



Crisp and Fuzzy Motif and Arrangement Symmetries in Composite Geometric Figures

A. E. KÖHLER

Lehrstuhl Biophysik, Institut für Biochemie und Biophysik
Friedrich-Schiller-Universität Jena, Philosophenweg 12, D-07743 Jena, Germany

(Received April 1993; accepted May 1993)

Abstract—The notions of motif and arrangement symmetries within composite geometric figures are defined. The relationships between these types of symmetry and the symmetry of the whole figure are clarified by making use of the crystallographic concepts of site symmetry and direction symmetry. From this, it has been deduced that a figure with arbitrary symmetry can be assembled from motifs of likewise arbitrary symmetries. If a motif with symmetry G_M is placed on a site having the site symmetry $G_S \subseteq G_M$, its contribution to the figure symmetry G is only a subgroup G_{MO}^* of its direction symmetry G_{MO} where $G_S = G_{MO}^* \subseteq G_{MO} \subseteq G_M$. Supernumerary symmetry elements of the motif give rise to *intermediate* or *latent* symmetries of the figure. A consequent decomposition of a geometric figure into its constituent *points* reveals that a large part of the $O(n)$ symmetry of every single point is lost when assembling these points to build up the figure. All “lost” symmetries can, however, be detected as *intermediate* symmetries of this figure. They can be displayed as *fuzzy symmetry landscapes* and *symmetry profiles* for a given figure showing all crisp and intermediate symmetries of interest.

1. INTRODUCTION

Symmetry of a geometric figure manifests itself most obviously in a regular repetition of certain motifs which are reproduced by reflections, rotations, translations and/or other symmetry operations of this figure (see, e.g., [1,2]). An example is given in Figure 1a. There are, however, instances where symmetries which lead to the repetition of a motif will afterwards *not* (within a fuzzy symmetry concept: *only partly*) appear in the symmetry of the resulting geometric figure. In Figure 1b, the mirror lines 2 to 5 are not part of the symmetry of the whole figure, they are only *local* symmetry elements: lines 4 and 5 are symmetry elements for two “I” motifs each, whereas lines 2 and 3 are only symmetry elements of the motifs they intersect. On the other hand, symmetry lines 0 and 1 coincide with the mirror lines of the whole figure, they are *global* symmetry elements. Shubnikov and Koptsik [3] describe a nice method of preparing figures with local symmetry lines by cutting out figures from irregularly folded paper.

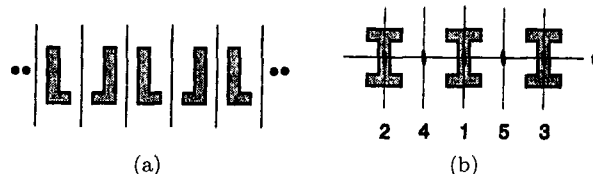


Figure 1. Endless repetition of an “L” motif by reflections and translations which are symmetry operations of the resulting infinite geometric pattern (a), and a geometric figure assembled from three “I” motifs (b). The mirror lines 2 to 5 and the C_2 axes (●) on them are not crisp symmetry elements of the whole figure, whereas the mirror lines 0 and 1 and the C_2 axis on them are.

From the viewpoint of *fuzzy symmetries* [4,5], a symmetry line which is a symmetry element of the *whole* figure is fully preserved in this figure. On the other hand, a symmetry line that is only a *local* symmetry element and is relevant for only a *part* of the figure is preserved only *partially* (to a degree below 100 per cent) during the composition of this figure, thus giving rise to an *intermediate symmetry*.

The fuzzy symmetry concept forms a sound basis for the qualitative and quantitative description of intermediate (approximate or latent) symmetries of a figure [4,5]. Such a description has been done in two ways: by using a Fourier series expansion of the form function [4] and by an approach involving fuzzy symmetry requirements [5]. Both methods give a degree of symmetry δ , which has been interpreted as degree of preservation of the respective symmetry element(s). Up to now, this fuzzy symmetry concept has been applied to simple geometric figures [4,5]. In this paper, it is used for the description and evaluation of fuzzy symmetries in composite geometric figures. The concept is applied to arbitrary geometric figures (not only figures that are regularly composed of repeated motifs). To this end, definitions of a degree of symmetry δ are developed which are especially suitable for discrete and continuous geometric figures. Then, δ will be displayed as *symmetry profile* or *symmetry landscape* for a given figure. This will reveal that there are fuzzy symmetries even in motifs which are conventionally termed asymmetrical. Before examining fuzzy symmetries in composite figures, however, the crisp symmetry relationships between motifs and the whole figure for regularly composed geometric figures have to be clarified.

2. MOTIF SYMMETRIES AND ARRANGEMENT SYMMETRIES IN FIGURES

2.1. Definition of Motif and Arrangement Symmetries

Parts of a geometric figure which are congruent, similar, or at least related to one another and by repetition build up the figure are termed “motifs” of this figure. Wolf [1,2] claims that a motif should be asymmetrical. A simple way to obtain an asymmetrical motif out of a symmetrical part of the figure is to cut this part along its symmetry elements—a method which R. B. Fuller used to produce the asymmetrical elementary motifs of symmetrical polyhedra [6]. Unfortunately, this method is *in praxi* not generally applicable: it fails, for example, in the case of a circle, a ring, or segments of them which *cannot* be cut along symmetry lines to give asymmetrical motifs. On the other hand, cutting a circle, ring, etc., *at will* results in pieces which do not *by repetition* form the whole figure, and therefore, could not be regarded as motifs. Since arbitrary geometric figures are to be considered in this paper, the condition of asymmetry of a motif has to be abandoned. This means, in turn, that the claim for repeatedness of a motif also has to be given up: a symmetrical motif does not need to be regarded as being built up by repetition of an asymmetrical element, and such a motif does not need to occur more than once in a figure¹. Therefore, I shall define a motif \mathcal{M} simply as a distinct part (a *logical unit*) or a subset of points of a geometric figure \mathcal{F} :

$$\mathcal{M} \subseteq \mathcal{F}, \tag{1}$$

regardless of its own symmetry or its repeatedness. With this definition, of course, the decomposition of a figure into motifs is not unique and can be adapted to the aims of the investigation, but this does not in any way restrict the general validity of the approach.

Figures that are composed of repeated motifs display two kinds of symmetries which I shall call *motif symmetry* and *arrangement symmetry*, respectively. A motif symmetry corresponds to all symmetry elements of a certain motif. They necessarily run through the centre of gravity of this

¹We will see that in a special position within a symmetrical geometric figure (namely, in the origin), a motif located there has to be unique and *cannot* be repeated. Generally, the number of repetitions of a motif will depend on its position within the figure (*vide infra*).

motif². The motif symmetries will normally be different for distinct sets of motifs within a figure; they often constitute only *local* symmetries. An arrangement symmetry, in turn, corresponds to all symmetry elements running through the centre of gravity of an n -tuple of motifs ($n \geq 2$, i.e., a pair, triple, quadruple, etc., up to the whole figure). It may in case of coincidence of local and global symmetry elements be equal to one or several motif symmetries. If a geometric figure can be reduced to mere asymmetrical motifs, then we have to deal exclusively with arrangement symmetries.

The relationships between motif symmetry and figure symmetry have been dealt with by Shubnikov and Koptsik [3]. They note that for a figure composed of geometrically different motifs (which cannot be converted into one another by motions or similarity transformations, e.g., a superposition of a square and a pentagonal sawtoothed star) with symmetries \mathbf{G}_1 and \mathbf{G}_2 (where none of these groups is a subgroup of the other), the symmetry \mathbf{G} of the resulting figure is given by the intersection $\mathbf{G} = \mathbf{G}_1 \cap \mathbf{G}_2$. During the formation of such a composite figure, a *dissymmetrisation* (symmetry reduction) of the system occurs. If, however, equivalent motifs are assembled in a regular manner, this results in a *symmetrisation*, i.e., the symmetry of the resulting figure is higher than the motif symmetry [3]. This is, however, not generally true. It is easy to convince oneself that it is impossible to assemble a finite number of icosahedra having the motif symmetry \mathbf{Y}_h ($2\mathbf{m}\bar{3}5$)³, to give a figure with a symmetry higher than \mathbf{Y}_h , or for cubes with symmetry \mathbf{O}_h ($\mathbf{m}\bar{3}\mathbf{m}$) to construct a figure with $\mathbf{G} \supset \mathbf{O}_h$. In other words, the above statement is true only for motifs with sufficiently low symmetries. In the following, I shall present a different approach to the description of the relationship between figure and motif symmetries by using the concepts of site symmetry [7,10–12] and direction symmetry [13] which are well-known in crystallography and solid state physics. Since a broader audience outside crystallographers may not be familiar with these notions, I shall describe them with examples in the following section.

2.2. The Concepts of Site Symmetry and Direction Symmetry

When using the site symmetry concept, the way of looking at the problem is from the finished figure backwards to the motifs which constitute it and not from the motifs towards the mode of assembling them. Therefore, the symmetry \mathbf{G} of the whole figure has to be pre-set. The notion of site symmetry, then, describes the symmetry properties of the motifs as *local* entities in relation to the *global* symmetry \mathbf{G} .

The main idea of the concept of site symmetry is as follows: if in a Euclidean space \mathbb{E}^n , a singular point (the origin of the coordinate system) is chosen in which the symmetry elements of a certain group \mathbf{G} are “installed,” then the points of \mathbb{E}^n group into disjoint classes corresponding to their position relative to the symmetry elements of \mathbf{G} [10]. For symmetry $\mathbf{C}_{2h}(\mathbf{2}/\mathbf{m})$, as an example, it is easy to see that we have four classes (Figure 2):

- (i) the origin (lying on the rotation axis *and* in the mirror plane),
- (ii) the points of the xy plane except the origin (lying only in the mirror plane),
- (iii) the points on the z axis except the origin (lying only on the rotation axis), and
- (iv) all other points (lying on no symmetry element).

A point in a mirror plane, then, has mirror-symmetrical surroundings, whereas a point on a rotation axis has rotationally symmetrical environs, and so on. To every point or position P ,

²This is only a necessary condition, since *arrangement* symmetry elements may also run through the centre of gravity of a motif, see Figure 1b.

