2014 · VOLUME 229 · ISSUE 3

ZEITSCHRIFT FÜR KRISTALLOGRAPHIE – CRYSTALLINE MATERIALS

DE GRUYTER

ABSTRACTED/INDEXED IN CCC, indexed in CAS.
Covered by Science Citation Index, SciSearch, Research Alert, Chemistry Citation Index, Materials Science Citation Index, Reaction Citation Index and Current Contents/Physical, Chemical and Earth Sciences.

ISSN 2194-4946 · e-ISSN 2196-7105

All information regarding notes for contributors, subscriptions, back volumes and orders is available online at www.degruyter.com/zkri.

JOURNAL MANAGER Birgit Zoglmeier, Oldenbourg Wissenschaftsverlag GmbH, a company of De Gruyter, Rosenheimer Str. 143, 81671 München, Germany, Tel.: +49 (0)89 76902-426, Fax: +49 (0)89 76902-491, Email: birgit.zoglmeier@oldenbourg-verlag.de

RESPONSIBLE FOR ADVERTISEMENTS Panagiota Herbrand, De Gruyter, Rosenheimer Str. 143, 81671 München, Germany.
Tel.: +49 (0)89 769 02-394, Fax: +49 (0)89 769 02-350, Email: Panagiota.Herbrand@degruyter.com

TYPESETTING Beltz Bad Langensalza GmbH, Bad Langensalza

DRUCK Franz X. Stückle Druck und Verlag e.K., Ettenheim
Printed in Germany

Graphical Synopsis

This Special Issue appears in two parts:
Part I appears as Issue 2 and Part II as Issue 3, Volume 229 (2014)

Special Issue: High Pressure Crystallography
Edited by Ross Angel, Francesca Fabbiani and Pierre Bouvier

Part II

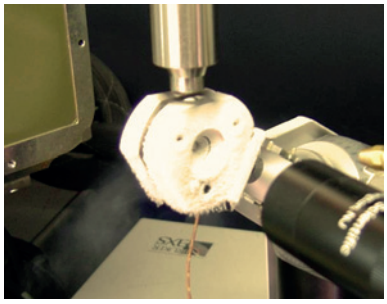
Preface

Original Papers

Christopher J. Ridley and
Konstantin V. Kamenev
High pressure neutron and X-ray diffraction at low temperatures

DOI 10.1515/zkri-2013-1673
Z. Kristallogr. 2014; 229(3): 171–199

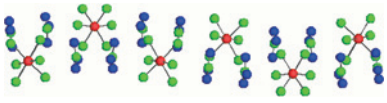
Synopsis: Collecting diffraction data from samples under extreme conditions poses many experimental difficulties. This paper presents a review of instruments for low temperature, high pressure diffraction studies, discussing the benefits/limitations of each.



Christopher A. Cameron,
David R. Allan,
Konstantin V. Kamenev,
Stephen A. Moggach, Mark Murrie and Simon Parsons
A pressure-induced displacive phase transition in Tris(ethylenediamine) Nickel(II) nitrate

DOI 10.1515/zkri-2013-1688
Z. Kristallogr. 2014; 229(3): 200–209

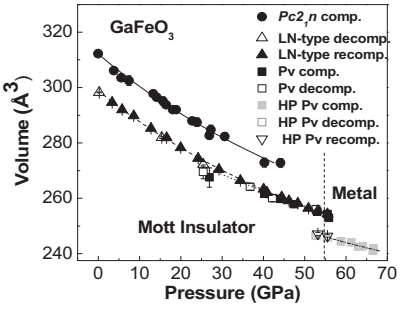
Synopsis: $[Ni(en)_3][NO_3]_2$ undergoes a displacive phase transition between 0.82 and 0.87 GPa in which the unit cell *c*-axis triples in length. A similar transition has been previously observed at 108 K ambient pressure, but with a reduced displacement amplitude.



Gregory Kh. Rozenberg, Weiming Xu and Moshe P. Pasternak
The Mott insulators at extreme conditions; structural consequences of pressure-induced electronic transitions

DOI 10.1515/zkri-2013-1644
Z. Kristallogr. 2014; 229(3): 210–222

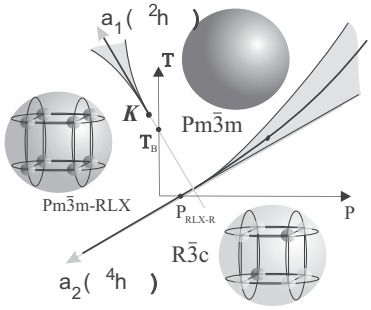
Synopsis: Pressure-induced electronic transitions and their structural consequences in Fe-based Mott insulators are the issue of this paper. We show the main scenarios which such strongly correlated systems may undergo on the way to a correlation breakdown.



