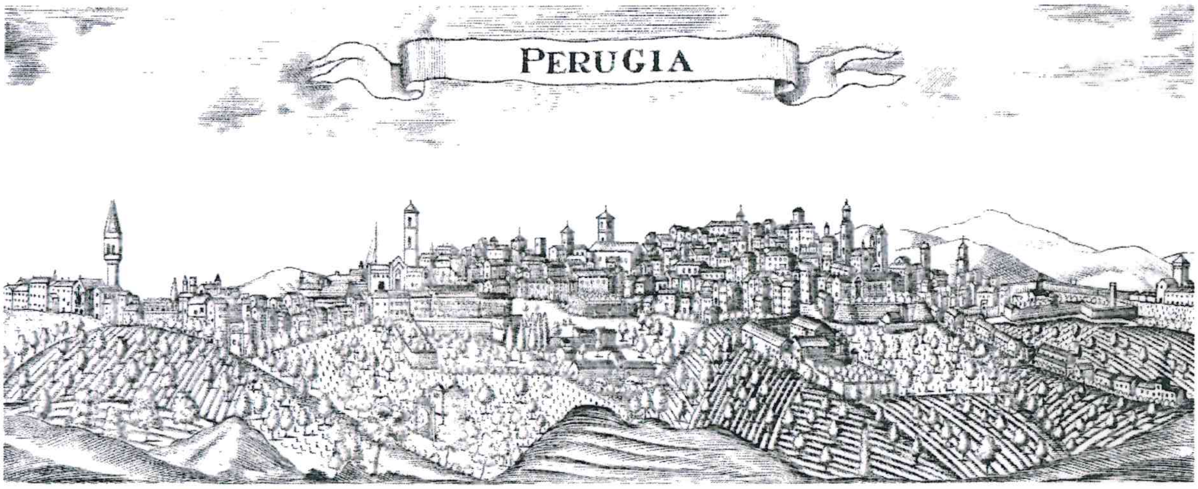
Abstacts and Programme Book

Associazione Italiana
di Cristallografia

Italian
Crystallographic
Association

XLVI Annual Meeting

Perugia, Palazzo Murena
June 26-29, 2017



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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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MARIO NARDELLI PRIZE

Microporous compounds at non-ambient (*P*,*T*) conditions: mechanisms of structure deformation, phase transitions and crystal-fluid interactions

Paolo Lotti

Dipartimento di Scienze della Terra, Università degli Studi di Milano, Milano, Italy
paolo.lotti@unimi.it

Microporous compounds are a class of open-framework materials; their structures contain cavities (in the form of channels or cages) with free diameters < 2 nm [1]. Zeolites, with their peculiar physical-chemical properties and diverse technological applications, are the most important group of this class, followed by feldspathoids and crystalline compounds with "hybrid" heterosilicate frameworks. The knowledge of the structural evolution of this class of materials under extreme conditions (*i.e.*, high/low temperature, high pressure) is of paramount importance, especially for the potential implications in materials science and Earth sciences. Zeolites, for example, are an important bulk commodity: the world production of natural zeolites in 2016 was about 2.8 million of tons (price: 100-230 dollars per ton) and the consumption of synthetic zeolites was approximately 1.6 million of tons.

Few decades of high-temperature and high-pressure studies of zeolites disclosed that a complex interplay between the framework topology and the extraframework constituents drives the structural response to (*T*,*P*)-variations. Isostructural compounds, which differs for the extraframework population only, are an ideal target for studying how strong may be the control exerted by ions and molecules (that fill the structural cavities) on the bulk behavior of the material. An X-ray diffraction study of four end-members of the cancrinite-group of minerals (feldspathoids), conducted by *in situ* high-*T* and high-*P* experiments, revealed that even slight changes in the extraframework population exert a control on the mechanisms of structure deformation, which are reflected on the bulk elastic behavior of the mineral [2-5].

Microporous compounds usually accommodate isostatic compression mainly by tilting of the framework tetrahedra, around the bridging oxygen atoms, which act as hinges. However, symmetry or chemical constraints may hinder this mechanism: displacive phase transitions can occur in zeolites and zeolite-like materials, in order to accommodate thermal, pressure and chemical stresses. In this respect, the high-*P* behavior of SiO_2-ferrierite is an interesting case study, as it undergoes, in a relatively narrow *P*-range, two displacive phase transitions with complex group-subgroup relationships ($Pmnn \rightarrow P12_1/n1 \rightarrow (P\text{-}1) \rightarrow P2_1/n11$, [6]).

In the last few years, a growing interest was devoted to the behavior of open-framework materials when compressed in the so-called "penetrating fluids", *i.e.* fluids in which molecules are small enough to be intruded at high pressure into the structural cavities. Once more, SiO_2-ferrierite may be considered an interesting case study. This zeolite has been compressed using three different *P*-media (*i.e.*, 16:3:1 methanol:ethanol:H_2O mixture, ethylene glycol and 2-methyl-2-propanol). The intrusion of the fluid molecules into the zeolite channels and cages was able to modify the bulk compressibility of the material and to prevent the transition to the $P2_1/n11$ polymorph, showing the strong control played by the extraframework population on the compressional behavior. Similar findings were also reported for other zeolites (*e.g.*, the zeolite $AlPO_4$-5 [7]). Several parameters were found to control the intrusion processes, among them: the sample size (*e.g.*, powder *vs.* single crystal) and the kinetics of compression. The first controls the magnitude of the intrusion process, whereas the second may prevent the intrusion, as confirmed by fast-compression experiments on zeolites [6].

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