³The first symbol is the Schoenflies symbol, followed by the abbreviated International (Hermann-Mauguin) symbol in parentheses (see, for instance, [7,8]). Schoenflies symbols for two-dimensional point groups will be marked with an asterisk; the corresponding Hermann-Mauguin symbols are: \mathbf{n} for \mathbf{C}_n^* , \mathbf{m} for \mathbf{D}_1^* , \mathbf{mm} for \mathbf{D}_2^* , \mathbf{nm} (\mathbf{nmm}) for \mathbf{D}_n^* with $n > 2$ and n odd (even) [9]. For symmetry operations, also both types of nomenclature will be used in several cases (without discriminating between three- and two-dimensional operations); the correspondence is as follows: rotation: $\mathbf{C}_n \hat{=} \bar{\mathbf{n}}$, rotation-reflection: $\mathbf{S}_n \hat{=} \bar{\bar{\mathbf{n}}}$, rotation-inversion: $\mathbf{A}_n \hat{=} \bar{\bar{\mathbf{n}}}$, reflection: $\sigma \hat{=} \mathbf{m}$. The orientation of rotation axes is denoted by an index; mirror planes will be characterised by their *normal direction* following [10] (i.e., m_x lies in the yz plane).

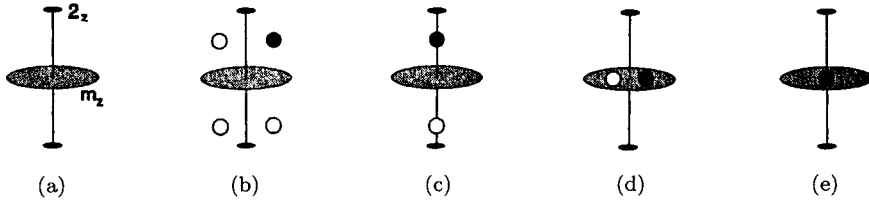


Figure 2. Symmetry elements of the group $C_{2h}(2/m)$ in perspective (a), and the four different sites within this symmetry: general position (b), and positions on the rotation axis (c), in the mirror plane (d), and on both symmetry elements, i.e., in the origin (e). In each case, a point (●) and its images (○) under the symmetry operations of C_{2h} , i.e., the symmetrically equivalent points forming an orbit (*vide infra*) are shown.

there will be ascribed a *site symmetry group* $G_S(P)$ which is the symmetry of the E^n seen from this very position. Thus, $G_S(P)$ characterises the *local* symmetry at this place. To be precise, the site symmetry of a point is given by the set of all transformations of G that leave this point invariant⁴ [7]. In the above example, the site symmetries range from the full symmetry C_{2h} (for the origin) down to symmetry C_1 (1) for the points of Class (iv).

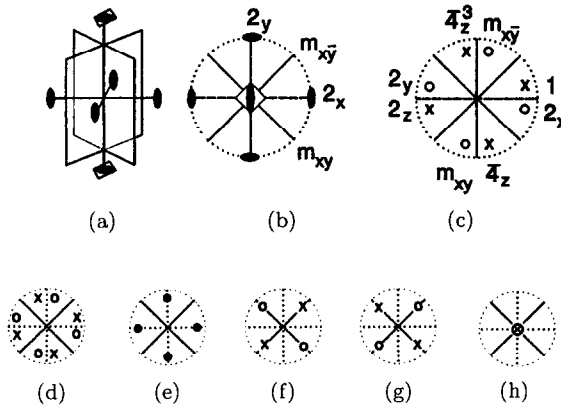


Figure 3. Symmetry elements of the group $D_{2d}(\bar{4}2m)$ in perspective (a), and in a stereogram⁵ (b). Symmetry operations resulting in the different points of orbit Ω_1 are given in (c). Orbit Ω_1 of a point of general position (d) and the orbits Ω_2 and Ω'_2 (both correspond to e), Ω_3 (f), Ω'_3 (g), Ω_4 (h), and Ω_5 (i) are shown. In the stereograms of the orbits, the symbols of the symmetry operations have been omitted for the sake of clarity.

The main task is, then, to find for a prescribed figure symmetry G , the different classes of points and their respective site symmetries. To this end, it is advantageous to introduce the *point group matrix* \hat{G} [10]. This is a $(g \times 3)$ -matrix (g : order of the point group G) with each row consisting of the coordinates of a point of general position (i.e., lying on no symmetry element) after transformation by one of the symmetry operations of G . For $G = D_{2d}(\bar{4}2m)$, as an example, we get⁶

⁴These transformations are not necessarily identical with the transformations corresponding to the symmetry elements on which this point is located. For points outside the origin, only rotations and reflections, but not rotation-reflections or rotation-inversions may occur in $G_S(P)$ [14].

⁵As a convention in stereograms, the paper plane will be drawn as a dashed circle if it does not represent a mirror plane; rotation axes lying in the paper plane are drawn as dashed lines, mirror planes oriented perpendicularly to the paper plane as solid lines. The contour square (\square) denotes an S_4 ($\bar{4}$) axis, filled lenses denote normal C_2 rotation axes. The symbols \times , \circ , and \bullet mean points above/below/in the paper plane, respectively.

⁶As usual in crystallography, a minus sign is put above the corresponding variable (e.g., $\bar{x} \equiv -x$).

Point group matrix $\hat{\mathbf{G}}$	Corresponding symmetry operations
$\hat{\mathbf{G}} = \begin{pmatrix} xyz \\ y\bar{x}\bar{z} \\ \bar{x}\bar{y}z \\ \bar{y}x\bar{z} \\ x\bar{y}\bar{z} \\ yxz \\ \bar{x}y\bar{z} \\ \bar{y}\bar{x}z \end{pmatrix}$	E (1)
	S_{4z}^3 ($\bar{4}_z$)
	C_{2z} (2_z)
	S_{4z} ($\bar{4}_z^3$)
	C_{2x} (2_x)
	σ'_d ($m_{x\bar{y}}$)
	C_{2y} (2_y)
	σ''_d (m_{xy})

(2)

The points resulting from the different symmetry operations have been depicted in Figure 3c.

Since the result of the transformation of the point coordinates (xyz) by a certain symmetry operation unambiguously characterises this operation, the point group matrix is a characteristic of the point group and, simultaneously, a shorthand for the transformation matrices of the individual symmetry operations⁷ [10]. The lines of the $\hat{\mathbf{G}}$ matrix correspond to the coordinate triples of all points which are symmetrically equivalent to a point of general position [10]. Such a set of symmetrically equivalent points is called an *orbit* ([7], cf., also [3,10]), the notion being taken over from permutation-group theory. Points of general position are said to belong to a *general orbit*, a point of special position belongs to a *special orbit* [7]. The different orbits for \mathbf{D}_{2d} are depicted in Figure 3d-i.

Summarising, the action of a group \mathbf{G} onto the points of \mathbb{E}^n defines an equivalence relation (\sim)⁸:

$$P' \sim P \iff \exists G \in \mathbf{G} : P' = \hat{G} \cdot P, \tag{3}$$

due to which these points subdivide into equivalence classes, the *orbits* $\Omega(P)$:

$$\Omega(P) := \{P' = \hat{G} \cdot P \mid G \in \mathbf{G}\}. \tag{4}$$

The site symmetry group $\mathbf{G}_S(P)$ of a site or point P is then

$$\mathbf{G}_S(P) := \{G \in \mathbf{G} \mid \hat{G} \cdot P = P\}. \tag{5}$$

The special point positions (sites) within a given point group can be found by specifically testing invariance properties of point positions under the symmetry operations of the group \mathbf{G} and combinations of them. To use \mathbf{D}_{2d} ($\bar{4}2m$) once more as an example, one may ask for a point position which is invariant under C_{2z} (2_z) operation. From

$$\hat{E} \cdot (xyz) = (xyz) \stackrel{!}{=} (\bar{x}\bar{y}z) = \hat{C}_{2z} \cdot (xyz), \tag{6}$$

follows

$$x = \bar{x} = 0 \quad \text{and} \quad y = \bar{y} = 0, \tag{7}$$

so that $(00z)$ is the point position which is invariant under C_{2z} . It is located, of course, on the C_{2z} axis. Positions on the other symmetry elements and on combinations of them can be found analogously. Taking these positions as headline in the point group matrix $\hat{\mathbf{G}}$ gives the

⁷The original transformation matrices can easily be reconstructed from the lines of the point group matrix, and these lines may also be symbolically multiplied in a one-to-one correspondence to the multiplication of the corresponding matrices [10].

⁸The operator or matrix corresponding to a symmetry operation G will be marked by a hat (\hat{G}).

Table 1. Point group matrices for general and special orbits Ω_i under symmetry D_{2d} ($42m$).

Operations		Ω_1	Ω_2	Ω'_2
E	1	$\begin{pmatrix} xyz \\ y\bar{x}\bar{z} \\ \bar{x}\bar{y}z \\ \bar{y}x\bar{z} \\ x\bar{y}\bar{z} \\ yxz \\ \bar{x}y\bar{z} \\ \bar{y}\bar{x}z \end{pmatrix}$	$\begin{pmatrix} x00 \\ 0x0 \\ \bar{x}00 \\ 0x0 \\ x00 \\ 0x0 \\ \bar{x}00 \\ 0\bar{x}0 \end{pmatrix}$	$\begin{pmatrix} 0y0 \\ y00 \\ 0\bar{y}0 \\ \bar{y}00 \\ 0\bar{y}0 \\ y00 \\ 0y0 \\ \bar{y}00 \end{pmatrix}$
S_{4z}^3	$\bar{4}_z$			
C_{2z}	2_z			
S_{4z}	$\bar{4}_z^3$			
C_{2x}	2_x			
σ'_d	$m_{x\bar{y}}$			
C_{2y}	2_y			
σ''_d	m_{xy}			
Locations		General position	On x axis on 2_x	On y axis on 2_y

Operations		Ω_3	Ω'_3	Ω_4	Ω_5
E	1	$\begin{pmatrix} xxz \\ x\bar{x}\bar{z} \\ \bar{x}\bar{x}z \\ \bar{x}x\bar{z} \\ xx\bar{z} \\ x\bar{x}\bar{z} \\ xxz \\ \bar{x}\bar{x}\bar{z} \\ \bar{x}\bar{x}z \end{pmatrix}$	$\begin{pmatrix} x\bar{x}z \\ \bar{x}\bar{x}\bar{z} \\ \bar{x}xz \\ xx\bar{z} \\ x\bar{x}\bar{z} \\ \bar{x}\bar{x}\bar{z} \\ \bar{x}xz \\ \bar{x}\bar{x}\bar{z} \\ x\bar{x}z \end{pmatrix}$	$\begin{pmatrix} 00z \\ 00\bar{z} \\ 00z \\ 00\bar{z} \\ 00z \\ 00\bar{z} \\ 00z \\ 00\bar{z} \\ 00z \end{pmatrix}$	$\begin{pmatrix} 000 \\ 000 \\ 000 \\ 000 \\ 000 \\ 000 \\ 000 \\ 000 \\ 000 \end{pmatrix}$
S_{4z}^3	$\bar{4}_z$				
C_{2z}	2_z				
S_{4z}	$\bar{4}_z^3$				
C_{2x}	2_x				
σ'_d	$m_{x\bar{y}}$				
C_{2y}	2_y				
σ''_d	m_{xy}				
Locations		Diagonal 1 on $m_{x\bar{y}}$	Diagonal 2 on m_{xy}	On z axis on $2_z, m_{x\bar{y}}, m_{xy}$	Origin on all elements

respective sets of symmetrically equivalent points in special positions (special orbits; see Table 1 and Figure 3).

