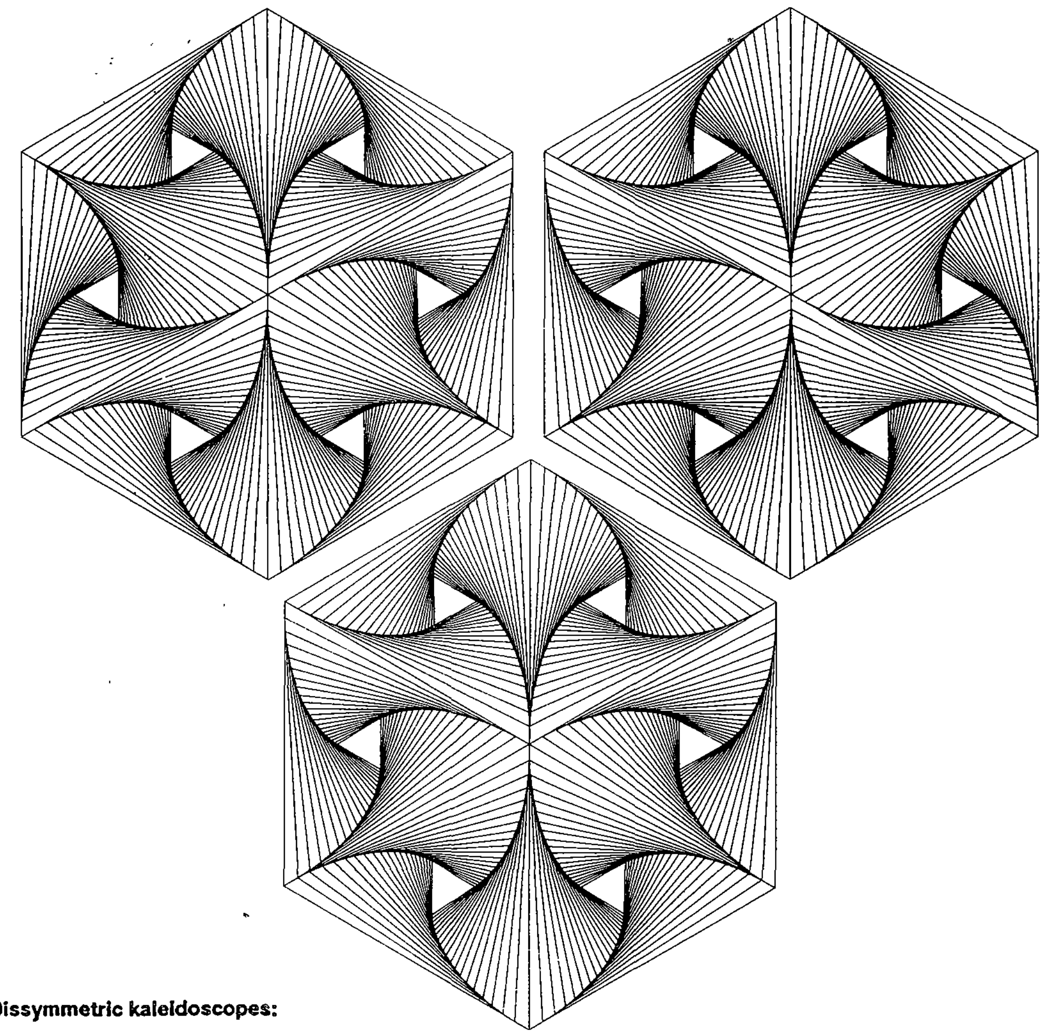
Symmetry: Culture and Science

SPECIAL ISSUE
Symmetry in a Kaleidoscope 3

The Quarterly of the
International Society for the
Interdisciplinary Study of Symmetry
(ISIS-Symmetry)

Editors:
György Darvas and Dénes Nagy

Volume 1, Number 3, 1990



Dissymmetric kaleidoscopes:
Hommage à Pasteur

Symmetry: Culture and Science
Vol. 1, No. 3, 1990, 313-318

SYMMETRY IN CRYSTALLOGRAPHY AND IN EVERYDAY LIFE

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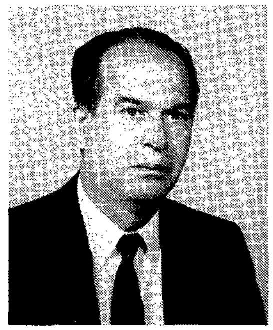


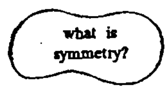
Fields of interest: Crystallography, mineralogy.

