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Higher-dimensional point groups in superspace crystallography

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Crystallographic puzzles not covered by the present crystallography, like integral indexing and crystallographic scaling of axial-symmetric biomacromolecules and icosahedral viral capsids and/or integral lattices, can possibly be explained by extending (n, d)-dimensional superspace crystallography to include finite subgroups of the higher-dimensional orthogonal group $O(n)$ and not only those of $O(d)$, as restricted by the physical dimension d.

1. Introduction

There are empirical observations of generic crystallographic properties of biomacromolecules, of icosahedral viruses, of quasicrystals and of three-dimensional crystals not covered by the present crystallography, not even if extended to higher dimensions according to the superspace approach. Generic means that these properties are not limited to a few isolated cases and, therefore, hardly represent marginal or accidental phenomena.

Examples of these unexplained properties are first of all the integral lattices which appear as sharp peaks in the frequency distribution of axial symmetric crystals as a function of the ratio $\gamma = c/a$ (Janner, 2004*a*; Gelder & Janner (2005*a*,*b*). In particular, in the case of inorganic hexagonal crystals, the most important peak occurs for $\gamma = 1$, which implies that the lattices of the ideal structures responsible for the peaked distribution are isometric hexagonal, with lattice parameters $c = a$. Normal hexagonal lattices certainly also contribute to the same peak. In axial-symmetric proteins (Janner, 2005*a*,*b*) and nucleic acids (Janner, 2001*a*), the striking property is represented by the possibility of assigning rational indices to the vertices of their enclosing forms, according to three- or higher-dimensional lattices. Again, these lattices, denoted *form lattices* for making a distinction with the crystal lattices arising from translational periodicity, are integral (at least in all cases investigated so far).

From the molecular point of view, the structural relevance of form lattices is already a puzzle, that of integral lattices an even greater one, despite the possibility of extending the crystallographic concepts to molecules, in analogy to what has been done for the aperiodic crystals (Janner, 2001*b*).

The first indication that something fundamental and unexplained is involved came from proteins, to begin with the decameric conformation of the cyclophilin–cyclosporin complex more than ten years ago, and observed since then in many other axial-symmetric proteins and nucleic acids. In axial projection, the external polygonal enclosing form appears to be related to that of the central hole by a polygrammal scaling as occurring in star polygons. Starting from a regular polygon with p vertices, one obtains a star polygon with Schäfli symbol $\{p/q\}$ by straight lines joining the q-successive vertices, whose intersections define a central polygon scaled from the external one by a factor $\lambda\{p/q\}$. The corresponding scaling transformation $S_{\lambda\{p/q\}}$ is expressible as an n-dimensional integral invertible matrix, where $n = \varphi(p)$ is the Euler φ function. Therefore, a polygrammal scaling generates a crystallographic point group of infinite order and the vertices of the polygrammal form can be indexed by a set of n integers. Similar crystallographic scalings occur in quasicrystals as well (Janner, 1992).

The capsid of an icosahedral virus is built up from an assemblage of coat proteins, which protect the viral genome inside a central hole. Considering axial-symmetric clusters of the coat proteins, one is back in the situation sketched above. In the particular case of various serotypes of the rhinovirus, the crystallographic properties mentioned above are observed, again and again: integral form lattices and crystallographic scalings (Janner, 2006*a*). Moreover, the vertices of the whole capsid could be indexed according to a single icosahedral lattice, invariant with respect to the scaling relating the polyhedral form of the external surface with that of the internal one, and expressible by a unimodular six-dimensional integral scaling matrix.

Last but not least, in the case of biomacromlecules the principle of a strong correlation could be observed (Janner, 2005*c*). This implies that the value of one single parameter suffices for fixing the metrical relation between structure and geometry. This is a property very natural for highly symmetric objects, but difficult to explain in theoretical terms.

2. Polygrammal superspace symmetry

For fixing the ideas, consider the pentagram {5/2}. Its Euclidean symmetry, the same as for a regular pentagon, does not take into account the specific scaling relations among the ten vertices (the golden mean, in particular). As one knows from the Penrose tiling and from the decagonal quasicrystals, these

scalings are crystallographic leaving invariant a four-dimensional lattice and the corresponding decagonal $\mathbb{Z}$-module M_{10} of rank $n = 4$ and dimension $d = 2$ obtained by projection. The scaling transformations are not symmetry of the pentagram because of infinite order, even if they allow an integral indexing of the vertices. They are possible symmetries of a decagonal (infinite) quasicrystal but are not elements of the superspace group because in the (n, d)-dimensional superspace approach the point groups are restricted by the physical dimension d to be finite subgroups of the orthogonal group $O(d)$ (Janssen *et al.*, 1999).