All relevant information about a certain position can be found by inserting the coordinates for this position into the point group matrix $\hat{\mathbf{G}}$. Generally, one has:

- (i) The point group matrix itself contains the positions of all general points which are symmetrically equivalent (the points of the general orbit).
- (ii) In special positions, the point group matrix contains n -tuples of points having the same coordinates. In orbit Ω_2 , for instance, there are only four different positions in contrast to eight in the general orbit: $\Omega_2 = \{(x00), (\bar{x}00), (0x0), (0\bar{x}0)\}$ (cf. Table 1). The order g_Ω of an orbit (number of symmetrically equivalent points) is given by $g_\Omega = g/g_S$ (g, g_S : orders of the point groups \mathbf{G} and \mathbf{G}_S). The multiplicity m of the orbit positions (number of points of the general orbit which merge into one point within the special orbit) is given by the order g_S of \mathbf{G}_S ($m = g_S$) [10]. For every orbit, the product of its order and its multiplicity equals the order g of the figure symmetry \mathbf{G} [10]. Data for the orbits of D_{2d} are given in Table 2.
- (iii) A point of general position always has a site symmetry of C_1 ($\mathbf{1}$), an orbit order of g , and a multiplicity of 1. In turn, a point at the origin has site symmetry $\mathbf{G}_S = \mathbf{G}$, multiplicity g , and its orbit has order 1. Other points have site symmetries which are subgroups $\mathbf{G}_S \subset \mathbf{G}$ with order g_S and multiplicity g/g_S (g_S is a factor of g).

- (iv) In special positions, different transformations result in the same point coordinates: in orbit Ω_2 , $(x00)$ is found with the identity 1 and also with 2_x ; $(\bar{x}00)$ is connected with 2_z and 2_y , and so on. This means that n -tuples of transformations become *equivalent* in so far as they transform the starting position into the same end-point. This defines a subdivision of the elements of \mathbf{G} into *equivalence classes*. These equivalence classes are identical with the *left cosets*⁹ $G \cdot \mathbf{G}_S$ of \mathbf{G} with respect to the site group \mathbf{G}_S . This is because all elements of \mathbf{G}_S leave a point P invariant, so that all products $G \cdot \mathbf{G}_S$ with fixed $G \in \mathbf{G}$ and variable $G_S \in \mathbf{G}_S$ ¹⁰ must become equivalent. Taking group \mathbf{D}_{2d} ($\bar{4}2\mathbf{m}$) as an example, we see that subgroups \mathbf{C}_1 , \mathbf{C}_{2v} , and \mathbf{D}_{2d} are invariant. For the noninvariant subgroup $\mathbf{C}_2 = \{1, 2_x\}$, the left and right coset decompositions are

$$G \cdot \mathbf{H} = \{1, 2_x\}, \{\bar{4}_z, m_{xy}\}, \{2_z, 2_y\}, \{\bar{4}_z^3, m_{x\bar{y}}\}, \quad (8)$$

$$\mathbf{H} \cdot G = \{1, 2_x\}, \{\bar{4}_z, m_{x\bar{y}}\}, \{2_z, 2_y\}, \{\bar{4}_z^3, m_{xy}\}, \quad (9)$$

where $G \cdot \mathbf{H}$ (in contrast to $\mathbf{H} \cdot G$) corresponds exactly to the equivalence classes for orbit Ω_2 which are evident from the point group matrix (Table 1).

- (v) Site-symmetry groups are always subgroups of the corresponding figure symmetry [10]. The site-symmetry groups of different points of the same orbit are conjugate subgroups¹¹ of \mathbf{G} [7]. Therefore, the site symmetry is taken to be the class of these conjugate subgroups [10]. In the example, \mathbf{D}_{2d} , the orbits Ω_2 and Ω'_2 belong to the conjugate subgroups $\{1, 2_x\}$ and $\{1, 2_y\}$, and Ω_3 and Ω'_3 to $\{1, m_{x\bar{y}}\}$ and $\{1, m_{xy}\}$, respectively.
- (vi) Outside the origin, only the groups \mathbf{C}_n (\mathbf{n}) including \mathbf{C}_1 ($\mathbf{1}$) and \mathbf{C}_{nv} ($\mathbf{mm2}$, \mathbf{nmm} , \mathbf{nm}) including $\mathbf{C}_{1v} \equiv \mathbf{C}_{1h} \equiv \mathbf{C}_s$ (\mathbf{m}) can appear as site-symmetry groups [14]; in \mathbb{E}^2 , the corresponding groups are \mathbf{C}_1^* ($\mathbf{1}$) and \mathbf{D}_1^* (\mathbf{m}). This is because a rotation-reflection (rotation-inversion) cannot be realized *locally* for points outside the origin, therefore, only rotations and simple reflections have to be considered when deriving site symmetries. In \mathbf{D}_{2d} , the site symmetry for orbit Ω_4 is \mathbf{C}_{2v} ($\mathbf{2m}$), though the axis is an S_4 ($\bar{4}$) axis, and \mathbf{C}_2 ($\mathbf{2}$) is only a subset of the corresponding transformations. The site symmetries which are possible under different point group symmetries are compiled in Table 3. Note that subgroups of the principal axis symmetry cannot appear as site symmetries. Therefore, \mathbf{C}_2 for example, is a site symmetry only in dihedral and cubic groups, but not in \mathbf{C}_{4h} , \mathbf{C}_{4v} , etc.
- (vii) The number of independent variables in the coordinates of the points of an orbit is termed its *degree of freedom*. The general orbit always has three degrees of freedom [10]. The degrees of freedom correspond to the geometric dimension of the symmetry element (the subspace of \mathbb{E}^n) on which the position can be moved without changing its local symmetry properties.

⁹For any subgroup \mathbf{H} of a group \mathbf{G} , there exists a system of left and right cosets:

$$G \cdot \mathbf{H} = \{G \cdot H \mid \forall H \in \mathbf{H}\} \text{ and } \mathbf{H} \cdot G = \{H \cdot G \mid \forall H \in \mathbf{H}\}$$

($G \in \mathbf{G}$), respectively [3,15,16]. These cosets constitute *equivalence classes*. Since cosets are always either identical or disjoint, the group \mathbf{G} is thus decomposed into $k = g/h$ classes with h equivalent elements in each (g, h : orders of \mathbf{G} and \mathbf{H} , respectively): using the left or right cosets, one gets a (left or right) *decomposition* of \mathbf{G} with respect to the subgroup \mathbf{H} . Left and right cosets are identical only for special subgroups (called *normal divisors* or *invariant subgroups*). If \mathbf{H} is an invariant subgroup (i.e., if it is conjugate to itself), then the set of cosets forms itself a group, the *factor group* denoted by the symbol \mathbf{G}/\mathbf{H} having the subgroup \mathbf{H} as identity element. (cf.[3,15,16]).

¹⁰Note that products of operations have to be executed from the right to the left according to a standard convention in group theory.

¹¹Two subgroups \mathbf{H} and \mathbf{H}' of \mathbf{G} are termed *conjugate* if they are related to one another by the transformation

$$\mathbf{H}' = G^{-1} \cdot \mathbf{H} \cdot G \quad (\forall G \in \mathbf{G})$$

(see reference [16]). In \mathbf{D}_{2d} ($\bar{4}2\mathbf{m}$), $\{1, 2_x\}$ is conjugate to $\{1, 2_y\}$, and $\{1, m_{x\bar{y}}\}$ is conjugate to $\{1, m_{xy}\}$, so that the corresponding site symmetries are taken to be \mathbf{C}_2 ($\mathbf{2}$) and \mathbf{C}_s (\mathbf{m}), respectively.

Table 2. Site-symmetry groups and their elements, their orders and the multiplicities of the positions for the orbits of symmetry group D_{2d} ($42m$).

Orbit	Site-symmetry group / Elements			Order	Multiplicity
Ω_1	C_1	(1)	{1}	8	1
Ω_2	C_2	(2)	{1, 2_x }	4	2
Ω'_2	C_2	(2)	{1, 2_y }	4	2
Ω_3	C_s	(m)	{1, m_{xy} }	4	2
Ω'_3	C_s	(m)	{1, m_{xy} }	4	2
Ω_4	C_{2v}	(mm)	{1, $2_x, m_{xy}, m_{xy}$ }	2	4
Ω_5	D_{2d}	($42m$)	{1, $2_x, 2_x, 2_x^3, 2_x, 2_y, m_{xy}, m_{xy}$ }	1	8

Table 3. Possible site symmetries under the different point groups G . The positions given in the head are: the origin; the z axis (except the origin; analogously for the other positions); n axial positions in the xy plane; n axial positions in the xy plane which are located *between* the foregoing ones; the xy plane, n vertical planes along the A'_\perp positions; n vertical planes along the A''_\perp positions. Mirror lines have been denoted by C_{1h} or C_{1v} depending on their orientation. Symbols in parentheses denote that the symmetry given is not the proper symmetry of this axis, but the symmetry of the *plane* containing this axis.

