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Point groups in crystallography

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Two dual spaces are extensively used in crystallography: the point space E^n, hosting the crystal pattern; and the vector space V^n, where face normals and reciprocal-lattice vectors are defined. The term "point group" is used in crystallography to indicate four different types of groups in these two spaces. 1) Morphological point groups in V^n: They can be obtained from maximal holohedries (holohedries not properly contained in another holohedry) by iteratively descending to proper subgroups: this gives 21 point groups in V^2 and 136 point groups in V^3, which are then classified into 10 and 32 point-group types, respectively (on the basis of which geometrical crystal classes are defined), and into 9 and 18 abstract isomorphism classes. 2) Symmetry groups of atomic groups and coordination polyhedra in E^n: They coincide with molecular point groups and fall into infinitely many different isomorphism classes, since due to the absence of periodicity these groups are not subject to the crystallographic restriction. 3) Site-symmetry groups in E^n: They are the finite subgroups of space groups. For each site-symmetry group, conjugation by the translation subgroup yields infinitely many different groups, but transforming the fixed point to the origin of E^n allows to classify them into geometric crystal classes exactly like point groups in V^n. A finer classification of site-symmetry groups into *species* is however introduced that takes into account their orientation in space: species of site-symmetry groups in E^n uniquely correspond to point groups in V^n. 4) Groups of matrices representing the linear parts of space group operations in E^n: They are isomorphic both to the point groups in V^n and to the factor groups G/T, where T is the translation subgroup of a space group G.

Keywords: point groups, Site-symmetry groups, symmetry

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Hierarchical structural analysis of supramolecular isomers of organic crystalline host compounds

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Supramolecular isomerism has attracted considerable attention currently in the field of supramolecular chemistry from the viewpoints of the development of new materials. However, the appearance of unexpected supramolecular isomers has been seen as a problem from the supramolecular architectural design. To better understand the isomerism, we have prepared the supramolecular isomeric crystals of host-guest complexes, and elucidated their crystal structures starting from the chiral host molecules hierarchically. Taking inclusion crystals of alkaloid for instance, here we describe the hierarchical interpretation of the supramolecular isomerism and chirality. Recrystallization from various organic solvents afforded the guest-induced supramolecular isomeric inclusion crystals composed of common 21 helical columnar assemblies. Thus, the inclusion crystallization can be interpreted hierarchically as follows; (i) fixing a conformation of host molecule with three-directional chirality for making the subsequent molecular architecture, (ii) forming a bimolecular aggregate, and piling up the bimolecular aggregates to form a helical columnar assembly with supramolecular tilt chirality, (iii) stacking the columns in a parallel or anti-parallel fashion to produce supramolecular isomeric bundles, (iv) accommodating guest molecules in the cavities of the bundles to yield host-guest complexes characterized by molecular recognition. Such an interpretation leads to a reasonable elucidation of supramolecular isomerism starting from molecules focused on intermolecular interactions, and will serve as models to better understand complicated self-assembled phenomena.

Keywords: alkaloid structures, helical structure, hydrogen bonds

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The (3+1)-dimensional scheelite structure type

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The concept of structure type (ST) is a well-known crystallographic term, which is widely used in physics, chemistry, and material science. This term refers to a family of periodic crystal structures sharing similar features [1]. In classical crystallography, the relations between structures belonging to the same ST are rather intuitive than quantitative. We propose to improve and extend the notion of ST by applying the concept of superspace symmetry. We show [2] that an incommensurately modulated structure (IMS) described in superspace can be used as a model, capable of generating and describing a family of compounds belonging to a unique higher dimensional structure type (HD-ST). This superspace model and the corresponding HD-ST are characterized by a superspace group (SSG), a number of building units in some basic unit cell occupying certain Wyckoff sites. The occupation and displacive atomic modulations along with variable coefficients of the vector **q** are able to uniquely specify any structure belonging to the HD-ST. An INS taken as a superspace model indicates the primary variable(s), which is (are) responsible for the structure manifold in the HD-ST family. The symmetry of the 3D structures and topological manifold in the structure type family are restricted by the SSG. The new concept of ST has been illustrated with the example of the scheelite-like incommensurately modulated structure (3+1)D $KNd[MoO_4]_2$. The concept has been applied for the description and derivation of scheelite-like compounds differing widely in chemical composition and topology [2].

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A model of decagonal Al-Cu-Co

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