Looking for finite point-group symmetry of the pentagram which takes into account its scaling properties, the idea came to extend the superspace approach to finite subgroups of $O(n)$ leaving, in projection, the $\mathbb{Z}$-module M invariant. One possible solution is shown in Fig. 1(*a*). All vertices of the pentagram are points of the decagonal $\mathbb{Z}$-module M_{10} and are obtained as [1100] orbit of the crystallographic point group $K = 54$ of order 20, generated by the two four-dimensional matrices of order 5 and 4, respectively,

$$R_5 = \begin{pmatrix} 0 & 0 & 1 & \bar{1} \\ 0 & 0 & 0 & \bar{1} \\ 0 & 1 & 0 & \bar{1} \\ 1 & 0 & 0 & \bar{1} \end{pmatrix}, \quad R_4 = \begin{pmatrix} 1 & 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 & 0 \\ 1 & 0 & 0 & \bar{1} \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad (1)$$

indicated by the isomorphism type 20.5 on p. 242 of the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (BBNWZ) (Brown *et al.*, 1978). In a similar way, the hexagram of Fig. 1(*b*) is generated from $[1\bar{1}0]$ by the cubic point group $m\bar{3}m$. The corresponding $\mathbb{Z}$-module M_6 is the hexagonal lattice, projection along the [111] direction of the cubic lattice. The star octagon {8/3} of Fig. 1(*c*) is obtained as [1100] orbit of the four-dimensional octagonal point group $K = 82$ of order 16 (indicated in BBNWZ as 16.13 on p. 245) generated by the two matrices of order 8 and 2, respectively:

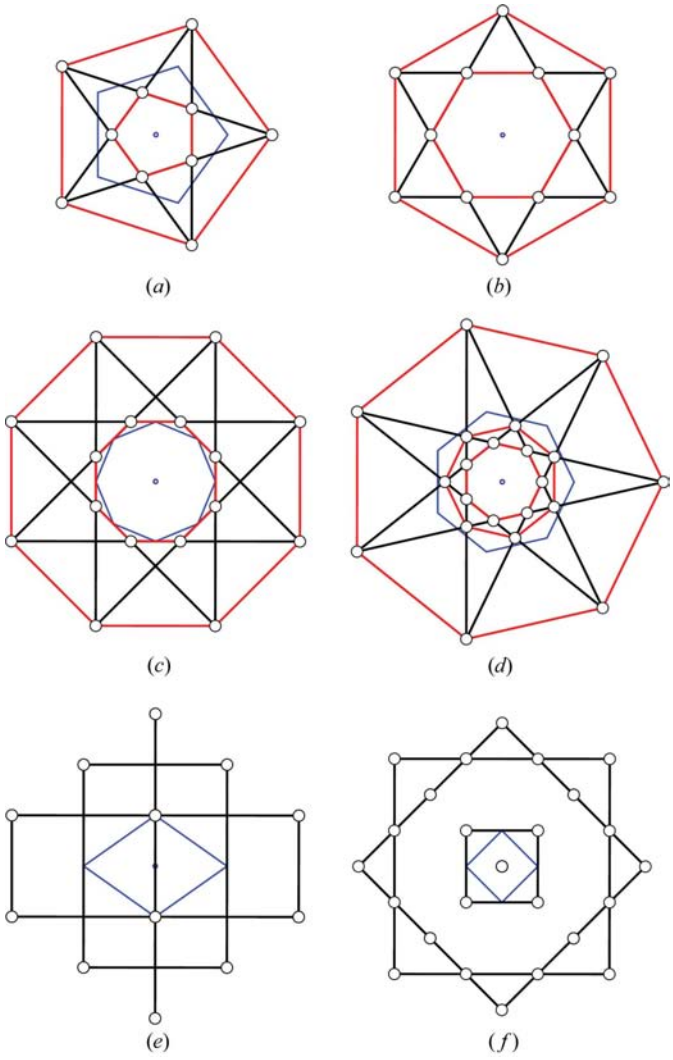

Figure 1
Orbit points of an n-dimensional point group K of order $|K|$ generated from an element P of a $\mathbb{Z}$-module of dimension 2 and rank n, with basis vectors pointing to the vertices of the (blue) polygon indicated. (*a*) Pentagram {5/2} ($n = 4$, $K = 54$, $|K| = 20$, $P = [1100]$). (*b*) Hexagram {6/2} ($n = 3$, $K = m\bar{3}m$, $|K| = 48$, $P = [1\bar{1}0]$). (*c*) Octagram {8/3} ($n = 4$, $K = 82$, $|K| = 16$, $P = [1100]$). (*d*) Heptagrams {7/2}, {7/3} ($n = 6$, $K = 73$, $|K| = 21$, $P = [111000]$). (*e*) Cluster of K-equivalent points of a $2^{1/2}$-rectangular lattice ($n = 3$, $K = m\bar{3}m$, $P = [120]$). (*f*) Cluster of K-equivalent points of a square lattice ($n = 4$, $K = 86$, $|K| = 384$, $P = [1110]$).