Award: Calouste Gulbenkian Foundation Scientific Award (1976).

Publications: A condensed way of representing inorganic close-packed structures, *Zeitschrift für Kristallographie*, 122 (1965), 346-358; Classification, notation and ordering on a table of inorganic structure types, *Journal of Solid State Chemistry*, 16 (1976), 7-20 (with Figueiredo, M.O.); Rules governing the layer organization of inorganic crystal structures, *Zeitschrift für Kristallographie*, 148 (1978), 1-5; Proper layer description and standard representation of inorganic structure types, *Acta Crystallographica*, B39 (1983), 317-323; A proposal for a structural classification of minerals, *Garcia de Orta: Serie de Geologia*, 6 (1983), 1-14.

Show: *Condensed models of crystal structures*, in the exhibition of teaching aids, organized by the Teaching Commission of the International Union of Crystallography, during the XII Congress of the International Union of Crystallography (Hamburg, 9-18 August, 1984).

QUESTION 1



Symmetry is a complex concept with various aspects and characteristics. There are several kinds of symmetry; one of these kinds of symmetry is crystallographic symmetry.

According to Bernal, Hamilton, and Ricci (1972, p. 9) : "The word [symmetry] is constructed of the Greek root *metron*, to measure, and the prefix *syn* (becoming *sym* before the letter *m*), along or together. To measure together? Two or more aspects of a symmetric figure do have the same measure. Symmetry is the characteristic of a pattern or object that leads us to say two or more parts of it are in some respects the same: this part is like that part." Therefore *symmetry means essentially repetition*.

Another important aspect is the fact that *there are several kinds of symmetry*. In the 18th century, symmetry, in a general sense, and in particular in art, expressed a well-proportioned, or well-balanced, figure or pattern. Only when crystallography developed, has the concept of symmetry been used with a different meaning: "a sort of concordance of several parts by which they integrate into a whole" (Weyl, 1952, p. 3). There are several definitions of symmetry suitable for the various purposes and kinds of objects concerned: decorative patterns, animals, plants (like flowers, some with fivefold symmetry), crystals, etc.

Moreover, *symmetry is a relative concept*, that is, it depends on the properties of the object we are considering. "Any particular object may or may not exhibit a specific symmetry, depending on the properties singled out and on the internal structure which we happen to be considering" (Shubnikov and Koptsik, 1974, p. 127).

We have considered some basic characteristics of symmetry. Now we shall look more deeply at its meaning. Although symmetry is essentially repetition, it is not only this. *The repetition has to be performed in a certain regular way*. For instance, Figure 1 shows clearly this aspect. According to Shubnikov and Koptsik (1974, p. 5): "A symmetrical figure must have, in addition to geometric equality of its parts (a), identical arrangement of the parts (b)" (Fig. 1).

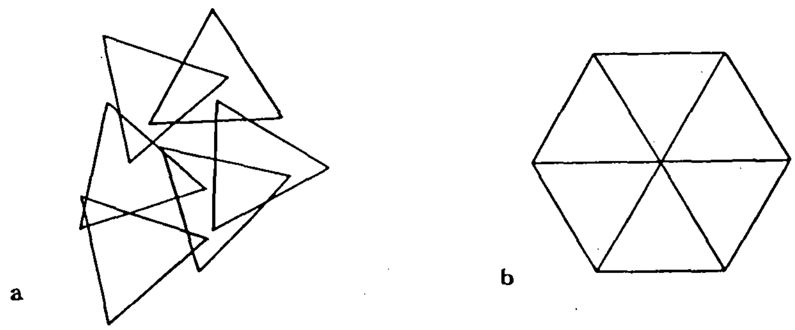


Figure 1: Asymmetrical (a) and symmetrical (b) figure (after Shubnikov and Koptsik, 1974).

Moreover, according to Helen Megaw (1973, p. 118): "An object possesses certain symmetry if after the application of a particular operation it looks exactly as it did before and continues to do so, however, often the operation is repeated. For instance, an hexagonal prism looks exactly the same after rotation through 60°". Therefore, as Fedorov (1901, p. 28) said: "Symmetry is the property of geometric figures to repeat their parts, or more precisely, it is the property of figures in different positions to bring them in coincidence with the figures in the initial positions".

