time for discussion, group meetings and collaborative work whilst enjoying the beautiful sunsets at Puerto de la Cruz.

We are looking forward to welcome you in Tenerife,

The organization team

Jorge Pasán
Javier González-Platas
Catalina Ruiz-Pérez



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**HIGH-PRESSURE BEHAVIOUR OF THE ZEOLITE PHILLIPSITE: AN *IN SITU*
SINGLE-CRYSTAL SYNCHROTRON DIFFRACTION STUDY**

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Phillipsite is one of the most common natural zeolites, found in “closed” or “open” hydrologic systems. Its Si/Al tetrahedral framework contains two main channel systems: an 8-membered ring channel along [100] and an 8-membered ring channel along [010], which intersect each other [1]. In order to investigate the high-pressure behavior of phillipsite and its structural evolution at the atomic scale, we performed an *in situ* single-crystal synchrotron X-ray diffraction experiment up to 10 GPa, using a nominally penetrating pressure-transmitting fluid (*methanol:ethanol:H₂O=16:3:1 mix*) [2] and a diamond anvil cell. The unit-cell parameters and the structure refinements within the *P*-range investigated show that: 1) phillipsite does not adsorb further H₂O molecules from the pressure fluid; 2) the configuration of the extra-framework population changes with pressure, affecting the elastic behavior of the mineral; in particular, two distinct compressional regimes have been observed; 3) phillipsite is crystalline at least up to 10 GPa, and this is surprising if we consider its microporous nature; all the *P*-induced effects are completely reversible.

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[1] G.D. Gatta, P. Cappelletti, N. Rotiroti, C. Slebodnick, R. Rinaldi. *American Mineralogist* **2009**; 94, 190–199.

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HIGH-PRESSURE BEHAVIOR AND PHASE TRANSITION IN COLEMANITE, AN INDUSTRIALLY RELEVANT INOBORATE

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Colemanite, $\text{CaB}_3\text{O}_4(\text{OH})_3 \cdot \text{H}_2\text{O}$, is a common constituent of natural borate deposits and a relevant mineral commodity, for its applications in the B-extraction processes and in the production of lightweight cements and ceramics [1,2]. Its crystal structure is monoclinic ($P2_1/a$, $a = 8.712 \text{ \AA}$, $b = 11.247 \text{ \AA}$, $c = 6.091 \text{ \AA}$, $\beta = 110.12^\circ$, $V = 560.4 \text{ \AA}^3$), characterized by infinite chains of B-polyhedra based on a fundamental ring-unit made by one triangular BO_3 and two $\text{B}(\text{O},\text{OH})_4$ tetrahedra. These chains are alternated with chains of Ca-polyhedra (coordination number, CN = 8), giving rise to sheets parallel to (010). Adjacent sheets are mainly interconnected through an H-bonding system involving hydroxyl groups and H_2O molecules. The links among structural polyhedra, both B and Ca, are all corner sharing in type [3].

Despite its relevance in industrial applications, the behavior of colemanite at high pressure has never been investigated. In this work, we have characterized the elastic behavior, the phase stability, the phase transition and the structural evolution with pressure of a natural colemanite single crystal based on an *in-situ* synchrotron X-ray diffraction study, performed at the P02.2 beamline of PETRA-III, Hamburg, Germany.

Colemanite, in its ambient conditions polymorph, is found to be stable up to 13.95 GPa. A III-order Birch-Murnaghan (III-BM) EoS fit leads to a refined bulk modulus (at ambient conditions) (K_{T0}) of 76(8) GPa [$K' = 4.4(10)$]. Comparative structure analysis, based on the refinements of the structure model at different pressures, shows that the B-polyhedra act as quasi-rigid units and the bulk compression is mainly accommodated by the compression of Ca-polyhedra and by polyhedral tilting.

Between 13.95 and 14.91 GPa, colemanite undergoes a reconstructive phase transition toward a monoclinic polymorph ($P2_1/n$, $a = 11.726(11) \text{ \AA}$, $b = 10.206(1) \text{ \AA}$, $c = 23.45(3) \text{ \AA}$, $\beta = 95.07(9)^\circ$, $V = 2796(4) \text{ \AA}^3$, at 14.91 GPa). The average coordination number of boron is found to increase: of the 18 independent B sites, 3 are triangularly coordinated and 15 are tetrahedra. Two independent infinite chains of B-polyhedra are alternated with two independent chains of Ca-polyhedra (CN = 8 or 9), by means of corner- and edge-sharing links. A II-BM EoS fit leads to a refined K_{T0} of 60(6) GPa for the high- P polymorph of colemanite.

X-ray diffraction patterns collected during P -release show that the phase transition is completely reversible and colemanite fully recovers its starting structural features.

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