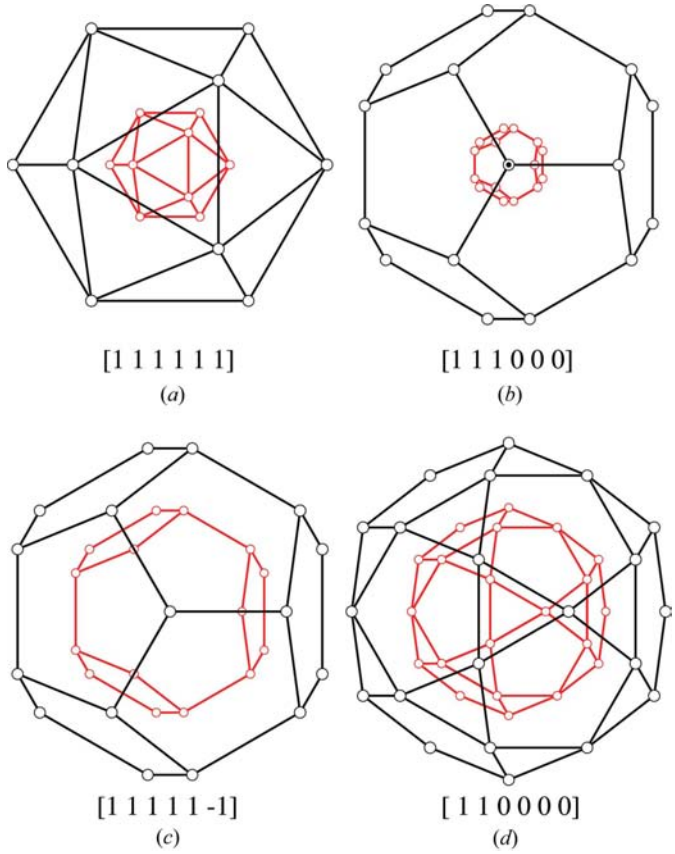

Figure 2
The six-dimensional point group $K = 2354$ of order 240 applied to the indexed elements indicated of the three-dimensional icosahedral $\mathbb{Z}$-module generates cluster models of a viral capsid enclosed between two scaled icosahedral forms. (*a*) τ^2-scaled icosahedra. (*b*) τ^3-scaled dodecahedra. (*c*) τ-scaled dodecahedra. (*d*) τ-scaled icosidodecahedra.

$$R_8 = \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad R_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (2)$$

In Fig. 1(*d*), one finds a more complex heptagonal arrangement involving both heptagrams {7/3} and {7/2} as a single [111000] orbit of the six-dimensional point group $K = 73$ of order 21 generated by the two matrices of order 3 and 7, respectively:

$$R_3 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad R_7 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \bar{1} \\ 1 & 0 & 0 & 0 & 0 & \bar{1} \\ 0 & 1 & 0 & 0 & 0 & \bar{1} \\ 0 & 0 & 1 & 0 & 0 & \bar{1} \\ 0 & 0 & 0 & 1 & 0 & \bar{1} \\ 0 & 0 & 0 & 0 & 1 & \bar{1} \end{pmatrix}. \quad (3)$$

3. Superspace holohedry of integral lattices

The peculiar rational value of the axial ratio squared, $\gamma^2 = (c/a)^2$, of integral lattices can possibly be implied by a higher-dimensional holohedry. In the present sketchy exemplification, the $\gamma = 2^{1/2}$ rectangular lattice appears as a $\mathbb{Z}$-module defined by the cubic lattice projected along the twofold axis [110], as shown in Fig. 1(*e*) in terms of the [120] orbit points of the cubic $m\bar{3}m$ point group. In a superspace characterization, the (3, 2)-dimensional holohedry of this integral lattice is $m\bar{3}m$. A less trivial example is given in Fig. 1(*f*), with points of a square lattice (which is of course integral) obtained as [211] projection of Frank's cubic hexagonal lattice with axial ratio $(3/2)^{1/2}$ (Frank, 1965; Janner, 2004*b*). In this case, the higher-dimensional holohedry is the four-dimensional hypercubic point group $K = 86$ of order 384 (indicated on p. 255 of BBNWZ as 384.1) generated by a matrix of order 8 and one of order 6:

$$R_8 = \begin{pmatrix} 0 & 0 & 0 & \bar{1} \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad R_6 = \begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (4)$$

acting on [1110]. These orbit points recall the (projected) vertices of the cubic form enclosing the RNA guanosine-5′-phosphate quadruplex (Janner, 2004*a*, 2007).

