

Article

# Structure Transformations in Broken Symmetry Groups—Abstraction and Visualization

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**Abstract:** The work reports the finding and the study of transformation groups with two conditional elements (binary transformations of abstract structures of the finite numerical sets with broken symmetry). The term Broken Symmetry Group (BSG) is introduced. Transformation examples of relevant structures are studied with computer visualization and application in real structure study. A special type of BSG was discovered, which describes the subsets of “evolutionary trees” with convergent and divergent properties of the oriented graph (orgraph) with structure-development direction edges and “growth spirals”.

**Keywords:** groups of substitution symmetry; Cayley tables; broken symmetry; permutation multiplying tables; orgraph; broken symmetry groups; convergent and divergent transformation graphs; evolutionary trees; growth spiral

## 1. Introduction

All the known physical effects in crystals are described based on the Curie-Neumann principle: the symmetry of the structure and the symmetry of the “impact” on the structure are summated in a way where only shared transformations remain. The growth of monocrystals in particular starts in one spot (nucleant-defect), where the symmetry of medium uniformity and isotropy is broken.

In a general case, systems interaction also results the transformations which break the symmetry and lead to the restructuring of each system [1]. This circumstance, as with many other factors, allows highlighting of the unity of two major principles of development, growth, accumulation, evolution, and stability of systems. These are, firstly, when expanded to all the systems, Curie’s Broken Symmetry Principle, which determines the cause of new occurrences, and secondly Le Chatelier’s symmetry conservation principle, which determines the system’s response, counteracting any infraction. The latter claims a conservation of the previous state or a transition to a new one, but also sustainable (symmetrical) state. According to the Noether’s theory, in a physical system of material particles, every differentiable symmetry of the action of a physical system has a corresponding energy-impulse conservation. In this case, the four-dimensional spatial occurrences continuum performs a “function” of possibility space. Lately, the following terms became common in scientific literature: phase space, economical space, personal psychological space, viral genome space, configurational space, informational space, and many others, which often are referred to as many-dimensional. Existing software tools such as Multidimensional Scaling (MDS) allow the projection of all the processed information on a familiar three-dimensional space. In all those

dimensions, formally abstract variables create an “image” of the system and its reactions, which becomes a method of abstraction “visualization”.

A substantial contribution to the studies of the symmetry and natural substances' properties within a crystal lattice state was made by Russian crystallographers [1,2]. These are the classic works of Fedorov (230 spatial groups of symmetry), Shubnikov (black-and-white symmetry), and Belov (color symmetry) etc. Starting midway through the last century, a numerous amount of works devoted to systems with broken symmetry had been written. In particular, super-symmetry groups and multidimensional groups [3] were introduced for the description of incommensurately modulated phases and quasicrystals. For more complex cases, a description based on “interlacement groups” [4] was introduced, which, in the final analysis, may depict the classic groups of substitutions. A research on pseudo-symmetry during a monocrystal growth may be referred to as an example [5].

Historically, symmetry groups theory takes the mathematical course starting with the work of Galois, describing the theory of symmetry of equation roots permutation. All the classic algebra [6] studies and combinatorics [7], geometry, and topology relate to the group theory basics. General classification of binary relation sets by groups, semi groups, field of scalars, vectors, tensor quantities and rings relate directly to the maze, diagrams, nets, graphs, orgraphs and other mathematical structures as well as to real objects. In particular, in modern quantum field theory a diagram technique of the description of the broken symmetry processes was offered by Feinman. The works of other Nobel Prize laureates, including Higgs, led to the understanding of the gauge symmetry of the physical vacuum state and of the moment of the “beginning” of the Universe [8], starting with the Higgs boson. Therefore, the accordingly reinterpreted quantum theory of nonabelian gauge fields with spontaneously broken symmetry lays the basis of scientific conceptions of this research area. Feinman's diagrams will be studied in further works within the scope of Broken Symmetry Group (BSG) analysis.

The article does not aim to present the fundamental essence of symmetry and the mechanisms of broken symmetry in different types of matter (physical, biological, social etc.), but attempts to search for a broken system elementary mathematical model and possible “visualization”, for which purpose some studies previously developed and presented in the field of computer techniques had been used [9,10]. Group theory shows that any finite symmetry group is isomorphic to a permutation group accordingly (Cayley theorem). Therefore, to describe symmetry, a “matrix representation” may be implemented as well as a two-rowed matrices substitution representation. In this article, the substitution is the choice due to, firstly, symmetry operation record simplicity and, secondly, substitution coding regardless of space characteristics. This has a particular importance when dealing with the state space or phase space, where topology and sizing may be indeterminate enough to enter a certain virtual possibilities space to visualize a calculation result.

As shown in the study [9], quaternion abstract symmetry, Pauli matrices, Dirac matrices and the local symmetry can be analyzed with substitution groups, and its visualization can be performed on periodic packing space discretion in the lattice [9]. This article will report the results describing translational symmetrical structures as well as non-periodic packing spaces structures and their discretion graphs. We will implement broken symmetry mathematical groups for restructuring processes description, in accordance with Curie's principle. This was briefly reported by the article's authors at the First Russian Crystallography Congress [11].

## 2. Transformation Models in Structures with Broken Symmetry

In our research, the first case of the broken symmetry group (BSG) finding and new properties showing up was the structure of the complex octahedral cation  $[\text{Me}(\text{urea})_6]^{2+,3+}$  (reference code “WOKNIT” in the database [12] with chelate hydrogen bonds [10,13]. Previously, the overview article [14] reported a crystallo-chemical research of possible combinations of directed H-bonds in different structures of complex compounds with carbamide. The description of the symmetry of complex cation [13] with double hydrogen bond required the “defect” substitutes entry to be in the form of two-rowed matrices as follows:  $\begin{pmatrix} 012345 \\ 223550 \end{pmatrix}$ , or, briefly, with the use of the “coding” (lower row):

$g[1] = (223550)$ . Therefore the classic multiplication substitution table (Cayley table) of a complex octahedral symmetry group in the orgraph model of directed bonds was not possible to apply. The octahedral symmetry was broken regarding directed bonds [12].

A series of computer experiments were performed to research such modifications in symmetry [11]. Now we will intentionally implement a defect (“accidental coding mistake”) in the entry of a certain substitution cyclic subgroup.

A regular pentagon (with a fixed central point) will be perceived as a classic symmetry simple geometric structure (Figure 1). A singular transformation  $g[0]$  will be left without the defect; however instead of a classic permutation ( $72^\circ$  turn), which is coded by matrix  $g[1]_{class} = (023451)$ , formally we will enter a different operation:  $g[1] = (023431)$ . Evidently a defect shows up within the fifth place in the permutation coding row.