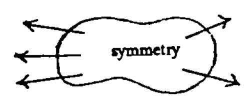
The repetition may be imagined as generated by a geometrical process, or symmetry operation, which brings the whole figure to another position coincident with the original figure. This can only be achieved if the shape, angles and size of its parts are equal.

Therefore, *equality of the parts, and coincidence of the whole figure* after a symmetry operation, *are also very important characteristics of symmetry.*

One of the kinds of symmetry is crystallographic symmetry. To describe the repetition of faces in a crystal, various symmetry operations were imagined, normally the simplest ones, the so called elements of symmetry, and it has been concluded that a reduced number of these elements of symmetry was sufficient to describe the different arrangements of equal faces in crystals. Later on, with the advent of the periodic theory, or lattice theory of the crystalline matter, a mathematical deduction of these elements was possible for the morphological domain, and it was found that only certain elements of symmetry and 32 combinations of them were compatible with the crystalline matter, the so called 32 crystal classes of symmetry. With the development of the study of the internal symmetry of crystal structures, other elements of symmetry, involving infinitely repeated translations, were considered, and the 230 space groups were established.

It was found that these elements of symmetry, either concerning the morphological aspect of a crystal or the internal crystal structure, form a group in the mathematical sense, and crystallographic symmetry could be expressed in terms of mathematical group theory. According to Wondratschek (1983, p. 714): "The properties (*a*) to (*d*) are the group axioms. Thus the set of all symmetry operations of an object form a group, *the symmetry group of the object* or its *symmetry*."

QUESTION 2



The measure of symmetry

In crystal chemistry we need quite often to compare the symmetries of two crystal structures, and to judge which has higher symmetry. To solve this problem it is necessary to be able to measure the symmetry.

The Laves principles of stability of crystal structures applied to alloys express two strong tendencies: one for higher symmetry (symmetry principle), and another for close packing of the atoms (space filling principle). It is relatively simple to measure the packing density, but to measure the symmetry is a difficult problem.

On the other hand it is well known that when dealing with phase transitions we also face the need of comparing symmetries. In fact, according to Helen Megaw (1973, pp. 510 and 472), "pseudo-symmetric structures are always likely to undergo transition to the high-symmetry form", and "a high-symmetry structure tends to have a higher entropy (and therefore lower free energy)", and again "the higher-temperature phase is not necessarily characterized by the higher symmetry".

In order to compare the symmetries of two structures one can use group-subgroup relations, but this subject has been treated only in an implicit manner (see, for instance, Vol. A of the *International Tables for Crystallography*, edited by Hahn, 1983, pp. 726-728 and 774-780) and can lead to ambiguous results. Therefore there is a real need for an explicit and precise definition of the measure of symmetry.

Although symmetry is essentially repetition in a certain regular way, repetition by itself can not be a measure of symmetry. In fact, if we compare a cube and a hexaoctahedron [see on p.318-eds.], the number of repeated faces in the cube is 6, and that in the hexaoctahedron is 48, but we cannot say that the hexaoctahedron has higher symmetry than the cube, because they have exactly the same symmetry.

What defines the crystallographic symmetry of these two forms is the group of elements of symmetry which is the same for both, and what should measure the symmetry is not the actual repetition of the faces, but the maximum number of repetitions generated by these elements of symmetry. This obviously occurs when the face is in a general position. This number measures the "power of repetition" or "symmetry capacity" of these elements of symmetry, and corresponds to the multiplicity of the general form (Lima-de-Faria, 1988), which is 48 in this case.

We can then purpose that the crystallographic symmetry of a pattern should be measured by the capacity of symmetry, or power of repetition of its elements of symmetry.

A pattern may be finite (a figure or a form), or infinite (in two or three dimensions). In the case of a figure or a form (e.g., a crystal in the morphological sense) the symmetry capacity of a group of its elements of symmetry corresponds to the multiplicity of the general form, or the *order of the point group* (Vol. A of the *International Tables for Crystallography*, edited by Hahn, 1983, p. 750).

For the two- and three-dimensional infinite patterns, using the same criterion, we have to order them by the *multiplicity of the general position* of the corresponding crystallographic *space groups* (Lima-de-Faria, 1988).

Applying our definition to the comparison of two infinite patterns corresponding to the plane groups *pm* and *cm* (we chose plane groups for reasons of simplification), we find that the multiplicity of *pm* is 2 and that of *cm* is 4, therefore the symmetry of *cm* is higher than that of *pm* (Fig. 2). Moreover, not only the multiplicity is higher in *cm* but more elements of symmetry are present, namely the glide lines.

