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It's all in the group

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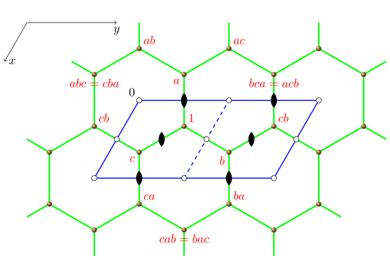
The space group of a crystal structure is usually given by augmented matrices representing the action as affine mappings on direct space, but can also be described by generators and defining relators, *i.e.* by a group presentation. Related to the latter, the Cayley graph of a group is constructed in which the vertices correspond to the group elements and two vertices are connected by an edge if one is the product of the other with one of the generators. Baburin [*Acta Cryst.* (2026), A**82**, 18–31] shows how combinatorial and geometric information about a crystal structure and its symmetry group can be derived from the interplay between the Cayley graph and the group presentation.

1. Computing with the symmetries of crystals

The description of crystal structures has gone through various phases and transitions, ranging from the observation of the macroscopic shapes via the determination of the internal structure by X-ray diffraction to more recent approaches investigating the self-assembly from building blocks. Throughout these different developments, it turned out to be extremely useful to take the symmetry properties of the crystals into account. The symmetry perspective not only describes and explains properties of a particular crystal, more importantly it provides a hierarchical framework organizing the zoo of individual crystal structures into different classes by abstracting from part of the individual properties.

The most common description of the symmetry of a crystal is by its space group. We note that the updated definition of a crystal (Brock, 2021) also includes aperiodic crystals in which the long-range order is not realized by translational invariance. In this commentary, however, we restrict ourselves to the large class of *conventional crystals* which are periodic in three independent directions (in the standard case) and we omit the attribute 'conventional' from now on. The abstraction from a crystal structure to its space group is a powerful step. It turns out that many important properties of the crystal can be derived solely from the group itself. For example, the representations of a space group provide information about the energy band structure or the Raman and infrared spectra, and many aspects of phase transitions are governed by the group–subgroup relations between space groups.

A fresh perspective to deduce interesting information from space groups, or more generally crystallographic groups (built from a finite point group acting on a normal subgroup that is isomorphic to a finite-dimensional lattice) has recently been presented by Baburin (2026). Here, the description of a group by generators and defining relators plays a crucial role. To put this into perspective, it is useful to take a short look at the development of the algebraic treatment of crystallographic groups. After Fedorov and Schoenflies had established the



correct list of 230 space group types in 1891, the fast development of general group theory led to a more systematic (and simpler) algebraic derivation. Important first steps were set by G. Frobenius, A. Speiser and J. J. Burckhardt and building on this a general method that is also applicable in dimensions higher than 3 was proposed by Zassenhaus (1948). The main ingredients of the Zassenhaus algorithm are the determination of the action of the point group on its invariant lattices, the solution of the Frobenius congruences (for which a presentation of the point group is required, see below) and the identification of orbit representatives under the action of the normalizer of the point group. In current computer algebra systems like *GAP* (The GAP Group, 2025) or *Magma* (Bosma *et al.*, 1997), all the required facilities are available as standard functions and an exercise like enumerating the almost 29 million crystallographic groups in dimension 6 (Plesken & Schulz, 2000) can by now be regarded as a routine task. As important as the enumeration of crystallographic groups is to get a complete overview of the different possibilities, in many cases one is more interested in specific properties of a single group. For that it is desirable to have available the full tool box from computational group theory. In particular, it often turns out to be advantageous to work with a *presentation* of a group, consisting of (abstract) generators and defining relators. For a group $\mathcal{G}$ generated by elements $g_1, \ldots, g_k$, a relator is a *word* in the g_i and their inverses g_i^{-1} that equals the identity element in $\mathcal{G}$. A set of defining relators is then a set of relators from which all other relators can be derived by insertion and deletion of the defining relators and of the trivial relators $g_i g_i^{-1}$ and $g_i^{-1} g_i$. For example, the dihedral group D_n of order $2n$ generated by two reflections whose composition is an n-fold rotation has the presentation $\langle r, s \mid r^2, s^2, (rs)^n \rangle$. If one omits the third relator, the element rs is turned into an element of infinite order and the group $\langle r, s \mid s^2, r^2 \rangle$ becomes the infinite dihedral group D_∞. This is realized for example as the frieze group $p1m1$ generated by two reflections in parallel lines having as their product $t = rs$ a translation by twice the distance between the reflection lines.