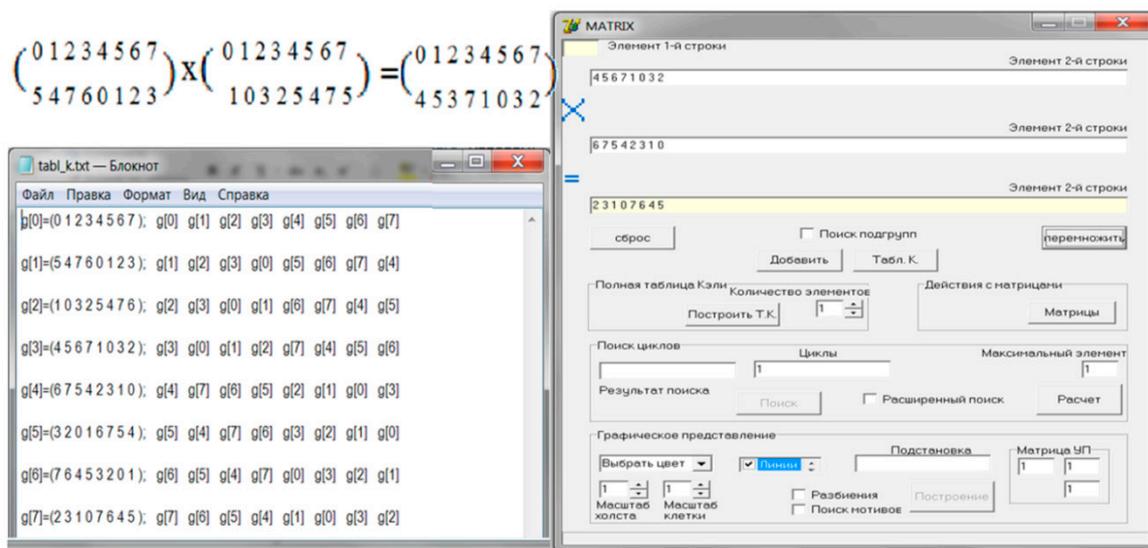


Figure 1. Groups calculation results with multiplication table and a program window screen shot.

If thereafter we use a simple rule of two-row matrices multiplication, then we will get an operations set  $g[1] = (023431)$ ,  $(g[1])^2 = g[2] = (034342)$ ,  $(g[1])^3 = g[3] = (043433)$  and  $(g[1])^4 = g[4] = (034344)$  as other elements of a substitution cyclic group.

We will “expand” this final subgroup up to the “9th order group” by the operation with a defect  $g[5] = (012343)$ . As a result we will get the final multiplication table of substitution with a defect (Table 1).

Table 1. Substitution operations with a defect subset and a multiplication table.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5);$	$g[0] g[1] g[2] g[3] g[3] g[5] g[6] g[7] g[8]$
$g[1] = (0\ 2\ 3\ 4\ 3\ 1);$	$g[1] g[2] g[3] g[4] g[3] g[1] g[2] g[3] g[4]$
$g[2] = (0\ 3\ 4\ 3\ 4\ 2);$	$g[2] g[3] g[4] g[3] g[4] g[2] g[3] g[4] g[3]$
$g[3] = (0\ 4\ 3\ 4\ 3\ 3);$	$g[3] g[4] g[3] g[4] g[3] g[3] g[4] g[3] g[4]$
$g[4] = (0\ 3\ 4\ 3\ 4\ 4);$	$g[4] g[3] g[4] g[3] g[4] g[4] g[3] g[4] g[3]$
$g[5] = (0\ 1\ 2\ 3\ 4\ 3);$	$g[5] g[6] g[7] g[8] g[7] g[5] g[6] g[7] g[8]$
$g[6] = (0\ 2\ 3\ 4\ 3\ 4);$	$g[6] g[7] g[8] g[7] g[8] g[6] g[7] g[8] g[7]$
$g[7] = (0\ 3\ 4\ 3\ 4\ 3);$	$g[7] g[8] g[7] g[8] g[7] g[7] g[8] g[7] g[8]$
$g[8] = (0\ 4\ 3\ 4\ 3\ 4);$	$g[8] g[7] g[8] g[7] g[8] g[8] g[7] g[8] g[7]$

For the structure, new operations with “a defect” cannot be considered permutations. However, at the same time they can still be called number substitutions, because the term “substitution” is wider than the term “permutation”. Permutation retains the numbers set, and substitution may change them.

Evidently, the resulting table is not a classic multiplication Cayley table, as inverse elements are absent and properties change “by rows” and “by columns”. Therefore, we may state that “a mistake” in element coding in symmetry groups led to a broken symmetry. We will consider [8] that each transformation from the elements of the transformation set may be visualized by analyzing the substitution itself.

Each modification [9] can be visualized by analyzing the substitution itself. Substitution visualization of three operations, randomly chosen from Table 1, is presented in Figure 2 [15].

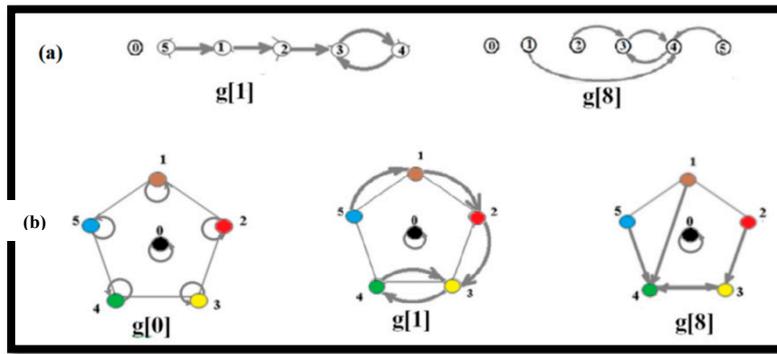


Figure 2. Visualization of substitutions g[1], g[8] Table 1 in one dimensional space (a) and g[0], g[1], g[8] in two-dimensional space (b).

**Definition 1.** The product set of two-rowed matrices of substitution numbers, which are not permutations, will be called broken symmetry groups (BSG). The order of the finite group broken symmetry is determined by the amount of transformations. The above example with nine operations can be marked as BSG 9.

