PS21.01.17 TWINNING AND PSEUDO-SYMMETRY IN BARIUM SUCCINATE.

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The crystal structure of barium succinate, $BaC_4H_4O_4$, shows a symmetry very close to space group $I4_1/amd$. The small deviations of the actual atomic arrangement from this high symmetry gives rise to multiple twinning, which leads to the tetragonal pseudo-symmetry observed in the crystal morphology. The deviations are associated with the low symmetry of the succinate molecule O_2 - CH_2 - CH_2 - O_2, which is incompatible with the site symmetry of 42m occupied in $I4_1/amd$. In quantity, however, these deviations of some carbon and oxygen positions from the "ideal" values are so small, that the crystal structure could be refined to R-values of about 6% in a lot of different space groups, for example Fddd, Pnma, $C222_1$, $P4_1$, C2/c or $P2_1$, all being subgroups of $I4_1/amd$ which share the same connectivity network of Ba^{2+}-ions and succinate chains along the pseudo-four-fold axis. The true space group C2 could only be found by optical experiments in conjunction with group-theoretical considerations. The twin law is represented by the "lost" symmetry elements, especially the 4-fold axis.

Twinned crystals of $BaC_4H_4O_4$ were grown from aqueous solution. They show tetragonal symmetry with faces {112} and {100}, as first described by Haushofer [1].The crystal structure was not investigated until now, in contrast to many other succinates [2]. A single crystal was prepared by cutting a twin under the polarizing microscope. X-ray-diffraction intensities (full sphere up to $2\Theta = 65°$, Mo Kα) were measured in tetragonal geometry (a = 7.601(1) Å, c = 10.293(1) Å) on a 4-circle diffractometer (AFC6R, RIGAKU/MSC). The deviation from tetragonal geometry is of the order of 0.2° as detected by optical means as misfit angle between faces of a twinned crystal.

PS21.01.18 TWO- AND THREE-DIMENSIONAL GROUPS OF HYPER TABLET P-SYMMETRIES AND THEIR APPLICATION.

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One of the first extensions of the notion of symmetry is Shubnikov theory of antisymmetry, used as the basis for various applications in geometrical crystallography and its generalizations. Interpretation of antisymmetry as two-colored symmetry resulted in the idea of p-symmetry; the other generalization of antisymmetry - the multiple antisymmetry is obtained ascribing to the points of a figure not only one, but several qualitatively different sign + or -. Diverse approaches to the colored antisymmetry introduced by Pawley, Neronova and Belov, and their further generalization - cryptosymmetry of Niggli and Wondratchek are the syntesis of the both.

The mentioned generalizations of antisymmetry and colored symmetry are included in P-symmetry, using arbitrary number of colors p (not only p=2, as antisymmetry) assigned to the points of a figure, and arbitrary group P of colorpermutations (not only cyclic groups, as Belov psymmetry. Belov p-symmetry is a particular case of P-symmetry with cyclic color-permutation group P={(12...p)}, and Shubnikov antisymmetry is treated as 2-symmetry.

Signs and indexes ascribed to the points of a figure posses the extra geometrical sense with regard to the space in which the symmetry group acts; in additional dimensions the signs and indexes can be interpreted geometrically. From this result the possibility to use two-dimensional and three-dimensional P-symmetry groups for modeling certain categories of multidimensional symmetry groups.

The more detailed explanation of the ideas mentioned, the recent methods of applying two-dimensional and three-dimensional symmetry groups of rosettes, tablets and hyper-tablets, as well, as crystallographic and hyper-crystallographic P-symmetry to the study of multidimensional symmetry groups will be given in this communication.

PS21.01.19 A QUASIPERIODIC PATTERN GENERATED BY MIXING DODECAHEDRAL AND ICOSAHEDRAL LATTICE.

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A 16 by 16 projection matrix is presented which produces basis vectors in pattern space as a combination or mixing of vectors from the center to vertices of a pentagonal dodecahedron and an icosahedron. The two polyhedrons are arranged such that the vectors of an icosahedron coincide with five-fold symmetry axes, and those of a dodecahedron with three-fold symmetry axes of an icosidodecahedron. The mixing ratio, the ratio of the length of basis vectors for an icosahedron to that for a dodecahedron can take any positive value and the 16-D unit cube projected to pattern space is an enneacontrahedron truncated by a triacontrahedron. The depth of truncation changes as the mixing ratio and for 1 to 1 mixing an equilateral truncated rhombic enneacontrahedron is obtained. Quasiperiodic patterns or tilings by the projection method using the 16 by 16 matrix are presented.

PS21.01.20 SYMMETRY IN MULTIPLE DIFFRACTION PATTERNS.

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It is well known that a multiple diffraction (m.d.) pattern has symmetry mirrors in certain azimuthal positions. In principle, peaks symmetrically positioned around a mirror have same intensity. Nevertheless, for two times in some of our experimental patterns we have unequivocally observed symmetrical peaks with different intensities. Casting about such peaks in experimental m.d. patterns in the literature, we have observed several pairs of them. In this work we make a systematic study about the appearance of such peaks in hexagonal, trigonal and cubic structures. Both experimental and simulated x-ray and neutron m.d. patterns were employed in the study. Plotting the data in circular plots allows immediate observation of the symmetry of the patterns. Two kinds of mirrors are observed: isomorphic mirrors, that produce symmetrical peaks with identical intensities, and anamorphic mirrors, where symmetrical peaks can have different intensities. The number of isomorphic mirrors equals the order n of the symmetry axis normal to the primary reflecting planes. Results show that in the cubic system n-fold axes, produce only isomorphic mirrors, for n even, and anamorphic mirrors intercalated between isomorphic mirrors, for n odd. For α–(trigonal) and β-quartz (hexagonal) results are opposite to those of cubic system. The 3-fold symmetry of reflection 00.1 from the hexagonal cell of α-quartz produces only isomorphic mirrors. For the 6- fold symmetry of same reflection from, β-quartz intercalation occurs.

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