4. Viral capsid

According to a (6, 3)-dimensional superspace approach, the capsid of icosahedral viruses, whose surface is delimited by an external and an internal form, respectively, can be characterized in terms of two polyhedra generated as an icosahedral cluster from one single point of the icosahedral lattice by the action of a six-dimensional point group, in a crystallographic scaling relation similar to that observed in the rhinovirus and in a few other viruses analysed so far (Janner, 2006*a*,*b*). Indeed, the models of viral capsid shown in Figs. 2(*a*), (*b*), (*c*), (*d*) represent the orbits of the icosahedral lattice points indicated, by the action of the group $K = 2354$ of order 240, semidirect product of the icosahedral group 235 by a cyclic group of order 4, generated by the six-dimensional integral matrices

$$R_3 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{1} \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \quad R_5 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

$$R_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \bar{1} \\ 0 & 0 & 0 & \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} & 0 & 0 & 0 \end{pmatrix}. \quad (5)$$

5. Concluding remarks

In the superspace crystallography extended to higher-dimensional point groups, the rational indices of enclosing forms of biomacromolecules and of icosahedral viruses and their crystallographic scaling properties appear to be the simple consequence of a higher-dimensional point-group symmetry. No form lattice is then required. Indeed, a crystallographic point group being faithfully represented by integral matrices transforms a given position with integral indices (which are the coordinates of the point in the corresponding lattice or $\mathbb{Z}$-module) into other atomic positions with integral indices. In a similar way, the rational indices of a regular hexagon are obtained by applying the two-dimensional matrix group 6 to the point [1, 0] without the explicit need of a hexagonal lattice. Moreover, the axial ratios of integral *d*-dimensional lattices, leading to a reduced number of lattice parameters, could follow from their (*n*, *d*)-holohedry, which is not a *d*-dimensional one. In the crystal case, the problem is not the finite width of the peak assigned to a given integral lattice. As remarked by one of the referees, the concept of the Bärnighausen family tree of crystallographic group–subgroup relations, the 'Stammbaum', is based on the fact that most real structures slightly deviate from ideal ones (Bärnighausen, 1980). Moreover, the Pearson symbol forms clouds in the parameter space, structures of the same structure type having a given number of atoms in the unit cell of a Bravais lattice. Interestingly enough, in the implementation of structure types adopted in the Inorganic Crystal Structure Database ICSD, the range of axial ratios $\gamma = c/a$ is one of the criteria adopted (Allmann & Hinek, 2007). The problem is that the two ideal cases, that of integral lattice and that of normal lattice, occur together in the same peak and cannot be distinguished by

means of the known crystallographic laws. If, however, the holohedry of an integral lattice is different from that of the corresponding normal lattice, then the Wyckoff positions are also different and, in principle at least, one should be able to identify a different behavior of structures involved in the given peaked distribution. Typical for the set of equivalent positions of higher-dimensional point groups is its composite character with respect to the Euclidean symmetry in the lower-dimensional space, as one can see in all the examples shown in Figs. 1 and 2. This is a hint to look at the content of a unit cell (as in Pearson's symbol). Analogous considerations arise from the molecular cases, where a distinction between enclosing form (geometric, symmetric and ideal) and content (where the real atoms are) is essential, as well as the composite character of the form which has external and internal boundaries in a mutual relation. So, for example, a hexagrammal form implies a regular hexagon inside an external one in a well defined scaling relation. As in the case of aperiodic crystals, higher-dimensional crystallography is not enough to be relevant to real structures. One has to find out the possible actions of an n-dimensional group in the d-dimensional physical space, which in fact are expressible in terms of group representations.

These considerations need not all be true and are, so to say, working hypotheses. In the same perspective, the examples given do not prove that all the crystallographic puzzles mentioned in the *Introduction* are covered by this superspace approach. Many implications, like those obtained by intersection, an operation dual to projection, have not even been mentioned and the conceptual foundation of the whole is not yet worked out. Potentially, however, these ideas open the possibility of applying to natural structures like crystals, quasicrystals and molecules the overwhelming wealth of the higher-dimensional crystallographic groups. These groups have already been classified by mathematicians up to dimension 6, and there are computer algebra programs allowing the consideration of higher dimensions as well (Brown *et al.*, 1978; Eick *et al.*, 1997; Opgenorth *et al.*, 1998; Thiers *et al.*, 1993; GAP, 2006). In addition to the conceptual basis of an extended (n, d)-dimensional crystallography, the implications of the approach (like extinction rules in diffraction, normal modes of vibration and so on) have to be worked out and verified to be applicable.

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