In one of the computer experiments [11] using a designed program of binary matrices multiplication with classic and non-classic substitutions (Figure 3) numerical set of 34 number values made a substitution set consisting of 91 BSG operations. Out of the set, two operations subgroups can be highlighted (including g[0]), which create small finite subsets (Table 2) BSG 6 and BSG 4.

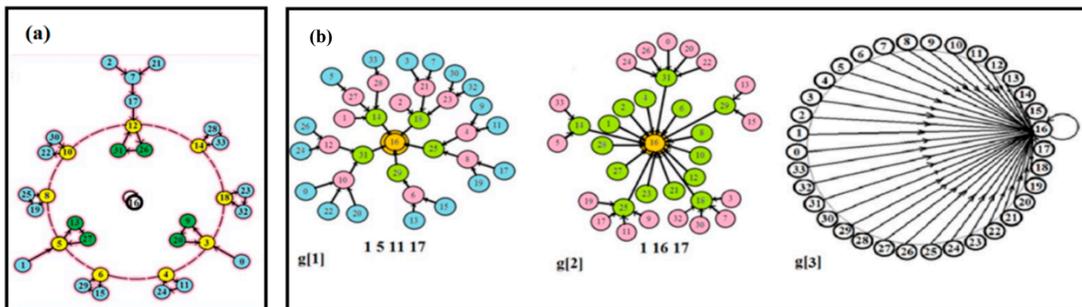


Figure 3. BSG 91 operations visualization as a model structure with 34 dots. Transformation structure g[1] Table 2 of the 6th order BSG subgroup (a) and transformation structures g[1]–g[3] Table 2 of the 4th order BSG 4 subgroup (b).

**Table 2.** 6 and 4 transformations subsets of BSG-91 and their multiplication tables.

g[0] = (0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33);	g[0]	g[1]	g[2]	g[3]	g[4]	g[5]
g[1] = (3 5 7 9 11 13 15 17 19 20 22 24 26 27 28 29 16 12 23 25 3 7 30 32 4 8 31 5 33 6 10 12 18 14);	g[1]	g[2]	g[3]	g[4]	g[5]	g[3]
g[2] = (9 13 17 20 24 27 29 12 25 3 30 4 31 5 33 6 16 26 32 8 9 17 10 18 11 19 12 13 14 15 22 26 23 28);	g[2]	g[3]	g[4]	g[5]	g[3]	g[4]
g[3] = (20 27 12 3 4 5 6 26 8 9 10 11 12 13 14 15 16 31 18 19 20 12 22 23 24 25 26 27 28 29 30 31 32 33);	g[3]	g[4]	g[5]	g[3]	g[4]	g[5]
g[4] = (3 5 26 9 11 13 15 31 19 20 22 24 26 27 28 29 16 12 23 25 3 26 30 32 4 8 31 5 33 6 10 12 18 14);	g[4]	g[5]	g[3]	g[4]	g[5]	g[3]
g[5] = (9 13 31 20 24 27 29 12 25 3 30 4 31 5 33 6 16 26 32 8 9 31 10 18 11 19 12 13 14 15 22 26 23 28);	g[5]	g[3]	g[4]	g[5]	g[3]	g[4]
g[0] = (0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33);	g[0]	g[1]	g[2]	g[3]		
g[1] = (10 14 18 21 25 27 29 21 25 4 31 4 31 6 16 6 16 8 16 8 10 18 10 18 12 16 12 14 14 16 23 16 23 28);	g[1]	g[2]	g[3]	g[3]		
g[2] = (31 16 16 18 16 14 16 18 16 25 16 25 16 29 16 29 16 25 16 25 31 16 31 16 31 16 16 16 18 16 18 14);	g[2]	g[3]	g[3]	g[3]		
g[3] = (16 16);	g[3]	g[3]	g[3]	g[3]		

Some transformations visualization from the table is presented on Figure 3. Of particular interest is the multiplication table of the 4th order subgroup from Table 2, i.e., product table  $g[i] \times g[k]$ , which can serve as the grounding for the following statement: subgroups with convergent properties of the transformation structure orgraph can exist within BSGs.

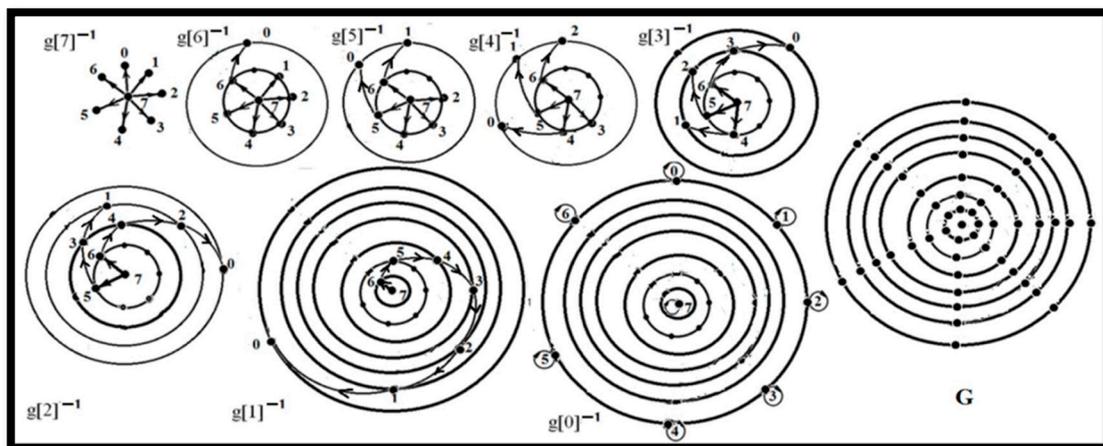
Evidently, for each table (with any finite number of elements), structurally created analogically with the multiplying table (Table 2, 4th order), there is always one transformation which inevitably exists, and which can be registered as a single value of integer R. A particular case of a group structure with such an inevitable operation is presented in Table 3. Operation  $g[R] = g[7] = (7 7 7 7 7 7 7 7)$ .