G	Origin	z	$n \cdot A'_\perp$	$n \cdot A''_\perp$	xy	$n \cdot \sigma'_v$	$n \cdot \sigma''_v$	Others	General
C_n	C_n	C_n	C_1	C_1	C_1	C_1	C_1	-	C_1
C_{nh}	C_{nh}	C_n	(C_s)	(C_s)	C_s	C_1	C_1	-	C_1
C_{nv}	C_{nv}	C_{nv}	(nC_s)	C_1	C_1	nC_s	C_1	-	C_1
S_n^{12}	S_n	$C_{n/2}$	C_1	C_1	C_1	C_1	C_1	-	C_1
D_n	D_n	C_n	nC_2	C_1	C_1	C_1	C_1	-	C_1
D_{nh}	D_{nh}	C_{nv}	nC_{2v}	(C_s)	C_s	nC_s	C_1	-	C_1
D_{nd}	D_{nd}	C_{nv}	nC_2	(nC_s)	C_1	C_1	nC_s	-	C_1
T	T	C_2	$2C_2$	C_1	C_1	C_1	C_1	$4C_3$	C_1
T_h	T_h	C_{2v}	$2C_{2v}$	(C_s)	C_s	$2C_s$	C_1	$4C_3$	C_1
T_d	T_d	C_{2v}	$2C_{2v}$	($2C_s$)	C_1	C_1	$2C_s$	$4C_{3v}, 4C_s$	C_1
O	O	C_4	$2C_4$	$2C_2$	C_1	C_1	C_1	$4C_3, 4C_2$	C_1
O_h	O_h	C_{4v}	$2C_{4v}$	$2C_{2v}$	C_s	$2C_s$	$2C_s$	$4C_{3v}, 4C_{2v}, 4C_s$	C_1
Y	Y	C_5	$5C_2$	C_1	C_1	C_1	C_1	$5C_5, 10C_3, 10C_2$	C_1
Y_h	Y_h	C_{5v}	$5C_{2v}$	($5C_s$)	C_1	C_1	$5C_s$	$5C_{5v}, 10C_{3v}, 10C_{2v}, 10C_s$	C_1

A concept which is closely related to the notion of site symmetry is the concept of *direction symmetry* [13]. The *direction-symmetry group* G_d^{13} for a direction $\mathbf{d} = [uvw]$ within a symmetry G contains all symmetry operations which leave this direction invariant [13]. These are all elements of G which are invariant under a similarity transformation involving an arbitrary translation along \mathbf{d} (cf. [10])

$$G_d := \left\{ G \in G \mid \hat{d}^{-1} \cdot \hat{G} \cdot \hat{d} = \hat{G} \right\}, \quad (10)$$

where \hat{d} is the *translation matrix*¹⁴ corresponding to vector \mathbf{d} . Since the symmetry operations of G_d transform \mathbf{d} into itself, they also leave all points P of \mathbf{d} fixed, hence, they are identical to

¹² n even; for odd, one has $S_n = C_{nh}$.

¹³I will discriminate between the direction-symmetry group for a motif G_{MO} where $\mathbf{d} = \mathbf{d}_{MO}$ is the direction \overrightarrow{MO} from the centre of gravity of the motif (M) to the centre of gravity of the figure, the origin (O), and the direction-symmetry group for the figure symmetry G_{OM} with $\mathbf{d} = \mathbf{d}_{OM} = \overrightarrow{OM}$ pointing from O to M (the index M may be replaced by i or ji to denote the i^{th} motif in the j^{th} orbit, if necessary).

¹⁴The notion of a translation *matrix* deserves some comment. For the combination of a translation \mathbf{t} and an orthogonal transformation \hat{R} , it is advantageous to replace the normal *additive* transformation equation $P' = \hat{R} \cdot P + \mathbf{t}$ by a *multiplicative* one: $P' = \hat{i} \cdot \hat{R} \cdot P$. This is possible when an additional (dummy) coordi-

the transformations leaving the P 's invariant:

$$\mathbf{G}_d = \mathbf{G}_S(P) \quad \forall P \in d. \tag{11}$$

The difference between both notions lies in the point of view: $\mathbf{G}_S(P)$ denotes the symmetry of \mathbb{E}^n in \mathbf{G} , seen from point P , and, likewise, the *local* symmetry of the surroundings of P , whereas \mathbf{G}_d describes the symmetry of \mathbb{E}^n , seen from the *origin* in direction \mathbf{d} . Both symmetries must, however, be identical. Note that the two direction symmetries \mathbf{G}_{OM} and \mathbf{G}_{MO} have different groups (\mathbf{G} and \mathbf{G}_M , respectively) to which they are related:

$$\mathbf{G}_{OM} = \left\{ G \in \mathbf{G} \mid \hat{G} \cdot P = P \quad (\forall P \in \overrightarrow{OM}) \right\}, \tag{12}$$

$$\mathbf{G}_{MO} = \left\{ G \in \mathbf{G}_M \mid \hat{G} \cdot P = P \quad (\forall P \in \overrightarrow{MO}) \right\}. \tag{13}$$

There are only two types of groups which can appear as direction symmetries in \mathbb{E}^3 : C_n and C_{nv} [13].

2.3. Relationships between Motif and Figure Symmetries

Having clarified the symmetry properties of the different positions within a figure, in the next step, the relationships between the symmetry of motifs located on such positions and the symmetry of the whole figure have to be considered. Since it seems that a figure of arbitrary symmetry can consist of motifs of likewise arbitrary symmetry (cf. Figure 4), there will be no restriction made concerning the symmetry of the motifs used, and the symmetry of the figure will be pre-set.

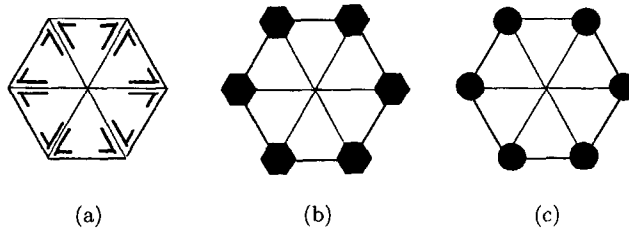


Figure 4. A planar hexagonal figure with symmetry D_{6h} ($6/mmm$) made from “1” motifs (a; motif symmetry C_s), from hexagons (b; motif symmetry D_{6h}), and from spheres (c; motif symmetry K_h) indicating that there is no restriction regarding the motif symmetry when the figure symmetry is pre-set.

If the figure is built up from geometrically different motifs, then each type of motif *must* belong to at least one separate orbit of the figure. Congruent motifs may or may not belong to the same orbit. Here, the notion of an orbit has been enlarged compared with its meaning in Section 2.2. If a motif is transformed by all symmetry operations of the figure symmetry \mathbf{G} , then one gets a set of symmetrically equivalent motifs which is equivalent to an orbit of positions. Therefore, I shall call this set an *orbit of motifs*.

The most important relationship between motif and figure symmetries is then: *the direction symmetry \mathbf{G}_{MO} of a motif in the direction $\mathbf{d}_{MO} = \overrightarrow{MO}$ from its centre of gravity to the origin*

nate is introduced, so that the augmented matrices for P , \hat{R} , and \hat{t} read:

$$P = \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} \quad \hat{R} = \begin{pmatrix} & & 0 \\ [R] & & 0 \\ & & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \hat{t} = \begin{pmatrix} 1 & 0 & 0 & x_T \\ 0 & 1 & 0 & y_T \\ 0 & 0 & 1 & z_T \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

where $[R]$ is the usual 3×3 orthogonal matrix, and $\mathbf{t} = (x_T, y_T, z_T)^T$ is the translation vector [7].

(the centre of gravity of the figure) must be a supergroup¹⁵ of the direction symmetry \mathbf{G}_{OM} of the figure in the reverse direction $\mathbf{d}_{OM} = \overline{OM}$:

$$\mathbf{G}_{MO} \supseteq \mathbf{G}_{OM}. \quad (14)$$

Otherwise, the motif would *destroy* the figure symmetry. From the explanations in Section 2.2, it follows that in this formulation, the direction symmetry of the figure can be replaced by the site symmetry of the location of the motif. Then, the condition reads $\mathbf{G}_{MO} \supseteq \mathbf{G}_S$. This is illustrated by Figure 4 where the direction symmetries of the different motifs (\mathbf{C}_s on \mathbf{C}_s sites in Figure 4a, and \mathbf{C}_{2v} or $\mathbf{C}_{\infty v}$ on \mathbf{C}_{2v} sites in Figures 4b,c) are equal to or higher than the necessary site symmetry. If the direction symmetry of the motif is a proper supergroup of \mathbf{G}_S ($\mathbf{G}_{MO} \supset \mathbf{G}_S$), then the supernumerary symmetry elements which do not belong to the site symmetry (i.e., the difference $\mathbf{G}_{MO} \setminus \mathbf{G}_S$) are only *local* ones, they form intermediate or latent symmetries of the figure¹⁶. Therefore, especially for later use in the following sections, I define an *effective direction symmetry group* $\mathbf{G}_{jiO}^* \subseteq \mathbf{G}_{jiO}$ of motif \mathcal{M}_{ji} which contains all elements of \mathbf{G}_{jiO} which are simultaneously *global* symmetry elements of the figure, i.e., which transform all motifs \mathcal{M}_{kl} of the figure \mathcal{F} into one another¹⁷

$$\mathbf{G}_{jiO}^* = \left\{ G_{ji} \in \mathbf{G}_{jiO} \mid \hat{t}^{-1} \cdot \hat{G}_{ji} \cdot \hat{t} \cdot \mathcal{M}_{kl} = \mathcal{M}'_{kl} \in \Omega_k \in \mathcal{F} \right\}. \quad (15)$$

Thus, \mathbf{G}_{MO}^* corresponds to the remaining (crisp) symmetry of the motif in the finished figure. Now the relationship between motif and figure symmetries can be written as

$$\mathbf{G}_S = \mathbf{G}_{MO}^* \subseteq \mathbf{G}_{MO} \subseteq \mathbf{G}_M. \quad (16)$$

In any figure symmetry \mathbf{G} , there are positions (namely, the general positions) which have a site symmetry \mathbf{C}_1 ($\mathbf{1}$). On the other hand, every possible motif symmetry has at least this group as one direction group. Therefore, the proposition made above is true: a figure of arbitrary symmetry \mathbf{G} can be composed of motifs of likewise arbitrary symmetry \mathbf{G}_M , at least by positioning g motifs with direction symmetries $\mathbf{G}_{iO} = \mathbf{C}_1$ ($i = 1, \dots, g$) in a set of symmetrically equivalent general positions (a general orbit).

Since rotation-reflection and rotation-inversion axes are not components of site symmetries, their respective symmetry requirements have to be fulfilled by the *arrangement* of the motifs. The simplest way to do so is to transform a motif on a chosen position by all symmetry operations of the figure symmetry group \mathbf{G} . This will, without any constraint, produce the proper orbit of symmetrically equivalent motifs.

