reflections observed for $T \leq 230$ K. The low temperature magnetic structure was found to be antiferromagnetic with both pyramidally and octahedrally coordinated Co ions in the intermediate spin state. The high and low temperature magnetic phases were found to coexist at 230 K.

Keywords: magnetic perovskite materials, magnetic phase transitions, neutron powder diffractometry

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The 'gillespite-III' phase - the key for understanding a famous high-pressure phase transition?

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The phyllosilicate gillespite, $BaFeSi_4O_{10}$ (space group *P*4/*ncc*), has attracted attention in high-pressure research due to displaying striking features related to its ferroelastic phase transition at high pressures. In particular aspects related to symmetry and elastic softening associated with the observed transitions give reason to speculations on additional possible polymorphs at high pressure. The evaluation of lattice properties of gillespite-type analogue phases (with Cr^{2+} and Cu^{2+} substituting for Fe^{2+}) by means of single-crystal XRD reveals first-order phase transitions in these analogue compounds, but the lattice symmetry of the high-pressure polymorphs clearly was found to be tetragonal. Both Raman and UV-VIS absorption spectroscopy investigations reveal features for the maintainance of local four-fold symmetries, in particular for the geometry of the planar MO_4-group, which is in contrast to the reported structural changes related to the orthorhombic high-pressure polymorph gillespite-II. Measurements of XRD intensities on the analogue-comounds in a diamond-anvil cell confirm the structure of a tetragonal high-pressure polymorph ('gillespite-III'), with a 3x3 superstructure showing a triplication of the tetragonal a-axis. Here we report on the single-crystal X-ray structural study based on a measurement in a low-background diamond-anvil cell, together with the results of measurements of in-situ high-pressure Raman spectroscopic investigations.

Keywords: high-pressure phase transition, gillespite structure, superstructure

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Crystallographic model of an atom and the dimension of real Euclidean space in Mendeleev's Table

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The dimension of real isotropic homogeneous Euclidean space is considered as the factor of self-organization of electrons of an atom into stable systems: into electron shells of an atom and periods of the Periodic Table of Chemical Elements. For revealing the role of the dimension of real space of it is considered the properties of the simplest polyhedron of n-dimensional space (a simplex of this space), the propositions of analytical geometry of three-dimension space. It is constructed crystallographic models of arrangement of electron shells of an atom as regular systems of interacting Coulomb particles on a sphere of three dimensional space. The positions of electrons of shells are modeled by vertices of the antiprisms inscribed in a sphere. The change in the number of electrons in neighboring shells always only by four electrons is the result of the fact that (n + 1)th vertices of a simplex fix a sphere in n-dimensional space. It is considering the Pauli principle from point of view three-dimensionality of Euclidean space. The limited number of the electron shells of the ground-state of an atom (s-, p-, d-, f-shells) and the periods are the results of three-dimensionality of real space too. So three-dimensionality of real space along with its homogeneity and isotropy, centrosymmetric field of atomic nucleus, the properties of electrons as the Coulomb quantum indistinguishable particles are responsible for the number of chemical elements equals to 118 and the periodicity of their physicochemical properties. The finite number of stable systems of electrons and their complication with increasing the number of electrons led to simplicity and hierarchy in the structure of electron system of an atom.

Keywords: crystallographic model of an atom, three-dimensional real space, the Periodic Table of Chemical Elements

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Application of corepresentations to magnetic structures and displacive crystallographic transitions

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Corepresentation theory provides a physical basis for the description and understanding of many characteristics in the solid state. Most known from its application to magnetic ordering and phonon spectra, its language also describes electronic states and the symmetry changes associated with displacive phase transitions (commensurate and incommensurate). In this way they can be used to construct a generalised framework for symmetry changes in the crystalline solids. Use of such a common language makes clear couplings between order parameters that may otherwise appear unrelated, such as in multiferroic materials, and allows symmetry rules to be developed. The use of corepresentations has been limited due to difficulties in generating a reliable source of the representations that form the basis of their construction, and the mathematical subtleties related to their use in the projection of their associated basis functions and application of antiunitary symmetry. The number of possible symmetry types and the observation that basis vectors are phased according to the wavevector of the ordering, requires their in situ generation by computer codes and libraries. At present there is no standard for the characterisation of these symmetries and the characters of the irreducible representations and corepresentations must to be explicitly stated, or reference made to some work of reference. We have verified the automorphism of the tables of Kovalev and converted their settings to those now used by the IUCr, and released them as a library within the computer program SARAh. These relationships and the protocols for the generation of the correct basis vector spaces for the different situations are discussed.

Keywords: magnetic ordering, non-crystallographic symmetry, symmetry theory generalization and applications