**Table 3.** Broken symmetry group with the “Rome” point on the 8 points set and the group multiplication table.

g[0] = (0 1 2 3 4 5 6 7);	g[0]	g[1]	g[2]	g[3]	g[4]	g[5]	g[6]	g[7]
g[1] = (1 2 3 4 5 6 7 7);	g[1]	g[2]	g[3]	g[4]	g[5]	g[6]	g[7]	g[7]
g[2] = (2 3 4 5 6 7 7 7);	g[2]	g[3]	g[4]	g[5]	g[6]	g[7]	g[7]	g[7]
g[3] = (3 4 5 6 7 7 7 7);	g[3]	g[4]	g[5]	g[6]	g[7]	g[7]	g[7]	g[7]
g[4] = (4 5 6 7 7 7 7 7);	g[4]	g[5]	g[6]	g[7]	g[7]	g[7]	g[7]	g[7]
g[5] = (5 6 7 7 7 7 7 7);	g[5]	g[6]	g[7]	g[7]	g[7]	g[7]	g[7]	g[7]
g[6] = (6 7 7 7 7 7 7 7);	g[6]	g[7]						
g[7] = (7 7 7 7 7 7 7 7);	g[7]	ROME						

The point where all the paths cross within the orgraph structure (as per Figure 3 for  $g[3]$ ,  $R = 16$ ) in a word will be called “Rome” (as per old saying: “All roads lead to Rome”), and the elements set of such a table, where “Rome” point exists, will be called “the Rome Transformations Set”.

A transition to the orgraph with divergent vectors (“All roads start in Rome”), formally can be seen as “reverse” operation,  $g[1]^{-1}$ , where upper and lower rows switch places in substitutional matrices [15]. A graphic representation of the reverse to the transformations from Table 3 operations is shown on Figure 4 as a divergent process (diverging “development spiral”).



**Figure 4.** Operations  $g[0]^{-1}$ – $g[7]^{-1}$  visualization in a virtual state space G,  $g[7]^{-1}$ —reverse modification with “Rome point”  $R = 7$ .

A virtual “possibility space”, or “latitude rate” (Figure 4) is necessary for such an “expansion”. Not a single system may develop without this condition. This circumstance requires additional systemic philosophical analysis (for instance within the “fractal-facet model” [16]).

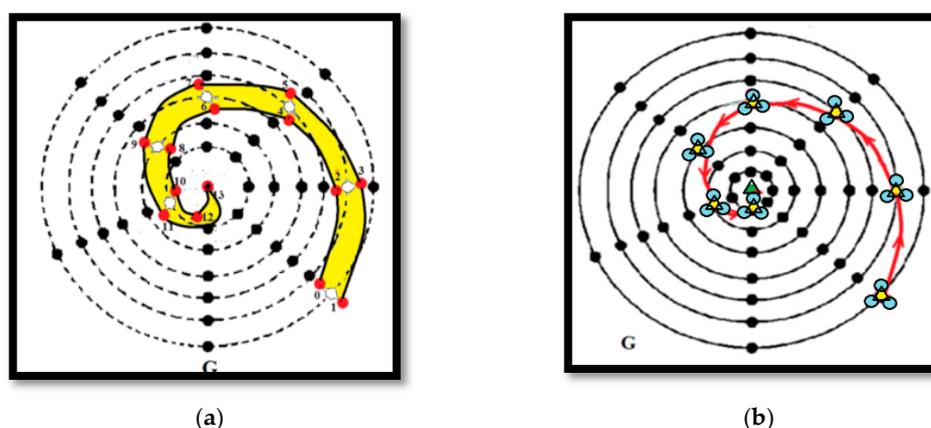
The  $g[7]$  operation in the Roman set from Table 4 acts as “zero”, since its application to other operations of the set of elements results in  $g[7]$ : “zero remains zero, regardless of how it is multiplied”. Therefore, the Roman set of binary operations has “unity” ( $g[0]$ ) and “zero” ( $g[7]$ ) but does not have inverse elements.

**Table 4.** Transformations types and a multiplying table for a 14 dots system.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13)$ ;	$g[0]\ g[1]\ g[2]\ g[3]\ g[4]\ g[5]\ g[6]$ ;
$g[1] = (2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 12\ 13)$ ;	$g[1]\ g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[6]$ ;
$g[2] = (4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 12\ 13\ 12\ 13)$ ;	$g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[6]\ g[6]$ ;
$g[3] = (6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13)$ ;	$g[3]\ g[4]\ g[5]\ g[6]\ g[6]\ g[6]\ g[6]$ ;
$g[4] = (8\ 9\ 10\ 11\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13)$ ;	$g[4]\ g[5]\ g[6]\ g[6]\ g[6]\ g[6]\ g[6]$ ;
$g[5] = (10\ 11\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13)$ ;	$g[5]\ g[6]\ g[6]\ g[6]\ g[6]\ g[6]\ g[6]$ ;
$g[6] = (12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13\ 12\ 13)$ .	$g[6]\ g[6]\ g[6]\ g[6]\ g[6]\ g[6]\ g[6]$ .

The orgraph divergent property leads to a situation where all the points of the structure become distinguishable (not identical), i.e., they only pass into themselves. This is the finite operation of “unity”  $g[0]^{-1}$  (Figure 4). On the contrary, the convergence leads to absolute symmetry when all points of the structure become indistinguishable (identical). This is the finite operation of “zero”  $g[R]$  (“Rome point”).

Table 4 and Figure 5a represent transformations types and a multiplying table for a 14 dots system ( $7 \times 2$ ) with 6 stages of the evolutionary spiral. The system expanding is done in accordance with the work’s formulations [9]. Similarly, Table 5 and Figure 5b represents a development spiral of the expanded system of 24 dots with 7 stages ( $8 \times 3$ ).



**Figure 5.** Two versions of “evolution spiral” in broken symmetry groups: (a) 7 steps in the structure of  $7 \times 2 = 14$  dots; and (b) 8 steps in the structure of  $8 \times 3 = 24$  dots.

The point of sets classification in mathematics, obtained by the broken symmetry method generally stand as symmetry subgroups, rings and semi groups grouping. There was no contravention of the associativity requirement detected in all the examined cases. Below are a few cases of BSG to describe symmetry and broken symmetry.

