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# Finite noncrystallographic groups, 11-vertex equi-edged triangulated clusters and polymorphic transformations in metals

**Alexander Talis[a] and Valentin Kraposhin[b]***

[a]A. N. Nesmeyanov Institute of Organoelement Compounds of the Russian Academy of Sciences, Vavilova Street 28, Moscow, 119991, Russian Federation, and [b]Bauman Moscow State Technical University, 2nd Baumanskaya Street 5, Moscow, 105005, Russian Federation. Correspondence e-mail: kraposhin@gmail.com

The one-to-one correspondence has been revealed between a set of cosets of the Mathieu group $M_{11}$, a set of blocks of the Steiner system $S(4, 5, 11)$ and 11-vertex equi-edged triangulated clusters. The revealed correspondence provides the structure interpretation of the $S(4, 5, 11)$ system: mapping of the biplane 2-(11, 5, 2) onto the Steiner system $S(4, 5, 11)$ determines uniquely the 11-vertex tetrahedral cluster, and the automorphisms of the $S(4, 5, 11)$ system determine uniquely transformations of the said 11-vertex tetrahedral cluster. The said transformations correspond to local reconstructions during polymorphic transformations in metals. The proposed symmetry description of polymorphic transformation in metals is consistent with experimental data.



## 1. Introduction

Classic crystallography cannot describe polymorphic transformations since the space group is the closed set of defined rigid motions (conserving distances between points). Different structures as interpretations of different tilings of the three-dimensional Euclidean space $E^3$ can belong to the same space group (Delgado Friedrichs *et al.*, 1999). On the other hand, widespread metal structures with the face-centred cubic (f.c.c.) and body-centred cubic (b.c.c.) lattices are representations of topologically equivalent tilings onto tetrahedra and octahedra but with different space groups and, specifically, these groups are not capable of mapping a breakdown of the edge-equality condition while passing from the f.c.c. to b.c.c. lattice. Generalized crystallography [the term was introduced by Mackay (2002)] overcomes the limitations of classic crystallography by means of an extension of its symmetry basis. The symmetry basis of generalized crystallography includes structural application of several theories: $n$-dimensional lattices, finite geometries, algebraic groups, combinatorial analysis and also closely related sections of mathematics. Base mathematic constructions are contained in fundamental monographs (Conway & Sloane, 1999; Coxeter, 1973; Dubrovin *et al.*, 1990). For example, it was suggested that one should use a polytope approach to describe structures of condensed phases (not only crystalline ones); in particular, such an approach allows one to generate structures by straightening into the $E^3$ three-dimensional fragments of four-dimensional polytopes (Kléman & Sadoc, 1979; Sadoc & Mosseri, 1993; Sadoc & Charvolin, 1992).

In the framework of the polytope approach there were also attempts to describe the polymorphic transformations between f.c.c., b.c.c. and h.c.p. (hexagonal close-packed) structures of metals. An action of the $2\pi$-disclination on the 'rhombus' formed by two adjacent triangular faces of a coordination polyhedron has been considered as an elementary act of any polymorphic transformation (Kraposhin *et al.*, 2002, 2003, 2006). The $2\pi$-disclination corresponds to the element $-1$ of the subgroup $G'$ of polytope symmetry group, where $G'$ is the lift of the point group $G$ into group SU(2) (Nelson, 1983). The result of that action is reduced to the substitution of the short rhombus diagonal (corresponding to a chemical bond in a structure) by the long diagonal, *i.e.* to change the number of edges meeting at a given vertex (Fig. 1). In this case numbers of vertices, edges and faces of the polyhedron are unchanged. Models by Kraposhin *et al.* (2002, 2003, 2006) predict as the natural consequence both rigid orientation relationships between transformation participants, and also a singular set of the symmetry-possible habit planes of the martensite in steels. It is remarkable that this set of habit planes contains all martensite habit planes experimentally observed in steels, including the {225} habit plane which cannot be explained by any of the other existing martensite theories (Kraposhin *et al.*, 2002, 2003). The agreement of these predictions with experiments is evidence of the adequacy of polytope models.

Such a description is in complete coincidence with the model by Lipscomb (1966) for the transition between two space isomers of the icosahedral $C_2B_{10}H_{12}$ molecule: this transition is considered as a cyclic sequence of transformations of the rhombus consisting of two triangular faces of an icosahedron into the square face of a cuboctahedron and *vice versa*.