Since points (circles, spheres) display the highest possible symmetry in \mathbb{E}^n ($\mathbb{E}^2, \mathbb{E}^3$), they are especially well suited for being used as motifs. Since their symmetry is $\mathbf{O}(n)$ (*vide infra*), their direction symmetry in arbitrary directions is $\mathbf{O}(n-1)$. This is a supergroup of all possible direction-symmetry groups within \mathbb{E}^n , so that they fit to arbitrary sites within a figure of given symmetry.

The freedom of creative work in producing ornaments and other geometric figures lies in the indeterminacy of the number of different motifs to be arranged, their forms and symmetries and the choice of suitable sites for arranging them. As we saw, the constraints are very mild, thus leaving plenty of room for the creative phantasy.

¹⁵Note that a certain group is considered both its own supergroup and its own subgroup.

¹⁶The problem of detecting these symmetry elements in an arbitrary figure will be addressed in Sections 3.1 to 3.3.

¹⁷The definition in equation (15) is more general than

$$\mathbf{G}_{MO}^* = \{G \in \mathbf{G}_{MO} \cap \mathbf{G}_{OM}\},$$

since it is also valid if a change in the arrangements of the motifs forces a change of the figure symmetry \mathbf{G} so that \mathbf{G}_{OM} is altered.

2.4. Changing Figure Symmetries by Varying Motif Orientations

The symmetry of a given figure may be changed in two ways: either the local symmetries of the motifs (strictly speaking, the direction symmetries \mathbf{G}_{jiO} of the motifs or at least their effective parts \mathbf{G}_{jiO}^*) are varied, or the figure will be deformed, thus altering the arrangement symmetry of the motifs. In both cases, the number of motifs is left fixed. In this section, the first possibility will be examined.

Considering the subdivision of the direction-symmetry elements of a motif into an effective and a “latent” part, the question arises how these parts respond to variations in the orientation of motifs. Here, only “collective” reorientations will be considered: a certain motif of an orbit will be reoriented, and afterwards it will be transformed by symmetry operations of the group \mathbf{G} , so as to construct a new orbit. In any case, the centres of gravity of the motifs will be left fixed.

A reorientation of a motif (especially by a rotation around some arbitrary axis) will normally change its direction symmetry¹⁸. The question is, then, which symmetry elements of \mathbf{G}_{MO} will be able to form *global* symmetry elements and thus constitute \mathbf{G}_{MO}^* . If the effective direction symmetry of the motif is changed by the new orientation, then the site symmetry \mathbf{G}_S and, hence, the figure symmetry \mathbf{G} will change in the appropriate manner. If the new effective direction symmetry is lower than the actual site symmetry, then the symmetry of the whole figure will be lowered. If it is higher, then the figure symmetry \mathbf{G} will be *enhanced*, if the new local symmetry operations become global ones. The condition for this to occur has been given in equation (15). Generally, the direction symmetry of a motif will be utilised *maximally*, i.e., *all* local symmetry elements of a motif which are compatible with elements of other motifs will become elements of \mathbf{G} .

An example is given in Figure 5. Here, it becomes clear that the resulting figure symmetry depends also on the symmetry element that is chosen for the transformation of the reoriented motif. In Figure 5, the starting point is a figure with \mathbf{D}_{4h} symmetry and four motifs with \mathbf{C}_{2v} direction symmetries on \mathbf{C}_{2v} sites (Figure 5a). Since this is the highest possible symmetry for such a figure, only descents in symmetry will be observed. A slight rotation of the upper motif around the y axis does not change its direction symmetry. However, both mirror planes become tilted against the xy plane, so that they can no longer form global symmetry elements. Consequently, the *effective* direction symmetry lowers to \mathbf{C}_2 . If this motif is duplicated by C_4 or the diagonal C_2' rotations, then a \mathbf{D}_4 configuration results (Figure 5b). On the other hand, after transforming the motif by S_4 or diagonal σ_v'' reflections, the resulting figure has \mathbf{D}_{2d} symmetry (Figure 5c). A slight rotation of the upper motif around a local z axis changes its direction symmetry to $\mathbf{G}_{MO} = \mathbf{G}_{MO}^* = \mathbf{C}_s$; a transformation by C_4 or S_4 gives \mathbf{C}_{4h} symmetry (Figure 5d), but a transformation by σ_v'' or C_2' results in \mathbf{C}_{2h} (Figure 5e). A slight rotation of the upper motif around a local x axis will give $\mathbf{G}_{MO} = \mathbf{G}_{MO}^* = \mathbf{C}_s$, so that C_4 or σ_v'' lead to \mathbf{C}_{4v} , whereas S_4 or C_2' lead to another \mathbf{D}_{2d} figure (neither shown). Lastly, a double rotation of the upper motif around both y and local z axes lowers its direction symmetry to $\mathbf{G}_{MO} = \mathbf{G}_{MO}^* = \mathbf{C}_1$, and application of the above operations leads to four different figure symmetries: C_4 leads to \mathbf{C}_4 (Figure 5f), S_4 to \mathbf{S}_4 (Figure 5g), σ_v'' to \mathbf{C}_{2v} (Figure 5h), and C_2' to \mathbf{D}_2 (Figure 5i). Taking other symmetry elements for the transformation of the reoriented upper motif, there will normally be only two or even one motif in the resulting orbit. This means that the orbit decomposes into 2 or 4 new orbits, and two (or all four) motifs may be reoriented independently. This way, the other subgroups of \mathbf{D}_{4h} may be generated also.

The symmetry transitions shown in Figure 5 may be displayed in a correlation table for the site symmetries in the different groups (Table 4). It shows that, starting from some subgroup

¹⁸This depends on the degrees of freedom at the positions within direction \mathbf{d} : if there are at least two degrees of freedom at positions in \mathbf{d} , then a differential rotation does not change the direction symmetry if it leaves the symmetry element containing \mathbf{d} fixed. If there exists only one degree of freedom, then it is in the direction \mathbf{d} itself, and every displacement perpendicularly to \mathbf{d} will change the direction symmetry.

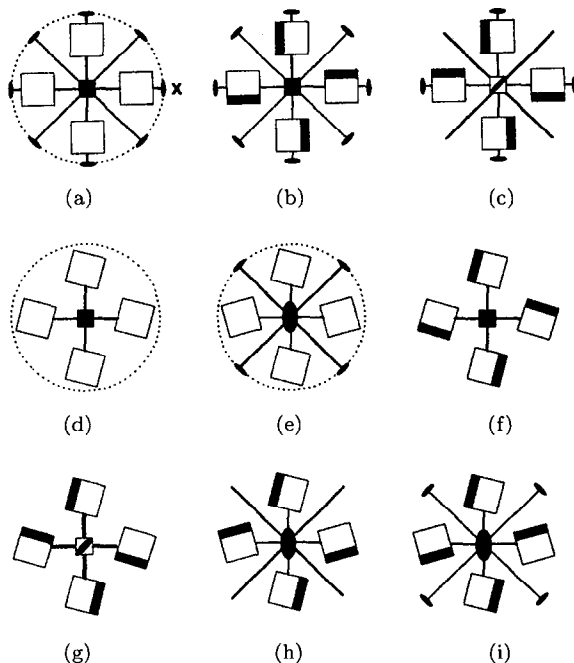


Figure 5: Variation of the figure symmetry by changing the orientation of the motifs leaving their centres of gravity fixed. The starting figure with symmetry D_{4h} (a), two figures with the upper motif rotated around the y axis having symmetries D_4 (b) and D_{2d} (c), two figures with the upper motif rotated around a local z axis having symmetries C_{4h} (d) and C_{2h} (e), and a series of figures with the upper motif rotated around both axes having symmetries C_4 (f), S_4 (g), C_{2v} (h), and D_2 (i) are shown. Edges of the motifs lying *above* the paper plane are drawn with bold lines.

of D_{4h} , both a descent and an ascent in symmetry is possible. For the latter, the motif must have a sufficient direction symmetry (at least C_{2v} in our case, since the motifs are located on the x, y axes, cf. Table 4). Since the maximum direction symmetry of the motif used is C_{4v} ($4mm$), a figure with cubic symmetry (at most O_h) may be assembled, but only if two more motifs are placed on the $\pm z$ axis. Otherwise, the C_4 symmetry will remain a local symmetry only.

Table 4. Correlation table for site symmetries of D_{4h} ($4/m\bar{m}m$) and its subgroups (S_4 to C_{2v} are not maximal subgroups).

Location	Point	D_{4h}	D_4	D_{2h}	D_{2d}	C_{4h}	C_{4v}	S_4	C_4	D_2	C_{2h}	C_{2v}
origin	(000)	D_{4h}	D_4	D_{2h}	D_{2d}	C_{4h}	C_{4v}	S_4	C_4	D_2	C_{2h}	C_{2v}
z axis	(00z)	C_{4v}	C_4	C_{2v}	C_{2v}	C_4	C_{4v}	C_2	C_4	C_2	C_2	C_{2v}
x, y axes	(x00)	C_{2v}	C_2	C_{2v}	C_2	C_{1h}	C_{1v}	C_1	C_1	C_2	C_{1h}	C_{1v}
diagonals	(xx0)	C_{2v}	C_2	C_{1h}	C_{1v}	C_{1h}	C_1	C_1	C_1	C_1	C_{1h}	C_1
xy plane	(xy0)	C_{1h}	C_1	C_{1v}	C_1	C_{1h}	C_1	C_1	C_1	C_1	C_{1h}	C_1
xz, yz planes	(x0z)	C_{1v}	C_1	C_{1v}	C_1	C_1	C_{1v}	C_1	C_1	C_1	C_1	C_{1v}
diagonal planes	(xxz)	C_{1v}	C_1	C_1	C_{1v}	C_1	C_{1v}	C_1	C_1	C_1	C_1	C_1
general	(xyz)	C_1	C_1	C_1	C_1	C_1	C_1	C_1	C_1	C_1	C_1	C_1

2.5. Changing Figure Symmetries by Deformation of the Figures

As stated above, changes of the arrangement symmetries in a given geometric figure by a displacement of the centres of gravity of the motifs without changing their local orientations relative to $\vec{d} = \overrightarrow{OM}$ can be described as *deformations* of this figure. Taking over the ideas from [17] to this problem, the deformation of a given figure may be described by attaching N local Cartesian tripods in the centres of gravity of the N motifs and seeking the *normal*

deformations for this figure. They will vary the global symmetry of the figure without changing the orientations (and hence the direction symmetries) of the motifs. Every figure generated by deformation will then correspond to a point in a $3N$ -dimensional *figure space* $\mathbb{F} = \mathbb{R}^{3N}$ ¹⁹. The points of this space, in turn, will cluster into disjoint *isosymmetric manifolds* consisting of points which correspond to figures of equal symmetry [17]. The coordinates of the form space may be chosen to be the Cartesian coordinates, but a simpler picture will arise when using the normal deformation coordinates mentioned above.