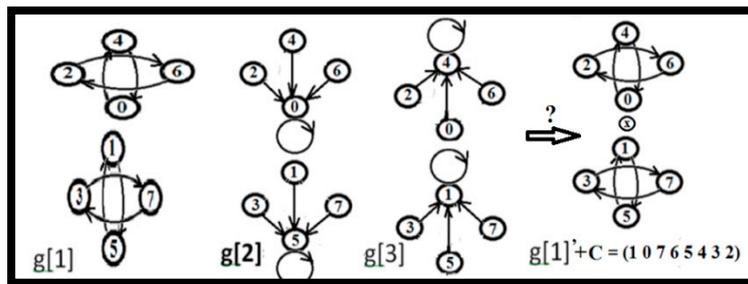
**Table 5.** Transformations types and a multiplying table for a 24 dots system.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23);$	$g[0]\ g[1]\ g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[7];$
$g[1] = (3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 21\ 21\ 21\ 21);$	$g[1]\ g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[7]\ g[7];$
$g[2] = (6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[7]\ g[7]\ g[7];$
$g[3] = (9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[3]\ g[4]\ g[5]\ g[6]\ g[7]\ g[7]\ g[7]\ g[7];$
$g[4] = (12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[4]\ g[5]\ g[6]\ g[7]\ g[7]\ g[7]\ g[7];$
$g[5] = (15\ 16\ 17\ 18\ 19\ 20\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[5]\ g[6]\ g[7]\ g[7]\ g[7]\ g[7]\ g[7];$
$g[6] = (18\ 19\ 20\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[6]\ g[7]\ g[7]\ g[7]\ g[7]\ g[7]\ g[7];$
$g[7] = (21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21\ 21);$	$g[7]\ g[7]\ g[7]\ g[7]\ g[7]\ g[7]\ g[7].$

**3. Applied Method of Symmetry Groups Visualization**

Example 1. As shown in the study [5], within the crystal growth the internal intermolecular interaction can convert the system with two local centers (LC) of symmetry into a system with one global center (GC) of symmetry without the property modifications (Figure 6, g[1]) (classic substitution). Suppose we have two subgroups: A (with a global symmetry center from Table 6 and B (with two LCs and broken symmetry from Table 7 and Figure 7.

We will calculate  $A \times B$  to assess a possibility of a joint existence of the structure with a global and local symmetry centers within one structure. The calculation result is presented in Table 8.



**Figure 6.** Global center (GC) regain  $g[1]' = g[1]$ .

**Table 6.** Subgroup A with broken symmetry with a global symmetry center.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7);$	$g[0]\ g[1]$	E
$g[1] = (1\ 0\ 7\ 6\ 5\ 4\ 3\ 2);$	$g[1]\ g[0]$	GC

**Table 7.** Subgroup B with broken symmetry and two local centers.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7);$	$g[0]\ g[1]\ g[2]\ g[3]$	E
$g[1] = (4\ 5\ 6\ 7\ 0\ 1\ 2\ 3);$	$g[1]\ g[0]\ g[2]\ g[3]$	LC
$g[2] = (0\ 5\ 0\ 5\ 0\ 5\ 0\ 5);$	$g[2]\ g[3]\ g[2]\ g[3]$	BS
$g[3] = (4\ 1\ 4\ 1\ 4\ 1\ 4\ 1);$	$g[3]\ g[2]\ g[2]\ g[3]$	BS

**Table 8.** BSG table of the group  $A \times B$  binary transformations and a multiplying table.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7);$	$g[0]\ g[1]\ g[2]\ g[3]\ g[4]\ g[5]\ g[6]\ g[7];$	E
$g[1] = (1\ 0\ 7\ 6\ 5\ 4\ 3\ 2);$	$g[1]\ g[0]\ g[3]\ g[2]\ g[5]\ g[4]\ g[7]\ g[6];$	GC
$g[2] = (4\ 5\ 6\ 7\ 0\ 1\ 2\ 3);$	$g[2]\ g[3]\ g[0]\ g[1]\ g[4]\ g[5]\ g[6]\ g[7];$	LC
$g[3] = (5\ 4\ 3\ 2\ 1\ 0\ 7\ 6);$	$g[3]\ g[2]\ g[1]\ g[0]\ g[5]\ g[4]\ g[7]\ g[6];$	TC
$g[4] = (4\ 1\ 4\ 1\ 4\ 1\ 4\ 1);$	$g[4]\ g[6]\ g[7]\ g[5]\ g[4]\ g[5]\ g[6]\ g[7];$	NC
$g[5] = (1\ 4\ 1\ 4\ 1\ 4\ 1\ 4);$	$g[5]\ g[7]\ g[6]\ g[4]\ g[5]\ g[4]\ g[7]\ g[6];$	NC
$g[6] = (5\ 0\ 5\ 0\ 5\ 0\ 5\ 0);$	$g[6]\ g[4]\ g[5]\ g[7]\ g[5]\ g[4]\ g[7]\ g[6];$	NC
$g[7] = (0\ 5\ 0\ 5\ 0\ 5\ 0\ 5);$	$g[7]\ g[5]\ g[4]\ g[6]\ g[4]\ g[5]\ g[6]\ g[7].$	NC

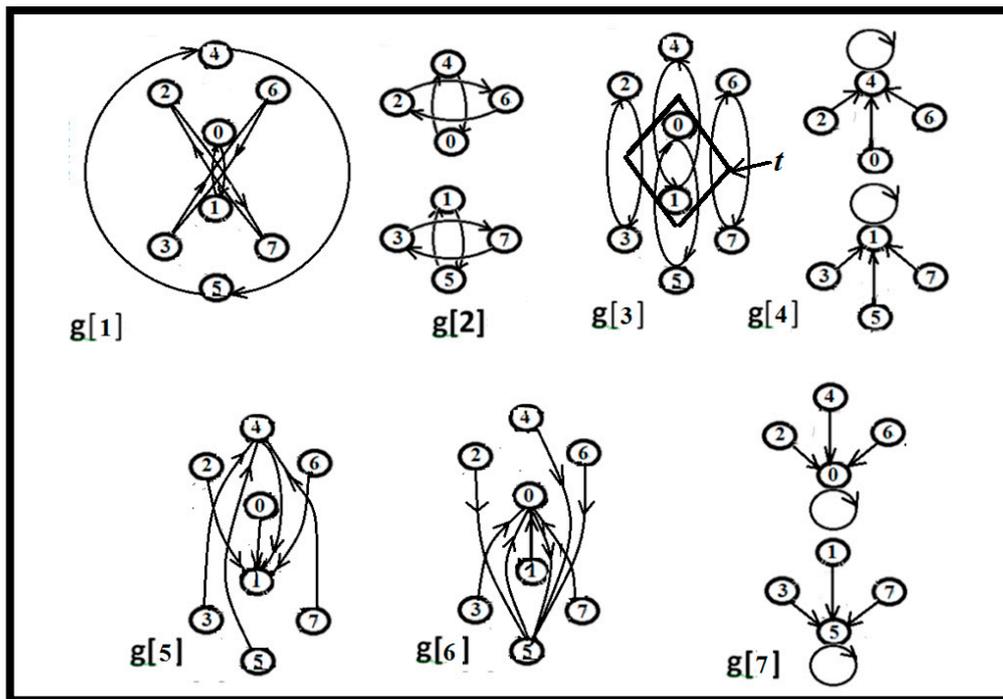


Figure 7. Structural images of transformation in a full group.