Since the manipulation of group presentations by hand is limited to very small examples, algorithms for finitely presented groups were among the first (besides algorithms for permutation groups) to be implemented on computers. Many of the fundamental methods were actually developed in the pre-computer era, such as Tietze transformations (Tietze, 1908) to simplify presentations and the Todd–Coxeter coset enumeration (Todd & Coxeter, 1936) to compute the permutation action on the cosets of a subgroup. An application of coset enumeration that is very useful for the analysis of group–subgroup relations is the determination of all subgroups with index up to a given bound (Dietze & Schaps, 1974). To obtain a presentation for a group can in general be a difficult task, but for crystallographic groups it is straightforward. For a group $\mathcal{G}$ with a normal subgroup $\mathcal{T}$ and known presentations for $\mathcal{T}$ and the quotient group $\mathcal{G}/\mathcal{T}$, a presentation for the full group can be constructed by extending those of the two parts by the conjugation action of generators for $\mathcal{G}$ on the generators of $\mathcal{T}$.

In terms of the state-of-the art facilities from computational group theory, crystallographic groups form a very accessible class of groups and it seems fair to say that in low dimensions (at least up to 6), basically every desired kind of information can be computed very quickly. This is exploited in various clever ways by Baburin (2026).

2. Cayley graphs for crystallographic groups

One of the advantages of working with presentations of groups is that only intrinsic properties of the groups are required. On the other hand, most groups are of interest because they act on certain types of objects. For crystallographic groups this can be points, lines or planes in direct or reciprocal space, but also the cells of a Voronoi tessellation or coordination polyhedra of a crystal structure. If in a crystal structure the focus is put on the atoms and the bonds between them, this can be described by the combinatorial structure of a graph, consisting of vertices (representing the atoms) and edges between some of them (representing the bonds). This graph is naturally embedded into space and an element of the space group of the crystal induces an automorphism of the graph if edges are mapped to edges and non-edges to non-edges (which is usually the case, since the types of atoms and their distances are preserved). One can, however, also proceed in the opposite direction: start with a graph and its automorphism group and try to construct an embedding of the graph into space, *e.g.* by a barycentric embedding (Delgado-Friedrichs & O'Keeffe, 2003), so that the graph automorphisms are realized by isometries and thus elements of a space group.

In this context, a very useful combinatorial object on which a group acts and which only requires the group itself for its definition is the *Cayley graph* (or *Cayley diagram*) of the group. This graph depends on a set S of generators for $\mathcal{G}$, the vertices are taken to be the elements of $\mathcal{G}$ and two elements $g, h \in \mathcal{G}$ are connected by an edge if $h = gs$ for some $s \in S \cup S^{-1}$ (so that $g = hs^{-1}$ gives the same edge). An important feature of the Cayley graph is that relators in the given generators S correspond to cycles in the graph. The action of $\mathcal{G}$ on its elements by left-multiplication gives an automorphism of the Cayley graph and this action is what is called a *regular action*: all vertices lie in a single orbit and the stabilizer of each vertex is trivial. Since $\mathcal{G}$ acts transitively on the vertices, the local configuration around each vertex is the same and looking at the cycles containing the identity element gives a complete overview of all the cycles in the graph. If, conversely, a group acts regularly on a graph, identifying one vertex with the identity element and taking the elements mapping this vertex to its neighbours as generators turns the graph into the Cayley graph of the group with respect to these generators. Baburin (2026) considers a slightly more general situation. If a graph has a transitive automorphism group, the stabilizers of the vertices are conjugate and in particular all have the same order. One can then look for a subgroup which acts regularly on the graph (for that its index in the full group must necessarily be equal to the order of the vertex stabilizers) and then the given graph can be identified with the Cayley graph of this subgroup. The advantage of starting with a graph and then identifying a group for which this is the Cayley graph is that for the graph of a crystal structure (that is *a priori* embedded into space) one gets an embedding of the Cayley graph for free.

A simple but illustrative example, borrowed from Baburin (2026), is based on the honeycomb net **hcb** as displayed in Fig. 1. Considered as a two-sided structure, its automorphism group is the layer group $p6/mmm$ having the point group $6/mmm$ of order 24. Since the stabilizer of a vertex is the site-symmetry group $\bar{6}m2$, a subgroup acting regularly on the net must have index 12. A suitable subgroup of type $p112/b$ is generated by the three elements $a = 2(0, 1/2, z) : -x, 1-y, z$, $b = \bar{1}(1/2, 1, 0) : 1-x, 2-y, -z$ and $c = 2(1/2, 1/2, z) : 1-x, 1-y, z$, where the coordinates are given with respect to the unit cell of the **hcb** net (small cell with one side dashed). Note that the point group of $p112/b$ has only index 6 in the point group of $p6/mmm$, the total index of this subgroup is 12 because the unit cell is doubled, the generating translations are $ca = t(1, 0, 0)$ and $(bc)^2 = t(0, 2, 0)$ [the element bc is the b glide $b(x, y, 0) : x, 1+y, -z$].