Such deformations will change the arrangement symmetry of the figure and, thus, the figure symmetry \mathbf{G} . On the other hand, they may also change the effective motif symmetry \mathbf{G}_{MO}^* when a coincidence between local and global symmetry elements occurs. As an example, consider two dumbbell motifs rotating independently around the x axis (Figure 6). The deformation normal coordinate (cf. [17]) shown in Figure 6a belongs to symmetry species A (totally symmetrical) under \mathbf{D}_2 symmetry (Figure 6b). This means that a deformation of the arrangement in Figure 6b along this normal coordinate will normally change the aspect of the figure, but not its symmetry. But as stated in [17], totally symmetrical deformations are under special conditions capable of transferring the figure to a supergroup symmetry. Here, the deformations Δ_+ and Δ_- (clockwise and counterclockwise relative rotation of the two motifs, respectively) lead to two *different* symmetries (they terminate the \mathbf{D}_2 isosymmetric manifold, cf. [17], as can be seen from Figure 6d) to \mathbf{D}_{2h} (Figure 6a) and to \mathbf{D}_{2d} (Figure 6c), respectively. In both cases, the ascent in symmetry is due to a mutual alignment of the mirror planes of the motifs' \mathbf{C}_{2v} direction symmetries which in the \mathbf{D}_2 configuration are *latent symmetries*, whereas the \mathbf{C}_2 subsymmetry of \mathbf{C}_{2v} is a crisp symmetry for any rotation angle. If, however, both motifs are replaced by paragraph-shaped motifs having only \mathbf{C}_2 direction symmetry (Figure 6e), there will be no symmetry transition to \mathbf{D}_{2h} or \mathbf{D}_{2d} along the angle coordinate since \mathbf{G}_{MO} is too low.

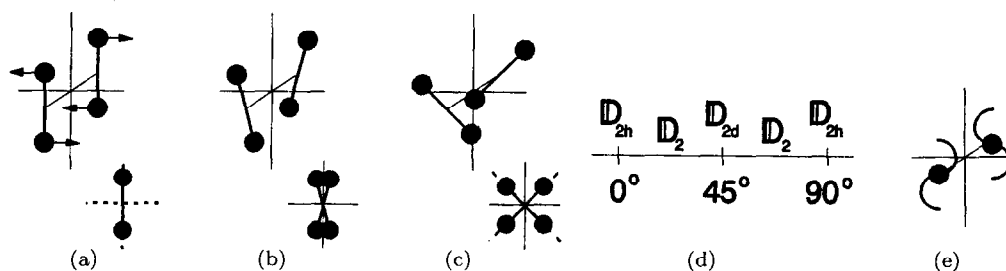


Figure 6. Ascent in symmetry from a \mathbf{D}_2 figure (b) to \mathbf{D}_{2h} (a) and \mathbf{D}_{2d} (c), respectively. Symmetry variations along the rotation angle α are shown in (d). A paragraph-shaped motif displaying no symmetry transition is sketched in (e), see text.

Generally one finds:

- A *descent* in symmetry by deformation of the figure is always possible if $\mathbf{G} \supset \mathbf{C}_1$. It gives a group \rightarrow subgroup transition in the figure symmetry and likewise in its site symmetries.
- An *ascent* in symmetry by deformation may enhance only the arrangement symmetry without changing the site symmetry of the motif's position (for example, during a $\mathbf{C}_2 \rightarrow \mathbf{C}_4$ transition in a figure with its motifs arranged only equatorially). However, in general both the arrangement and site symmetries will change. Then, the transition to a supergroup symmetry will be possible if the motif exhibits symmetry elements in proper orientation. A necessary condition for this to occur is that the direction symmetry \mathbf{G}_{MO} is a supergroup of the site symmetry for the starting (lower-symmetry) figure.

¹⁹In [17], \mathbb{F} has been termed *form space* since the aspect of the forms was given priority. There is equally a one-to-one correspondence between the points of \mathbb{F} and all possible *figures* that may be generated by deformations of a starting figure.

3. FUZZY MOTIF AND ARRANGEMENT SYMMETRIES

3.1. Arbitrary Decompositions of Figures and Fuzzy Symmetries

As stated above, the decomposition of a geometric figure into pieces is, in principle, arbitrary. It can be done by any section of the motifs of this figure. The resulting pieces may have a higher symmetry than the figure or its motifs. In Figure 7a,b, a two-dimensional “b”-shaped figure belonging to symmetry group C_1^* ($\mathbf{1}$) has been cut into pieces displaying D_2^* (\mathbf{mm}) and D_1^* (\mathbf{m}) symmetries, respectively. As a second example, a rectangle with a side lengths ratio $a/b = 2$ may be cut into two squares with symmetries $D_4^* = \mathbf{4mm}$ (Figure 7c). Just as well, this rectangle may be decomposed into rectangular slices with D_2^* (\mathbf{mm}) symmetries (Figure 7d). In all such cases, the resulting pieces may have symmetry elements which are not present in the whole figure, namely, if they are assembled in a way where their symmetry elements do not coincide and, therefore, are in a crisp sense not preserved in the whole figure. The same is true for arrangement symmetries as has been shown in Figure 1b: there two mirror lines between two motifs each are not preserved in the resulting figure. Nevertheless, these symmetry elements are valid for two motifs and, thus, must constitute a fuzzy symmetry of the figure. The same is true for all symmetry elements shown in Figure 7.

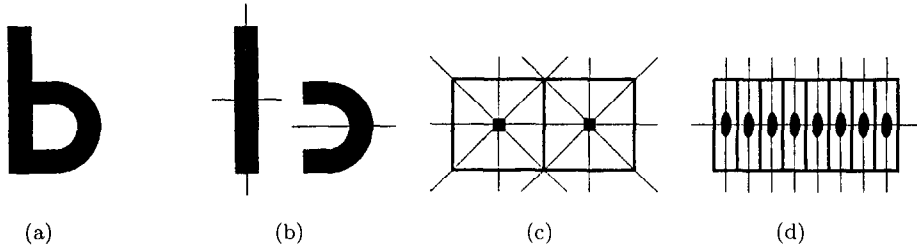


Figure 7. A “b”-shaped figure with symmetry $C_1^* = \mathbf{1}$ (a) has been cut into pieces with symmetries D_2^* (\mathbf{mm}) and D_1^* (\mathbf{m}), respectively (b). A special rectangle has been cut into two squares (c) and rectangular slices (d), the mirror lines and rotation points of which are shown, see text.

Generally, if by decomposition of a geometric figure \mathcal{F} , we find a particular symmetry element \mathbf{g} which is valid for at least a piece of this figure, it must be a fuzzy symmetry element of \mathcal{F} . The extent to which \mathbf{g} is preserved can be quantitatively described by a degree of symmetry (degree of preservation) δ with $0 \leq \delta \leq 1$ (see [4,5]). This degree of symmetry must be proportional to the relative weight of the piece within the figure. This means if one finds a symmetry element \mathbf{g} which is valid at least for some piece \mathcal{P} of this figure, then the degree of symmetry $\delta(G)$ for the corresponding symmetry operation G must in \mathbb{E}^2 be given by

$$\delta(G) \geq \frac{A_P}{A_F} \quad (17)$$

(A_P , A_F : areas of the piece and the whole figure, respectively). In \mathbb{E}^3 , the areas A have to be replaced by the corresponding volumes. The degree of symmetry defined this way is the *lower limit* for the degree of symmetry corresponding to \mathbf{g} , since the very same element may also be shared by other pieces of the figure.

3.2. Fuzzy Symmetries of Point Sets

In this section, the ideas of Section 3.1 will be used to evaluate the degrees of various symmetries in *finite* sets of points. To describe *all* possible fuzzy symmetries within such a set, we must use an unambiguous decomposition of the figure. This can be performed by adopting a consequently “atomic” point of view by using the *points* of the figure as its elementary units. Therefore, I

shall define a geometric figure \mathcal{F} as a set of points of \mathbb{E}^n which (extending the notion of a geometric object in [4]) need not necessarily be connected

$$\mathcal{F} \subset \mathbb{E}^n. \tag{18}$$

In the end, the symmetry of each particular point must be found in the geometric figure as a *fuzzy* or *intermediate* symmetry. For the sake of simplicity, I will use examples in \mathbb{E}^2 .

The symmetry of a Euclidean space \mathbb{E}^n is given by $\mathbb{E}(n)$, the *Euclidean group* in n dimensions of all isometries of \mathbb{E}^n (i.e., all transformations leaving the metric properties of the space invariant). The operations of $\mathbb{E}(n)$ are of the type $\{\mathbb{R} | t\}$ ²⁰, i.e., they are combinations of an $(n \times n)$ orthogonal transformation matrix \mathbb{R} and a translation t [3]. When a certain point of \mathbb{E}^n is made to stand out by demanding its invariance under all transformations, then the symmetry of the space lowers to $\mathbf{O}(n)$, the orthogonal group in n dimensions, the operations of which leave at least this point (the origin) invariant [3]. In physics, the group $\mathbf{O}(3)$ is synonymously denoted by \mathbf{K}_h (complete symmetry group of the sphere). This means that the symmetry of a single point in \mathbb{E}^n is described by $\mathbf{O}(n)$. In \mathbb{E}^2 , the symmetry of a point is $\mathbf{O}(2) \equiv \mathbf{D}_\infty^*$ (∞/\mathbf{mm}), with one infinite-fold rotation point and an infinite number of mirror lines.