Evidently, in a joint BSG,  $g[1]$  and  $g[2]$  visualize a global symmetry center (inversion) (1) and (2) two LCs of inversion.  $g[3]$  describes a structure with 4 centers and  $t$ -transfer (TC).

Example 2. Let the two subsets of elements—dots numbered from 0 to 14 and from 15 to 25—interact in various ways. The possible three scenarios of its “behavior” are: (1) with the symmetry center (equality) between the dots of internal convergence (“Rome points” 0 and 15); (2) with numbers 0 and 15; (2) without the local symmetry center of convergence dots and (3) with a directed bond between them (Figure 8). First, let's refer to the case dynamics of the third scenario (Table 9).

Scenario 3. Directed bond.  $15 \rightarrow 0$ . Ultimately Rome  $g[4]$ .

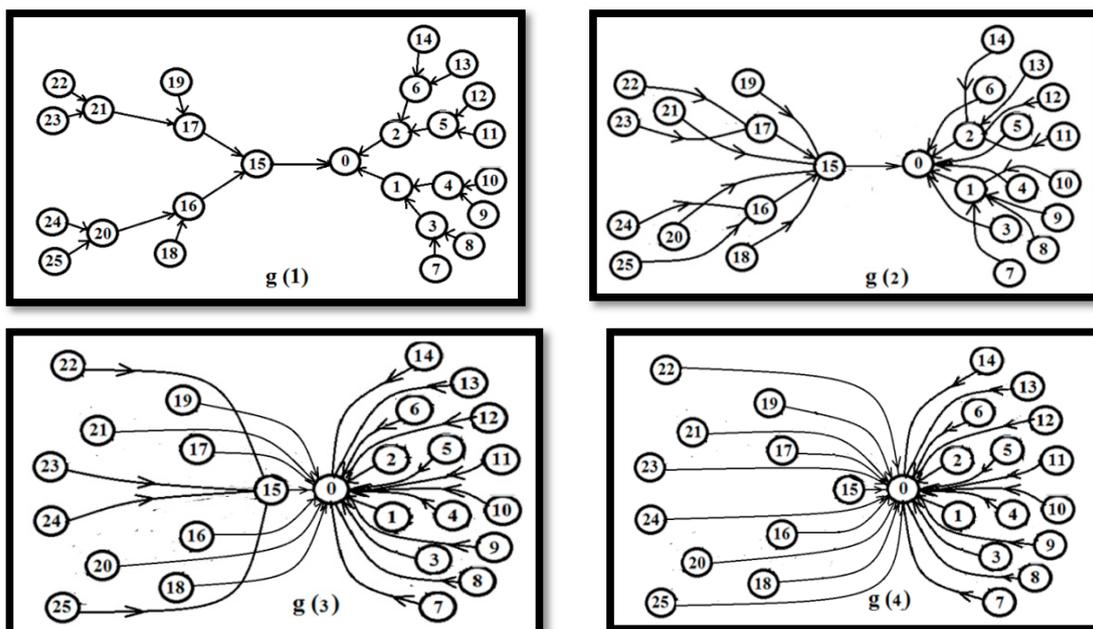


Figure 8. Step by step system dynamics in Scenario 3.

**Table 9.** Step by step system dynamics in Scenario 3.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23\ 24\ 25);$	$g[0]\ g[1]\ g[2]\ g[3]\ g[4];$
$g[1] = (0\ 0\ 0\ 1\ 1\ 2\ 2\ 3\ 3\ 4\ 4\ 5\ 5\ 6\ 6\ 0\ 15\ 15\ 16\ 17\ 16\ 17\ 21\ 21\ 20\ 20);$	$g[1]\ g[2]\ g[3]\ g[4]\ g[4];$
$g[2] = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 2\ 2\ 2\ 2\ 0\ 0\ 0\ 15\ 15\ 15\ 15\ 17\ 17\ 16\ 16);$	$g[2]\ g[3]\ g[4]\ g[4]\ g[4];$
$g[3] = (0\ 15\ 15\ 15\ 15);$	$g[3]\ g[4]\ g[4]\ g[4]\ g[4];$
$g[4] = (0\ 0);$	$g[4]\ g[4]\ g[4]\ g[4]\ g[4].$

Figure 8 represents a visualization of the transformation scenario.

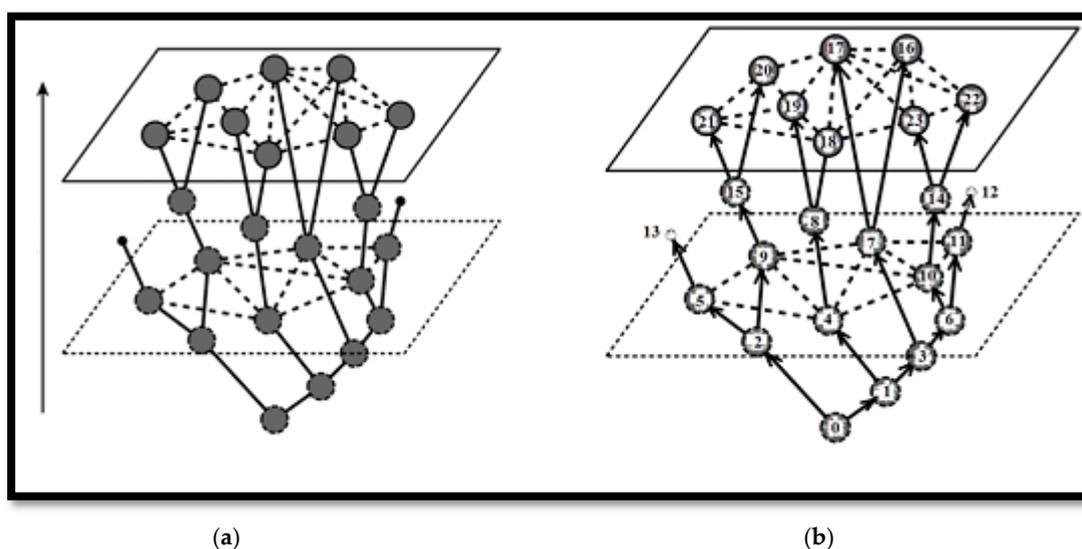
In microbiology in particular, the development model can characterize two branches of interaction (“archaea” and “viruses” in  $g[1]$ ) with a formation of a single “viruses’ life tree” (in  $g[4]$ ) with possible transformation stages in the genome space.