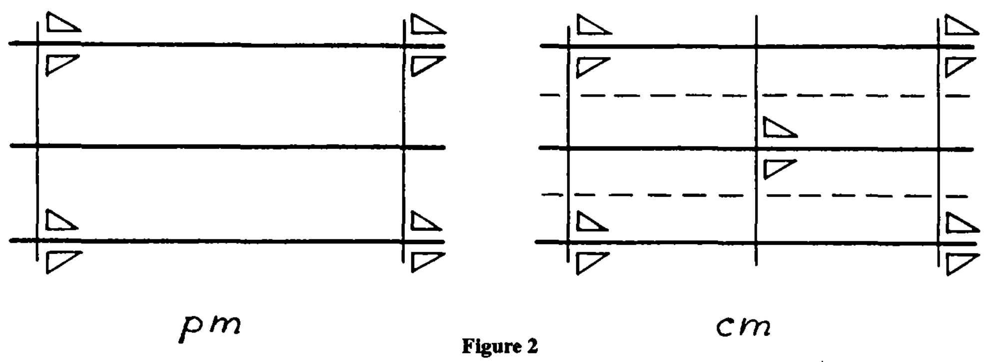
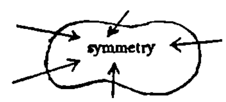


Figure 2

Group-subgroup relations when applied to these examples may give rise to contradictory results, depending on the sense and mechanism of the transition we use. It seems that in group-subgroup relations there is an interconnectivity between symmetry and density of symmetry which gives rise to this ambiguity. Such situation might possibly be solved if symmetry and density of symmetry are treated separately.

Our proposal, which is independent of the symmetry density, is in complete agreement with the group-subgroup theory in what regards the comparison of point groups. Only in respect to space groups there is divergence. Moreover, this proposal of the definition of the measure of symmetry corresponds to the natural extension, from point group to space group. In fact, the multiplicity of the general form in point groups corresponds to the multiplicity of the general position in space groups.

QUESTION 3



Symmetry in everyday life. Symmetry and harmony.

Symmetry has been a synonym of harmony, in the sense that it corresponds to a certain balance between change and invariance. In everyday life there are several examples of harmony which may be considered as a certain kind of symmetry.

If one looks at the word harmony in a dictionary, one realizes that a possible synonymous is symmetry. Harmony and symmetry are in general interconnected in common language.

According to Shubnikov and Koptsik (1974, p. ix) "[Symmetry] has two opposing aspects: transformation (change) and conservation (invariance)" ... "the set of transformations which keeps something invariant is its symmetry group". As Goethe (1808, p. 273) said "in the beginning was action", and the Portuguese poet Camões (16th century, p. 143) also stated that "all the world is made of change". It is clear that the essence of life and existence is the difference. However this does not mean that too much difference is the best. It is also important to keep a certain base unchanged, a certain continuity where this difference is settled and gets significance. One needs change (or action) to feel alive, but one also needs security (invariance, something already known) to feel that the action is in a good sense. Complete change, or disorder, is very painful. Therefore the *harmony in life* seems to correspond to the balance between change and permanence (invariance), which may be considered as a kind of symmetry.

There are many other aspects of symmetry in everyday life, and one common example is the harmony of clothes. In fact, there is a general tendency to use similar colours in the different parts of the clothes, which again may be considered as a certain kind of symmetry.

The strait relationship between harmony and symmetry has already been emphasized by Shubnikov and Koptsik (1974, pp. 309 and 373): "Ideas of symmetry (literally *proportionality*) arose among the ancient Greek philosophers and mathematicians in connection with their study of *harmony* of the world", and furthermore "The magic land of harmony and symmetry lies open for exploration".

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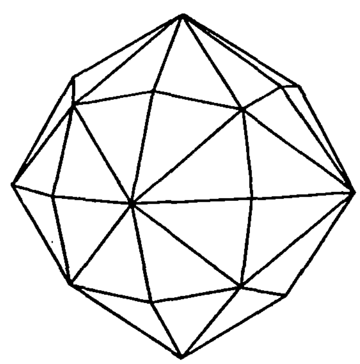
Editors' note:



The *hexoctahedron*, or *hexakisoctahedron*, is a polyhedron shaped by 48 (= 6 × 8) faces – see Figure. It has a remarkable property: all the faces of the polyhedron are equal (congruent). In a forthcoming issue we will return to the topic of *equifaced polyhedra*.