Making *two* points of \mathbb{E}^3 stand out, the symmetry lowers to $\mathbf{D}_{\infty h}$ (∞/\mathbf{mm}). In \mathbb{E}^2 , the two points display \mathbf{D}_2^* (\mathbf{mm}) symmetry. In the latter case, only two coinciding mirror lines of the two times infinite many of the two starting points are (in a crisp sense) preserved in the combination of the two points, whereas both the mirror line and the two-fold rotation point between the two points are arrangement symmetries. The assembly of *three* points in a regular manner will give a three-fold rotation point as an arrangement symmetry and three mirror lines which are in part motif symmetries and arrangement symmetries, respectively. In sum, for points taken as motifs of a geometric figure, the following is true:

- (i) In \mathbb{E}^2 , a *single* point defines infinitely many mirror lines as motif symmetries. A *pair* of points defines two additional mirror lines (the connection line and a perpendicular halfway between the two points) as arrangement symmetries. Arrangement symmetry elements of triples, quadruples, etc., of points can be traced back to those of point pairs.
- (ii) A *single* point defines an ∞ -fold rotation point as motif symmetry. A *pair* of points defines one two-fold rotation point and, furthermore, pairs of rotation points of all orders $n \geq 3$ as arrangement symmetries: given a pair of points in a plane (Figure 8), there exists a two-fold rotation point (for which the degree of symmetry is $\delta(C_2) = 1$) halfway between the two points. Moreover, there are rotation points of arbitrary foldness on the perpendicular, their distances x from the connection line (see Figure 8) are given by

$$x = \frac{d}{(2 \cdot \tan(\frac{\pi}{n}))} \tag{19}$$

(d : distance of the two points). Both the rotations C_n^1 and C_n^{n-1} ($n \geq 3$) around these points transform one point of the pair into the other. Since the degree of symmetry δ for a rotation C_n is given by

$$\delta(C_n) = \frac{1}{n} \cdot [\delta(E) + \delta(C_n^1) + \dots + \delta(C_n^{n-1})] \tag{20}$$

(E : identity operation) [5], the degrees of symmetry for these rotation points are

$$\delta(C_n) = \frac{2}{n}. \tag{21}$$

For a C_n point ($n \geq 3$), $n - 2$, more suitably arranged points are needed to arrive at $\delta(C_n) = 1$.

²⁰ $\{\mathbb{R} | t\}$ is the so-called Seitz symbol for general motions in \mathbb{E}^n [18].

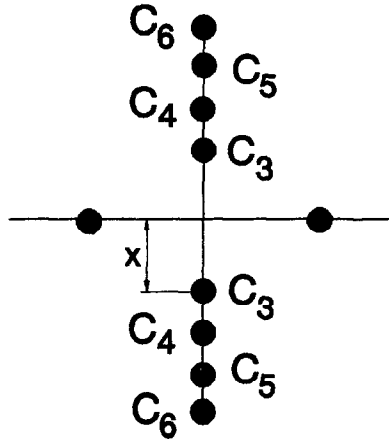


Figure 8. Scheme of two points in the plane and the (fuzzy) rotation points they define (see text). The C_n rotation points are shown up to $n = 6$.

These findings are made the basis for a method for evaluating *fuzzy symmetry landscapes* and *symmetry profiles* for point sets. A symmetry landscape of a two-dimensional figure in \mathbb{E}^2 is one-dimensional (“symmetry profile”) for one-dimensional symmetry elements (mirror lines) in \mathbb{E}^2 , and two-dimensional for zero-dimensional symmetry elements (rotation points). In contrast to the symmetry profiles in [5], here I shall use reflection symmetry profiles along straight lines instead of radially oriented directions and also two-dimensional profiles in the case of rotations. For geometric figures composed of a finite number of points, I propose a third definition of the degree of symmetry δ adding to the definitions given in [4,5]: the degree of symmetry δ for such figures will be defined by the relative number N_C of coincidences between original and transformed points²¹

$$\delta(G) = \frac{N_C}{N_P} = \frac{N\{P \in \mathcal{F} \mid \hat{G} \cdot P = P' \in \mathcal{F}\}}{N\{P \mid P \in \mathcal{F}\}} \quad (22)$$

(N_P : number of points in the figure, N : cardinal number of the finite set indicated [19]), or, identically,

$$\delta(G) = \frac{N(\mathcal{F} \cap \mathcal{F}')}{N(\mathcal{F})}, \quad \mathcal{F}' = \hat{G} \cdot \mathcal{F}. \quad (23)$$

In general, since the degree of symmetry is in essence a *vectorial* property (see [4]), it cannot be evaluated and represented in full, but only for selected symmetries of interest. Figure 9 gives an example in \mathbb{E}^2 . Here, the fuzzy symmetries give a *symmetry profile* or a *symmetry landscape* which is a detailed picture of the symmetry properties of the geometric figures under study. It can be seen that both motif symmetries and arrangement symmetries may appear as intermediate symmetries of the whole figure. In geometric figures consisting of many points, the degree of symmetry stemming from a symmetry element of one single point will, of course, be visible in the symmetry landscape only if this symmetry element is shared by sufficiently many other points. In Figure 9, the fuzzy symmetries of symmetry elements which are only local, but to different degrees, are clearly visible: elements which are valid for only one motif (20% of the whole figure), have a degree of symmetry of 0.2, symmetry elements which are valid for 2 motifs (they are arrangement symmetries in this case) correspond to $\delta = 0.4$, etc. Interestingly, the profile displays as well the degree of symmetry for all other points of the plane, which in the traditional way of looking at such figures are not regarded as containing a mirror plane or rotation point.

²¹In this definition, there has been no discrimination between points on the boundary or contour $\partial\mathcal{F}$ of the figure \mathcal{F} and points within its interior $\mathcal{F} \setminus \partial\mathcal{F}$ since the condition $P \in \partial\mathcal{F} \Leftrightarrow \hat{G} \cdot P = P' \in \partial\mathcal{F}$ is only true for *crisp* symmetry operations.

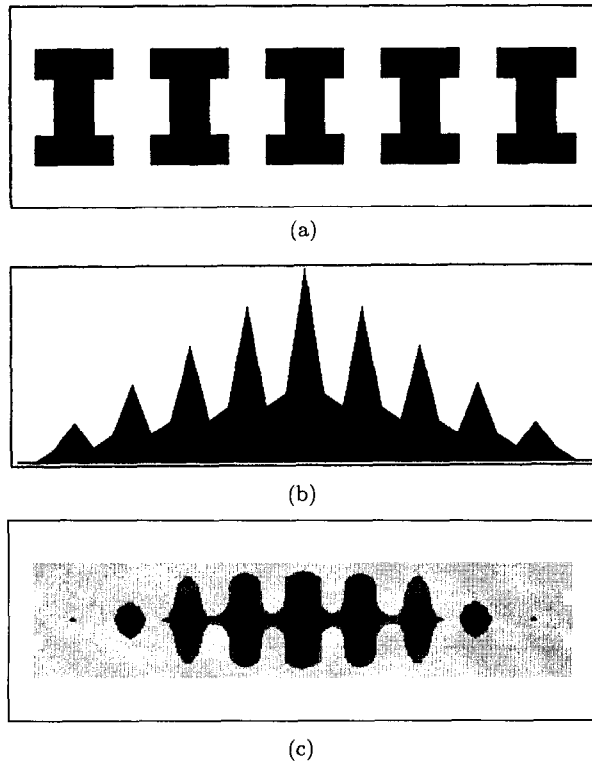


Figure 9. Reflection symmetry profile for vertical mirror lines (b) and rotation (C_2) symmetry profile (c) for a figure composed of five identical "I" motifs (a). The C_2 symmetry landscape is a contour plot for values of $\delta(C_2)$ in steps of 0.2, darker shades of grey mean higher degrees of symmetry.

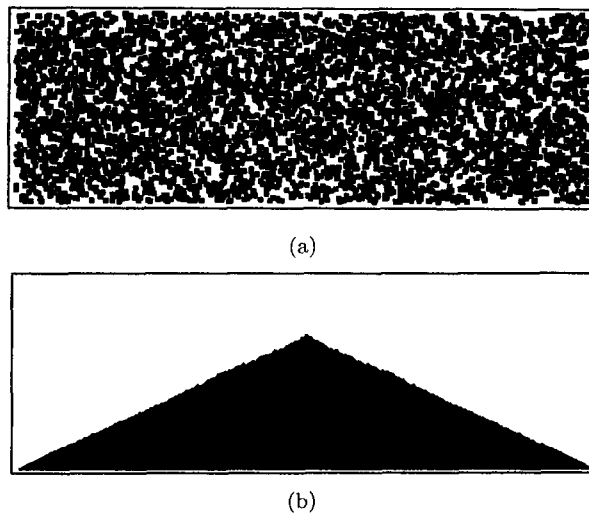
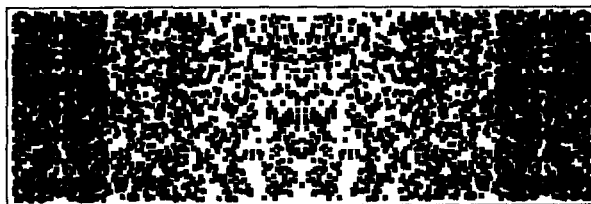


Figure 10. Mirror-symmetry profile for a figure made from 5000 randomly arranged points. Every point has been drawn with 4 pixels to enhance its visibility.

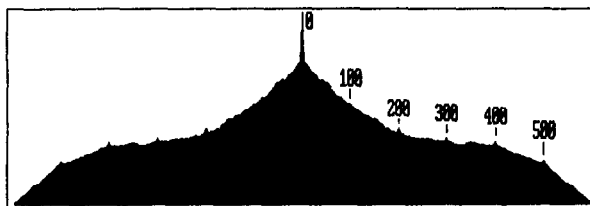
In Figure 10, the mirror-symmetry profile of a picture made from randomly set points is shown. It has a nearly triangular shape, the maximum degree of symmetry being proportional to the point density (number of points). In the extreme case, the picture becomes an ordinary rectangle without gaps for which the symmetry profile is given in Figure 12b. In both cases, the triangular shape of the profile is due to the fact that a mirror line is shared by more points the nearer to the centre line it is.

In contrast, Figure 11 shows two figures where points are set randomly, but afterwards are repeated by reflection at some pre-set local mirror lines. The centre line has been chosen to be a

crisp (global) mirror line, so that the local mirror lines outside it have been duplicated themselves by reflection. N_j points have then been arranged symmetrically to local mirror line j , and N_0 points symmetrically to the centre line. The resulting picture is analogous to the figures made by the method of Shubnikov and Koptsik mentioned in the Introduction. The coarse shape of the profile depends on the gradation of the numbers of points N_j corresponding to the individual mirror lines. If the number of points is inversely proportional to the distance of the mirror line from the centre line, then the profile displays maxima at the locations of the mirror lines rising somewhat higher than the triangular basis profile (not shown). For the number of points being proportional to the mirror line distance, the global triangular profile is disturbed, giving *local* triangular shapes in the extreme case (Figure 11d).