Evolution within the genome space is studied separately in reference [17].

The calculation process of the evolution within BSG convergent model is registered in BSG-7 table (Table 10). Figure 9b represents a reverse divergent process of the evolutionary development by time axis (Figure 9a). Each of the few highlighted columns in the multiplying table characterizes a separate “branch” of the process. The direction in each group is “interpreted” consequentially “from bottom-up”.

**Table 10.** Transformation group BSG-7 multiplying table (Figure 9b).

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23);$
$g[1] = (0\ 0\ 0\ 1\ 1\ 2\ 3\ 3\ 4\ 2\ 6\ 6\ 11\ 5\ 10\ 9\ 7\ 7\ 8\ 8\ 15\ 15\ 14\ 14);$
$g[2] = (0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 0\ 3\ 3\ 6\ 2\ 6\ 2\ 3\ 3\ 4\ 4\ 9\ 9\ 10\ 10);$
$g[3] = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 1\ 3\ 0\ 3\ 0\ 11\ 1\ 1\ 2\ 2\ 6\ 6);$
$g[4] = (0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 3\ 3);$
$g[5] = (0\ 1\ 1);$
$g[6] = (0\ 0);$

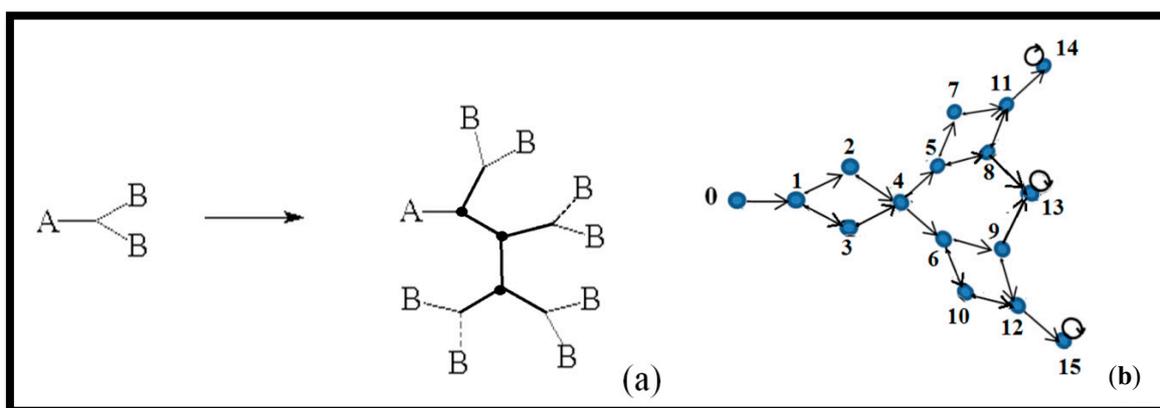


**Figure 9.** The process of prokaryotes’ “life tree” formation within the genome space (a) and a digital model of the process (b) based on BSG.

The presented example scientifically and objectively confirms the validity of the studied methods of broken symmetry visualization in biological systems

Example 3. Currently, a new field of supramolecular bonds chemistry is being developed which relates to the synthesis of three-dimensional branched polymers and oligomers called dendrimers (1. Hoffman Allan S. The origins and evolution of “controlled” drug delivery systems // J. Contr. Release. 2008. V. 132. pp. 153–163. 2. Nanoparticulate Drug Delivery Systems/Ed. by D. Thassu;

M. Deleers; Y. Pathak.—Informa Healthcare, 2007, p. 352). This type of bond is of particular interest since with each elementary growth event of a dendrimer the amount of branching in a simple case increases exponentially. With the increase of molecular mass of such bonds the shape and density of the molecules also changes and generally it occurs along with the modifications of dendrimers' physicochemical properties such as viscosity, solubility, density etc. Dendrimers can create complexes with other molecules, moreover the stability of such complexes is controlled by the external environmental state. This opens a potential for dendrimer use in medicine as a vehicle for a directed delivery of genes or pharmaceutical substances (vectors). The initial stage of this process is presented in Figure 10a. The formation of "branches" of dendrimers gives a task its mathematical description with the consideration of the directions of the process, which is, from a mathematical point of view, a directed graph; it is sort of a "labyrinth" (Figure 10b) or even a net if bonds between the branches form.



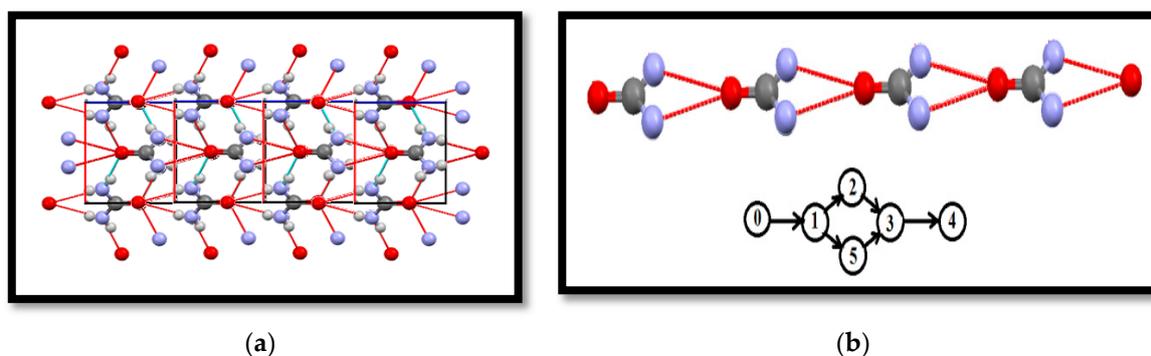
**Figure 10.** The initial stage of dendrimers synthesis (a) and a "labyrinth" with bonds (b).

Hypothetically, in a liquid crystal state, carbamide molecule chains which diverge from the "center" could have created a dendrimer.

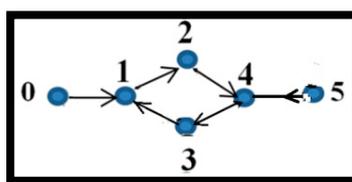
A simple fragment of such a chain, highlighted in Figure 3b, is structurally like such an element of the labyrinth structure (Figure 10b), if an end atom (marked as dot 5) will not interact with the external cycle, therefore the bond direction has changed.

For the highlighted element we will find a BSG with an initial (non-identical) transformation  $g[1]$ .