There are some peculiarities of polymorphic transformations which cannot be rationalized in the framework of the polytope approach. In accordance with the model of the b.c.c.–h.c.p. transition (Kraposhin *et al.*, 2006) the transfer from the 14-vertex rhombic dodecahedron of the b.c.c. structure to the 12-vertex cuboctahedron of the h.c.p. is effected successively through two intermediate 11-vertex joins of polyhedra (clusters): three distorted octahedra sharing a common edge (Fig. 2*a*) and eight regular tetrahedra sharing common faces (Fig. 2*b*). In this paper we name as a cluster the join of equi-edged triangulated polyhedra. Both intermediate clusters possess the threefold rotation axis and the mirror plane orthogonal to this axis. Although the number of vertices is 'noncrystallographic', both 11-vertex clusters are very abundant in experimentally observed crystal structures. The octahedral 11-vertex variant is the structural fragment of the hexagonal high-pressure phase of Ti and Zr metals and can be preserved at atmospheric pressure by alloying (the so-called $\omega$-phase). The octahedral 11-vertex cluster is also a fragment of the structure type $AlB_2$. The 11-vertex join of three octahedra forms a continuous network in the (0001) plane of the $\omega$-phase structure and $AlB_2$ structures as the common part of three adjacent hexagonal prisms. In the structure of the $CsMgD_3$ deuteride the octahedral 11-vertex polyhedron exists as an isolated cluster with deuterium-occupied vertices, while Mg atoms centre each octahedron (Renaudin *et al.*, 2003). The tetrahedral 11-vertex cluster is the common part of three intersecting icosahedra in the crystal structures of several intermetallic compounds such as $Al_5Co_2$, $Al_{10}Mn_3$, $\gamma$-brass, $Ti_2Ni$ and others (Schubert, 1964). The isolated tetrahedral 11-vertex cluster of In and Tl metals (Fig. 1*b*) exists in the structure of $K_8In_{11}$ and $K_8Tl_{11}$ compounds (Sevov & Corbett, 1991; Xu & van der Lugt, 1993), and neutron diffraction data evidence the preservation of the tetrahedral $Tl_{11}$ cluster in the liquid state (Xu *et al.*, 1993). A summary of the abundance of 11-vertex clusters is given in Table 1. This table does not claim to be exhaustive. One must note that both variants of the 11-vertex cluster are present as isolated clusters or as fragments of a continuous network.

Utilization of $2\pi$-disclinations in the framework of the polytope approach by Kraposhin *et al.* (2002, 2003, 2006) was limited intrinsically by clusters with symmetries determined by the subgroups of the polytope symmetry groups. In particular, in Kraposhin *et al.* (2002, 2006) an adequate description for certain types of cluster transformations was obtained by using the eight-dimensional $E_8$ lattice (Conway & Sloane, 1999) in which both four-dimensional polytopes and three-dimensional crystallographic lattices can be embedded. A tetrahedron is the simplex of the $E^3$ space; thus to map the symmetry of the specific tetrahedra face-to-face joins is a very urgent problem, especially for metallic structures. The face-to-face joins of tetrahedra are simplicial complexes, and one section of modern geometry is dedicated to mapping the symmetry of such joins (Dubrovin *et al.*, 1990). In particular, Babiker and Janeczko have fulfilled an examination of the algebraic structure of tetrahedral chains with face-to-face joining (Babiker & Janeczko, 2012).

The aim of this paper is to define a singular class of 11-vertex triangulated equi-edged clusters in the framework of generalized crystallography. We are presupposing a unique determination of polymorphic transformation in metals by the symmetry-possible transformations of clusters belonging to this class.

As will be shown, these transformations can be determined in the frameworks of generalized crystallography. We are starting from the assumption that this task can be solved by

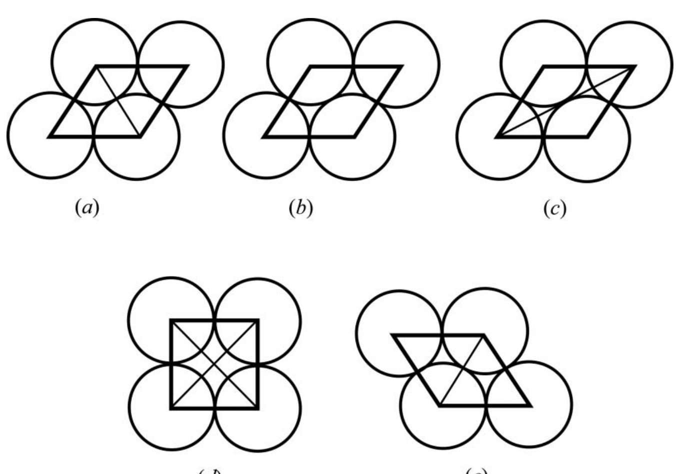


**Figure 1**
The elementary act of a polymorph transformation is developed through the sequence (*a*) to (*e*): a $2\pi$-disclination changes a short diagonal by the long one in the rhombus consisting of two equilateral triangles, thus changing the rhombus orientation in a plane. When two diagonals become equal the intermediate square configuration arises. The action of the $2\pi$-disclination on the dual of the shown structure coincides with the T1-process by Rivier (1999).