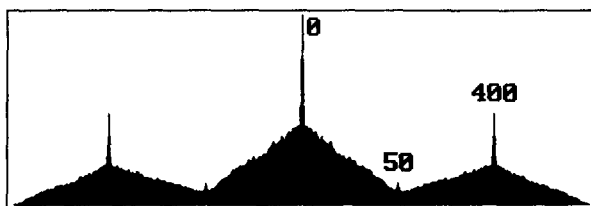
(a)



(b)



(c)



(d)

Figure 11. Mirror symmetry profiles (b,d) for two figures (a,c) made from random points duplicated by reflection at arbitrarily chosen local mirror lines which are themselves arranged symmetrically relative to the centre line. The numbers of points reflected in each mirror line is given about the respective maximum.

Generally, the fuzzy symmetry landscape of a figure has its own symmetry which is identical to the crisp symmetry \mathbf{G} of that figure. This is because symmetry-equivalence of points under the operations of \mathbf{G} also includes equality of the degree of symmetry at these points.

3.3. Symmetry Profiles for Ordinary Geometric Figures

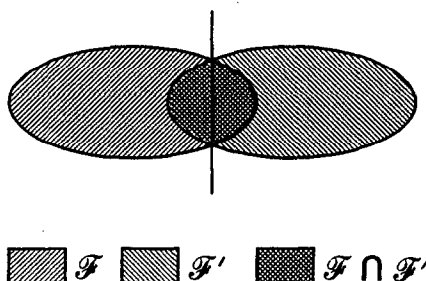
The method described in the foregoing section can be transferred to the description of ordinary geometric figures. Here, the definition of the degree of symmetry is adapted conveying the sense

of it: since the arithmetic for (transfinite) cardinal numbers of *infinite* sets differs from that for finite sets [19], the cardinal numbers of the finite sets have to be replaced by the areas of the corresponding figures

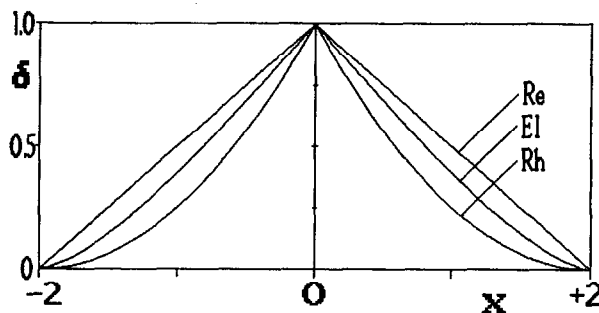
$$\delta = \frac{A(\mathcal{F} \cap \mathcal{F}')}{A(\mathcal{F})}, \quad (24)$$

where $\mathcal{F}' = \hat{G} \cdot \mathcal{F}$ is the figure transformed by the symmetry operation G tested (cf. Figure 12a). Here, $A(\mathcal{F} \cap \mathcal{F}')$ lies between zero if the tested symmetry element is outside the figure, and $A(\mathcal{F})$ if the transformed figure will fully coincide with the original one. On the other hand, $A(\mathcal{F})$ is equal to the maximum possible area difference Δ_{\max} [4], this difference will be reached if the trial symmetry element is outside the figure.

Examples of symmetry profiles obtained this way are given in Figure 12b. Here, a continuous version of the decomposition of a rectangle shown in Figure 7d is performed by shifting a trial symmetry line over the rectangle and measuring the respective degree of symmetry in dependence of the location of this line. The respective areas are evaluated by integration. The same has been done with an ellipse and a rhombus, each with an axis ratio of $x/y = 2$. It can be seen that there are only minor differences between these symmetry profiles. They are dominated by the fact that in all three cases, $A(\mathcal{F} \cap \mathcal{F}')$ increases monotonically from the border to the centre of the figures.



(a) Scheme for the evaluation of the degree of symmetry for geometric figures under reflection (see text). The original figure \mathcal{F} , its reflected image \mathcal{F}' , and the intersection of both point sets ($\mathcal{F} \cap \mathcal{F}'$) have been differentiated.



(b) Reflection symmetry profiles for different related geometric figures: a rectangle (Re), an ellipse (El), and a rhombus (Rh), all with axis ratios of $x/y = 2$. A vertical trial mirror symmetry line has been moved over the figure along the x axis.

Figure 12.

4. CONCLUSIONS

The main points made in this paper are the following:

- (i) A geometric figure \mathcal{F} with prescribed arbitrary symmetry \mathbf{G} can be built up from motifs of likewise arbitrary symmetries. The relationships governing the assembly of the motifs are clarified by using the concepts of site symmetry and direction symmetry.
- (ii) For the analysis of site symmetries, a study of the point group matrix $\hat{\mathbf{G}}$ is advantageous. It provides all necessary information about general and special points (sites) within a given

- symmetry (equivalence classes of symmetry operations, multiplicity of points, orders of orbits and so on).
- (iii) If a motif with symmetry \mathbf{G}_M is placed on a site with site symmetry \mathbf{G}_S , then only a part (\mathbf{G}_{MO}^*) of the direction symmetry \mathbf{G}_{MO} of the motif towards the origin of the figure is effective, so that one has $\mathbf{G}_s = \mathbf{G}_{MO}^* \subseteq \mathbf{G}_{MO} \subseteq \mathbf{G}_M$. The complement $\mathbf{G}_M \setminus \mathbf{G}_S$ becomes an *intermediate symmetry* of the figure. If the direction symmetry of the motif is changed by variation of its orientation, then all symmetry operations which are compatible with the other motifs of the figure will become global symmetry operations. Thus, it may happen that the symmetry of the whole figure will be *enhanced*.
 - (iv) Strictly speaking, the *elementary* motifs of a certain geometric figure are the *points* from which it is made. This is a special (extreme) case of the decomposition of a figure into motifs. Since a single point in \mathbb{E}^n has the symmetry $\mathbf{O}(n)$, all its symmetry elements, which are not (in a crisp sense) preserved in the superposition with other points when assembling the figure, must form intermediate symmetries of the figure. The degree of symmetry of a certain symmetry element, then, is higher the more points are sharing this symmetry element.
 - (v) The analysis presented here is valid for arbitrary geometric figures. Motif and arrangement symmetries are treated in an equal manner, when they form crisp or intermediate symmetries of the geometric figure under study.
 - (vi) All symmetries of a given figure, be they crisp or intermediate, can be found by evaluating symmetry landscapes or symmetry profiles using the definitions for the degree of symmetry δ given in this paper. The symmetry profile or landscape has the crisp symmetry of the geometric figure. Since δ , in essence, is a *vectorial* property comprising the symmetry properties of the figure under all possible symmetry groups, it can be displayed only for selected groups.
 - (vii) The fuzzy symmetry concept gives a much more detailed insight into symmetry properties (especially into *intermediate*, i.e., *local* symmetries) of geometric figures than the traditional crisp notion of symmetry can provide.

REFERENCES

1. K.L. Wolf and R. Wolff, *Symmetrie*, Böhlau Verlag, Münster, p. 4, (1956).
2. K.L. Wolf and D. Kuhn, *Gestalt und Symmetrie*, *Die Gestalt* **23**, 7 (1952).
3. A.V. Shubnikov and V.A. Koptsik, *Symmetry in Science and Art*, pp. 29,69,127,242,328, Plenum Press, New York, (1974).
4. A.E. Köhler, A fuzzy symmetry concept for forms with imperfect symmetry, *Computers Math. Applic.* **22** (9), 35–50 (1991).
5. A.E. Köhler, A second approach to fuzzy symmetries: Fuzzy symmetry requirements, *Computers Math. Applic.* **25** (1), 17–34 (1993).
6. A.C. Edmondson, *A Fuller Explanation*, Chapter 13, Birkhäuser, Boston, (1987).
7. T. Hahn, Editor, *International Tables for Crystallography, Vol. A: Space-Group Symmetry*, pp. 71,724, Chapter 8.3.2, Chapter 10.2, D. Reidel, Dordrecht, (1987).
8. N.F.M. Henry and K. Lonsdale, Editors, *International Tables for X-Ray Crystallography*, Chapter 3.3, Kynoch Press, Birmingham, (1965).
9. K. Klemm, *Symmetrien von Ornamenten und Kristallen*, Springer-Verlag, Berlin, p. 5, (1982).
10. H. Burzlaff and H. Zimmermann, *Symmetrielehre*, G. Thieme Verlag, Stuttgart, pp. 42,59,62–64,330, Chapter 3.1.1, (1977).
11. R.S. Halford, Motions of molecules in condensed systems: I. Selection rules, relative intensities, and orientation effects for Raman and infra-red spectrum, *J. Chem. Phys.* **14**, 8–15 (1946).
12. R.L. Flurry, Jr., The use of site symmetry in constructing symmetry adapted functions, *Theoret. Chim. Acta* **31**, 221–230 (1973).
13. R.V. Galiulin, Classification of directions in crystallographic point groups according to the symmetry principle, *Acta Cryst.* **A36**, 864–869 (1980).
14. L.L. Boyle, The method of ascent in symmetry I. Theory and tables, *Acta Crystallog* **A28**, 172–178 (1972).
15. S. Fujita, *Symmetry and Combinatorial Enumeration in Chemistry*, pp. 32,36, Springer-Verlag, Berlin, (1991).

16. A. Speiser, *Die Theorie der Gruppen von endlicher Ordnung*, Birkhäuser Verlag, Basel, pp. 26,29, Chapter 8, (1956).
17. A.E. Köhler, Isosymmetric manifolds in form spaces and the normal deformations of polygonal forms, *Computers Math. Applic.* **25** (9), 67–89 (1993).
18. M. Belger and L. Ehrenberg, *Theorie und Anwendung der Symmetriegruppen*, p. 43, BSB B.G. Teubner Verlagsgesellschaft, Leipzig, (1981).
19. W. Gellert, H. Küstner, M. Hellwich, H. Kästner, Editors, *Kleine Enzyklopädie Mathematik*, p. 701, Bibliographisches Institut, Leipzig, (1965).