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Barium Ternary Fluorides Ba*M*F_4 (*M* = Mn, Zn, or Mg) at Non-ambient Conditions. Jose Maria Posse[a], Andrzej Grzechnik[a], Karen Friese[a]. [a]*Dept. of Condensed Matter Physics, University of the Basque Country, Bilbao, Spain.*
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The compounds Ba*M*F_4 (*M* = Co, Fe, Mn, Ni, Zn, or Mg) crystallize in space group $Cmc2_1$ (Z = 4) at ambient conditions. The cation *M* is surrounded by six fluorine atoms forming an irregular octahedron. Four of the octahedra are connected via common corners with others, generating puckered layers perpendicular to the *b* axis. The neighbouring layers are shifted with respect to each other by a translation of *a/2*. The barium atoms are located in the interlayer spaces [1]. These compounds are interesting due to the fact that some of them (M = Mn, Fe, Co, or Ni) exhibit a multiferroic behaviour [2]. $BaMnF_4$ has a second-order phase transition to an incommensurate phase at low temperatures (T ~ 250 K) supposedly with superspace group $C2_1(½\ ½\ \gamma)$ [3]. In addition, it exhibits magnetic anomalies at about 50 K and 27 K, the latter being due to a formation of an antiferromagnetic phase [4].
The aim of our study is to examine the structural instabilities [5] in $BaMnF_4$, $BaZnF_4$ and $BaMgF_4$ at low temperatures and high pressures.
Powder x-ray diffraction (ID31 beamline, ESRF) and single-crystal x-ray diffraction (SCD beamline, ANKA; our laboratory in Bilbao) experiments were carried out on $BaMnF_4$, $BaZnF_4$ and $BaMgF_4$ from 290 K to 10 K at atmospheric pressure. Both $BaZnF_4$ and $BaMgF_4$ do not undergo any phase transitions at low temperatures. On the other hand, our diffraction data on $BaMnF_4$ indicate that it transforms to an incommensurate monoclinic phase which is affected by twinning. In contrast to the earlier investigations [3], our data indicate the superspace group $X2_1(½\ ½\ \gamma)$ with X = (½, ½, 0, ½) as the correct choice. Upon lowering the temperature, the γ component of the modulation wave vector increases and reaches a constant value $\gamma \approx 0.3948$ below 50 K, i.e., in the temperature range in which the magnetic anomalies occur [4].
We also performed high-pressure measurements using single-crystal x-ray diffraction in our laboratory and in HASYLAB/Hamburg ($BaZnF_4$ and $BaMgF_4$) as well as Raman spectroscopy ($BaZnF_4$). The Raman data suggest pressure-induced phase transition in $BaZnF_4$ at about 5 GPa. Currently, we are analyzing our diffraction data to elucidate the high-pressure structures of $BaMgF_4$ and $BaZnF_4$.
Our intention is to perform high-pressure single-crystal diffraction experiments to examine the structural behaviour of $BaMnF_4$.

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Keywords: multiferroic; modulated structure; high pressure

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Modulated Structures in Aluminate Sodalites. Wulf Depmeier. *Institute of Geosciences, University of Kiel, Kiel, Germany.*
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Aluminate sodalites $|\mathbf{M}_8(\mathbf{X}O_4)_2|[Al_{12}O_{24}]$-**SOD**, with **M** = Ca^{2+} or Sr^{2+}, and **X** = S^{6+}, Cr^{6+}, Mo^{6+}, W^{6+}, usually undergo phase transitions from a cubic high temperature phase to one or several non-cubic low temperature, often ferroelastic or ferroelectric, phases. The majority of the low symmetry phases can be described as modulated phases. Commensurately and incommensurately modulated phases with dimensions of the superspace varying between (3+1) and (3+3) have been found. Even small disturbances lead to quite complicated T – x phase diagrams. The reason for the occurrence of the modulations is believed to be due to the fact that the structure of sodalites in general can be broken down into three partial structures, viz. i) the sodalite framework, ii) an interpenetrating net of cations, and iii) cage anions at the centres of the sodalite cages. In the case of tetrahedral cage anions competitive interactions occur between these partial structures. The system is frustrated and its free energy can be lowered by a modulation. Cascades of phase transitions especially in the Ca-bearing members of the aluminate sodalite family can be rationalized by the fact that the phase transitions from the cubic phase usually happen at the N-point of the body-centred Brillouin zone meaning that the corresponding order parameter has six components. In real space the cascades can be rationalized by interplay of rotational and translational potentials becoming subsequently deeper or shallower as a consequence of the above-mentioned interactions. Chaotic phases and phases due to sliding of modulation waves are anticipated as well.

Keywords: sodalites; modulated phases; phase transitions

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Molecular Structure of 4-(9-Anthryl)-1-phenylspiro[azetidine-3,90-xanthen]-2-one. İsmail Çelik[a], Mehmet Akkurt[b], Aliasgar Jarrahpour[c], Edris Ebrahimi[c], Orhan Büyükgüngör[d]. [a]*Department of Physics, Faculty of Arts and Sciences, Cumhuriyet University, 58140 Sivas, Turkey.* [b]*Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey.* [c]*Department of Chemistry, College of Sciences, Shiraz University, 71454 Shiraz, Iran.* [d]*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey.*
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The β-lactam ring of the title compound, $C_{35}H_{23}NO_2$, is nearly planar with a maximum deviation of 0.003 (3) Å from the