Transformation visualization is presented in Figures 11 and 12 and corresponds with Table 11 group fragment data.



**Figure 11.** Tetragonal carbamide structure (a) and carbamide molecules "chain" (b).



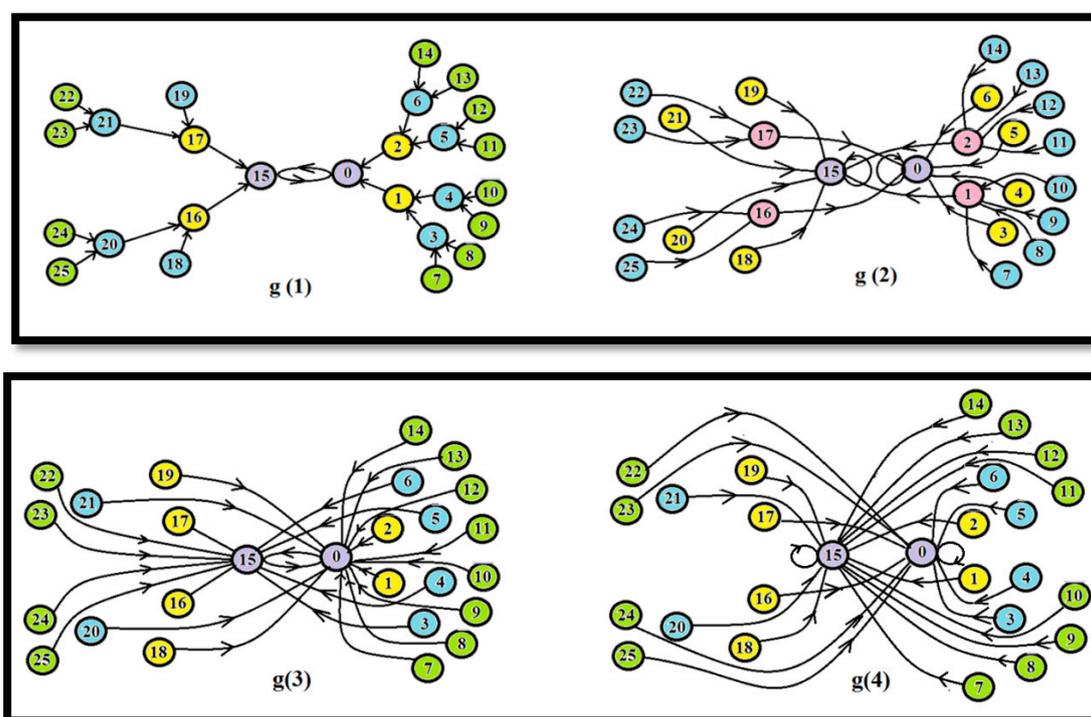
**Figure 12.** An element of the structure with a cycle (by Figure 10b).

**Table 11.** BSG transformations within the 5 dots structure 5.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5);$	$g[0]\ g[1]\ g[2]\ g[3]\ g[4]$
$g[1] = (1\ 2\ 4\ 1\ 3\ 4);$	$g[1]\ g[2]\ g[3]\ g[4]\ g[1]$
$g[2] = (2\ 4\ 3\ 2\ 1\ 3);$	$g[2]\ g[3]\ g[4]\ g[1]\ g[2]$
$g[3] = (4\ 3\ 1\ 4\ 2\ 1);$	$g[3]\ g[4]\ g[1]\ g[2]\ g[3]$
$g[4] = (3\ 1\ 2\ 3\ 4\ 2);$	$g[4]\ g[1]\ g[2]\ g[3]\ g[4]$

**Example 4.** We shall investigate the case of a more complicated structure of two dendrimers with 11 and 15 branching dots, which at the initial stage have a bond only between the directed graph tree “roots”.

As the result of the interaction, a phased rearrangement of the bonds occurs (Figure 13) and this visual data fully matches the BSG structure presented in the table of the general group of 26 elements-dots (Table 12).



**Figure 13.** Visualization of the process stages (by the first scenario, example 2) in a BSG (26 dots).

Broken symmetry research becomes relevant not only for structural chemistry and modern physics of elementary particles, which appear to be a quantum theory of nonabelian gauge fields with spontaneously broken symmetry, but also for other real micro- and macro systems, including biological as well as socioeconomical. Each of them has its own symmetry infractor “defect”, which causes the creation of new properties, along with evolution process occurrence. Therefore, further scientific confirmation is required.

**Table 12.** BSG table (26 dots, 4th order) with the local symmetry center.

$g[0] = (0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 17\ 18\ 19\ 20\ 21\ 22\ 23\ 24\ 25);$	$g[0]\ g[1]\ g[2]\ g[3]\ g[4];$
$g[1] = (15\ 0\ 0\ 1\ 1\ 2\ 2\ 3\ 3\ 4\ 4\ 5\ 5\ 6\ 6\ 0\ 15\ 15\ 16\ 17\ 16\ 17\ 21\ 21\ 20\ 20);$	$g[1]\ g[2]\ g[3]\ g[4]\ g[3];$
$g[2] = (0\ 15\ 15\ 0\ 0\ 0\ 0\ 1\ 1\ 1\ 1\ 2\ 2\ 2\ 2\ 15\ 0\ 0\ 15\ 15\ 15\ 15\ 17\ 17\ 16\ 16);$	$g[2]\ g[3]\ g[4]\ g[3]\ g[4];$
$g[3] = (15\ 0\ 0\ 15\ 15\ 15\ 15\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 15\ 15\ 0\ 0\ 0\ 15\ 15\ 15\ 15);$	$g[3]\ g[4]\ g[3]\ g[4]\ g[3];$
$g[4] = (0\ 15\ 15\ 0\ 0\ 0\ 0\ 15\ 15\ 15\ 15\ 15\ 15\ 15\ 15\ 15\ 0\ 0\ 15\ 15\ 15\ 15\ 0\ 0\ 0);$	$g[4]\ g[3]\ g[4]\ g[3]\ g[4].$

#### 4. Conclusions

A computer experiment with tables of binary transformation sets with a “defect” discovered new transformation sets with zero, with unity, without the reverse elements, with convergent and with divergent properties of the structure orgraph. They were called BSG. A possibility of a transition from the structure group with convergent orgraph properties to a group with divergent properties. A developed approach clearly demonstrates a creation of evolutionary trees and growth spirals of the orgraph structure; therefore, it emphasizes a general aspect of scientific studies.

The researched method of visualization allows easy presentation of the points and transitions of broken symmetry in designated transformations.

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