A presentation of $p112/b$ on the generators a, b, c is $\langle a, b, c \mid a^2, b^2, c^2, (abc)^2 \rangle$. Putting the identity element of $p112/b$ on the vertex at $\frac{1}{3}, \frac{2}{3}, 0$, the **hcb** net is precisely the Cayley graph of $p112/b$. The elements given by words up to length 3 are given (in red) in Fig. 1. The three hexagons around the identity element correspond to the relators $(abc)^2$, $(bca)^2$ and $(cab)^2$ (where the second and third ones are simply cyclic rotations of the first one).

To obtain a Cayley graph that has a meaningful geometrical interpretation, the choice of generators is crucial. Since the generators correspond to the edges having as one endpoint the identity element of the group, generators should be chosen for which the geometric elements are located close to each other and so that they map the vertex of the identity element to a vertex nearby. This has the side effect that short translations will be generated as short words in the generators. Note that this principle for the choice of generators for the space groups is different from that followed in the *International Tables for Crystallography* (Aroyo, 2016). There, the generators are chosen along an ascending chain of subgroups (starting from the translation subgroup) so that adding the next generator yields a supergroup that lies in a crystal system of higher symmetry. Although a presentation along this chain provides a lot of information about the group, it often requires more generators and more and longer relators than necessary and a Cayley graph based on these generators is typically of little geometric significance.

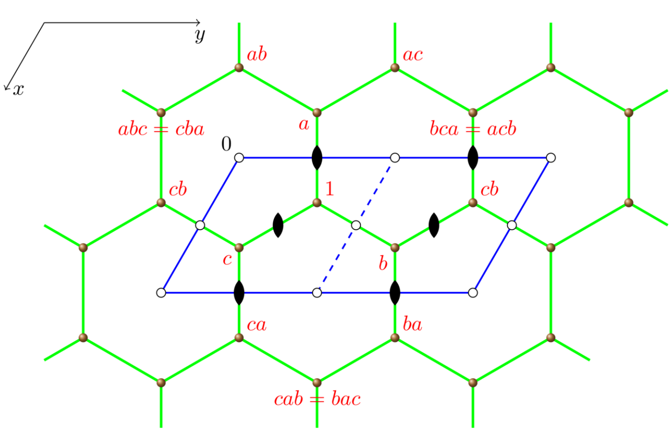


Figure 1
Realization of the honeycomb net **hcb** as the Cayley graph of a layer group of type $p112/b$. Figure adapted from Baburin (2026).

It is demonstrated by Baburin (2026) that the Cayley graphs corresponding to short presentations of crystallographic groups, *i.e.* presentations on few generators with a small number of short relators, often correspond to periodic graphs that are relevant for the investigation of crystal structures. With the presentation and the Cayley graph at hand, useful combinatorial and geometric information can be derived. For example, the lengths of cycles attached to a vertex and their number can be determined, because cycles correspond to relators in the presentation. Also, relations between the cycles become transparent. A simple example already observed in the example of the **hcb** net are the cyclic rotations of a relator, which immediately give cycles of the same kind starting at the same vertex. Only slightly more complex, splitting a relator into a product $r = r_1 r_2$ of two subwords gives the relation $r_1 = r_2^{-1}$ and if one of the parts is found in a different relator, then replacing this subword by the other gives rise to a new cycle.

The interplay between the Cayley graph and the presentation of its group can be taken much further. In general infinite graphs, local automorphisms are characterized by the property that the distance between each vertex and its image is bounded. A typical example are the translations in a periodic graph. A compact representation of a graph is obtained by forming the quotient graph with respect to a subgroup of local automorphisms (Eon, 2005), where the orbits of the subgroup on the vertices are taken as vertices of the quotient graph. In some cases, such a quotient graph has itself a physical realization such as a nanotube formed from the honeycomb net by rolling it up along a suitable translation. The corresponding operation in the group is to divide out the normal subgroup generated by the translation and in the presentation of the group this simply means to add the word representing the translation as a new relator.

Summarizing, the article by Baburin nicely demonstrates several novel ways to derive interesting information about crystal structures and their symmetry groups by a clever combination of methods from computational group theory and graph theory. In some cases, the new perspective simplifies the derivation and clarifies the understanding of known properties, but it also leads to new results. It can be expected that further creative ideas on the interplay between crystallographic groups, their presentations and their Cayley graphs will provide valuable insights for the investigation of crystal structures.

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