Dmitry Chernyshov, Vadim Dyadkin, Vladimir Dmitriev and Alexey Bossak
Pressure evolution of $PbMg_{1/3}Nb_{2/3}O_3$ relaxor ferroelectric

DOI 10.1515/zkri-2013-1642
Z. Kristallogr. 2014; 229(3): 223–229

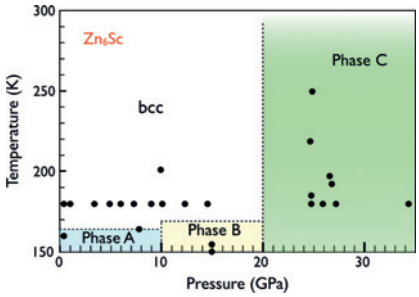
Synopsis: The relaxor-specic diffuse scattering is observed for $p > 40$ kbar and parametrized with a model of polar correlations. The transition between non-polar and relaxor phases is considered as an iso-structural crossover.



Tsunetomo Yamada, Gaston Garbarino, Hiroyuki Takakura, Cesar Pay Gòmez, Ryuji Tamura and Marc de Boissieu
***In-situ* high-pressure X-ray diffraction on the $Zn_6Sc\ ^1/_1$ periodic cubic approximant to a quasicrystal**

DOI 10.1515/zkri-2013-1684
Z. Kristallogr. 2014; 229(3): 230–235

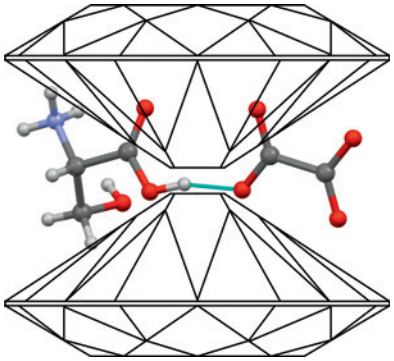
Synopsis: $Zn_6Sc\ ^1/_1$ cubic approximant to a quasicrystal has been studied in-situ at high pressures by X-ray diffraction. In the pressure range up to 35 GPa, two new superstructures were observed. The resulting pressure-temperature phase diagram is presented.



Elena V. Boldyreva
Multicomponent organic crystals at high pressure

DOI 10.1515/zkri-2013-1699
Z. Kristallogr. 2014; 229(3): 236–245

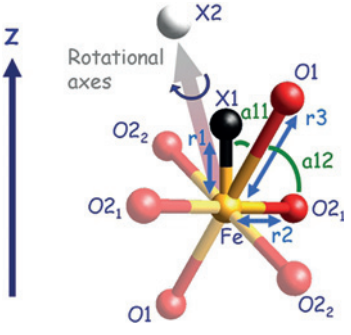
Synopsis: What changes in respond of a crystal structure to external stimuli, if several components form a co-crystal, a salt or a solvate?



Martin Etter, Melanie Müller, Michael Hanfland and Robert E. Dinnebier
Possibilities and limitations of parametric Rietveld refinement on high pressure data: The case study of $LaFeO_3$

DOI 10.1515/zkri-2013-1668
Z. Kristallogr. 2014; 229(3): 246–258

Synopsis: Four competitive crystallographic approaches are applied to high pressure powder diffraction data of the orthoferrite $LaFeO_3$ in order to investigate the possibilities and limitations of parametric Rietveld refinement.

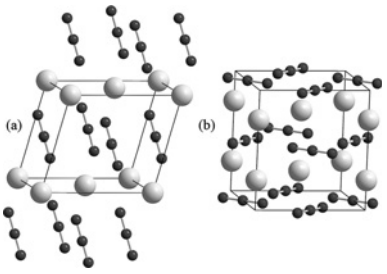


David I. A. Millar, Christopher Barry,
William G. Marshall and
Colin R. Pulham

Structural characterization of sodium azide and sodium bifluoride at high pressures

DOI 10.1515/zkri-2013-1660
Z. Kristallogr. 2014; 229(3): 259–275

Synopsis: High-pressure studies of NaN_3 and $NaDF_2$ show that both adopt the archetypal *I*4/*mcm* structure shared by the heavier Group 1 azides and bifluorides. The transition in NaN_3 is sluggish at ambient temperature, but occurs readily at 3.33 GPa and 393 K.



Part I

Original Papers