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VRML General Position Diagrams of non-Cubic Magnetic Space Groups
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We have developed three-dimensional general position diagrams of the 1502 non-cubic magnetic space groups in VRML (virtual reality modeling language) format. Each diagram can be rotated and zoomed to aid in its visualization and includes both the general positions of the atoms and the general orientations of the associated magnetic moments.
Keywords: magnetic space groups, general position diagrams, 3-dimensional visualization

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Database of the Subperiodic Rod Groups on the Bilbao Crystallographic Server
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Recently, we have started the development of databases for the subperiodic groups: the crystallographic data for the 80 layer groups including generators, general and special positions and maximal subgroups are already accessible on the Bilbao Crystallographic server (www.cryst.ehu.es) [1]. The aim of this contribution is to announce the development of a database for the 75 rod groups. In addition to the basic crystallographic data as found in the International Tables for Crystallography, Vol. E [2], the complete information on maximal subgroups of rod groups is made available. All maximal subgroups of index 2, 3 and 4 are listed individually whereas the infinitely many maximal isotypic subgroups are presented as infinite series. For each subgroup either its General position or a set of generators is given. The conjugacy relations of the subgroups in the original group are indicated. The transformation to the conventional coordinate system of the subgroup is available as a matrix for the change of the basis and a column for the origin shift. The symmetry information has been stored in XML and provisional CIF formats.

[1] Aroyo M.I., Capillas C., Perez-Mato J.M., Konstantinov P., Wondratschek H., *Acta Cryst*. , 2004, **A60**, s297. [2] *International Tables for Crystallography*, Volume E: Subperiodic Groups, Kopsky V., Litvin D., Kluwer Acad. Publ., 2002.
Keywords: Bilbao Crystallographic Server, subperiodic rod groups, crystallographic database

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Fibration-defined Integer and Non-integer Axes
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Axis of rotation on the angle $2\pi d/p$ is determined by partition of p vertices of the regular polygon on the p subsets with d+1 vertices for each. When $1<d<p/2$ then polygon is a star-polygon. The sides of the star-polygon intersect in certain extraneous points, which are not included among the vertices. Crystallographical and quasicrystallographical axes (d=1) are determined by cyclic subgroups (of order p=2,3,4,5,6,7...) of the Weyl groups of the root lattices of simple Lie groups. The root lattice E_8 incorporates (or they can by embedded in it) all types of root lattices and gives possibility for building of the special algebraic construction – fibre space. L points of fibre space correspondence b points of base and N points of fibre.

By Hopf fibration for E_8 the N points of the fibre can be split into m sets with 1 or 2 special points for each set; therefore:

$L=b\cdot N=m\cdot b(k+c)$, (1)

where $N=m(k+c)$, c=0, 1, 2. The set of b(k+c) points can be split into subsets from k points which define k vectors. Thus, fibration (1) defines an axis of the order:

$p/d=(1/\gamma)\cdot(b(k+c)/k)=(1/\gamma)\cdot(L/N-mc)$ (2)

where γ=1 or 2 if a cover for fibre group is one or two-sheeted. The choice of L, N, m and c practically defines one of the subsystems of the E_8 root vectors [1].

Equation (2) defines crystallographical and quasicrystallographical (d=1) and non-integer (d>1) axes in the framework of the unique algebraic construction. The non-integer axes are realized in some rod substructures; for instance the collagen structure has 10/3 axis – rotation on the 108°. All non-integer axes, which are determined Hopf fibration for E_8 lattice are considered.

[1] Samoilovich M.I., Talis A.L., *Nanostructures and photon crystals*, "Tehnomash" Publisher, Moscow, 2004, 5-114.
Keywords: fibration, non-integer axes, algebraic construction

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A Fibre Bundle Approach to the Description of the Symmetry of Magnetic Structures in a 6-dimensional Space
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We consider the magnetic symmetry groups in terms of the fibre bundles. To describe magnetic symmetry one needs a 6-dimensional space $\mathbf{E_6}$. This space has the structure of the **fibre bundle** with $\mathbf{R_3}$ as a **base space**, and a 3-dimensional vector space $\mathbf{V_3}$ as a **fibre**. $\mathbf{R_3}$ is the position space of the magnetic structure, while $\mathbf{V_3}$ is spanned by the orthogonal unit vectors $\mathbf{e_1}$, $\mathbf{e_2}$, $\mathbf{e_3}$ and is the space of the magnetization vector. In the simplest case the space $\mathbf{E_6}$ becomes the Cartesian product of the $\mathbf{R_3}$ and $\mathbf{V_3}$. In this formalism one can describe a magnetic structure as a certain subspace **S** of $\mathbf{E_6}$. The subspace **S** in terms of the fibre bundles is called the **section of $\mathbf{E_6}$**. Therefore the corresponding magnetic symmetry group becomes a symmetry group of **S**. In this case the problem of formulating the different magnetic symmetry groups consists in searching the corresponding symmetry groups of **S**. These symmetry groups are defined as groups, which conserve the unique structure defined by the magnetization vector. The magnetic symmetry group in this approach is the **structure group of the bundle $\mathbf{E_6}$.** To illustrate the above approach a ferromagnetic, an antiferromagnetic and both different spiral magnetic structures and spin waves are considered. This approach can serve for the determination of all the other magnetic symmetry groups as well as for the determination of the symmetry groups of all the other aperiodic structures (like the modulated nonmagnetic structures, quasicrystals etc.).
Keywords: fibre bundles, magnetic groups, aperiodic structures

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Validation of a Twinned Pseudo Symmetric Crystal using a Hierarchical Pathway
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An apparently monoclinic crystal of $[Mn(cyclam)(NCO)2]^+.ClO_4^-$, (cyclam is the tetradentate ligand 1,4,7,11-tetraazacyclotetradecane) was shown to be a 0.545(1) : 0.455 twin, space group *C-1*, $Z = 16$, that is best described as a commensurate occupational and displacive modulation of a $Z = 4$ idealised parent structure with space group *A2/a* and $\mathbf{a}p = \mathbf{a}/2$, $\mathbf{b}p = \mathbf{b}/2$, $\mathbf{c}p = \mathbf{c}$.

The quality of refinement is very pathway dependent. Success requires using constraints inspired by the pseudo symmetry. A hierarchical approach to solution and refinement obtained sequentially structures in space groups *A2/a*, $P2_1/n$, *P-1* and finally *C-1*. Major and minor components of the reflection intensities could be identified using irreducible representations of *A2/a* and $P2_1/n$ to symmetrise the scattering density so that any reflection is associated with two