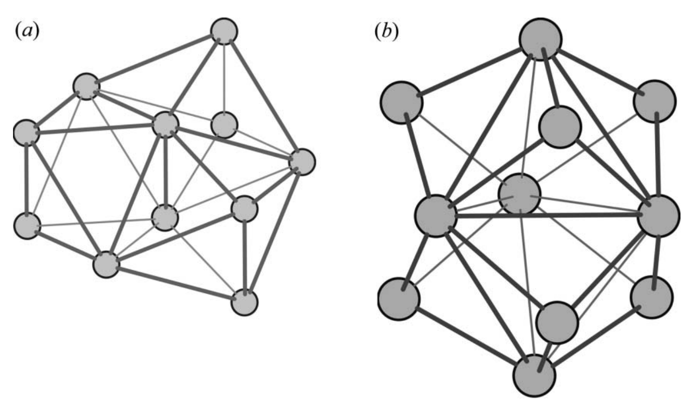


**Figure 2**
Two variants of the 11-vertex triangulated cluster. (*a*) The straightened fragment of the {3, 4, 3} polytope: three octahedra sharing a common edge (a polytope projection starting from an edge). This variant coincides with crystalline structure fragments of the high-pressure phase of Ti and Zr metals ($\omega$-phase), and compounds $AlB_2$, $Ni_2In$, $CsMgD_3$. (*b*) The straightened fragment of the {3, 3, 5} polytope: eight regular tetrahedra joined in the face-to-face mode (a polytope projection starting from a face). It is in coincidence with crystalline structure fragments of compounds $K_8In_{11}$, $K_8Tl_{11}$, $Al_5Co_2$, $Al_{10}Mn_3$ *etc.*

**Table 1**
Presence of 11-vertex cluster in different structures.

| Tetrahedral variant (Fig. 2*b*) | | Octahedral variant (Fig. 2*a*) | |
|---|---|---|---|
| Phase (structure type) | Mode of presence in crystalline structure | Phase | Mode of presence in crystalline structure |
| $K_8In_{11}$, $K_8Tl_{11}$ (present in liquid state also) | Isolated 11-vertex cluster | $CsMgD_3$ | Isolated 11-vertex cluster |
| $Al_{10}Mn_3$, $Al_5Co_2$ ($D8_{11}$), $Al_{24}V_3$, and many isomorphic compounds | Continuous network of 11-vertex tetrahedral clusters as intersection of three icosahedra | $\omega$-Ti, $\omega$-Zr (high-pressure modifications), $\omega$-phase ('monatomic' C32) is an intermediate product of martensitic transformation in the multitude of commercial Ti- and Zr-based alloys | Continuous network of 11-vertex octahedral clusters in tiling of hexagonal prisms |
| $\gamma$-brass $Cu_5Zn_8$ ($D8_2$), $Ti_2Ni$, $Al_{13}Cr_4Si_4$ $(Fe,W)_6C$ ($E9_3$), $Th_6Mn_{23}$ ($D8_a$) and many isomorphic compounds, $CsBi_2F_7$ | Continuous network of 11-vertex clusters as intersection of four icosahedra | $AlB_2$ (C32) $Ni_2In$ ($B8_2$) and many isomorphic compounds | Continuous network of 11-vertex octahedral clusters in tiling of hexagonal prisms |

the use of a specific projective linear $PSL_2(11)$ group of the 11 × 60 = 660 order which is defined over the Galois field of order 11. The Galois field of the $p$ order GF($p$) is the set of all residues 0, 1, ..., $p - 1$ after division of positive integers by prime number $p$, and the laws of addition and multiplication by $p$ modulus are introduced in this set. That assumption permits us to seek the symmetric solution of the polymorphic transformation problem in the framework of the $t$-($v$, $k$, $\lambda$) design formalism; here the $t$-($v$, $k$, $\lambda$) design is the set of $v$ elements subdivided into $k$ element subsets (blocks) such that every $t$ element is contained in exactly $\lambda$ blocks (Conway & Sloane, 1999). This paper will show the existence of a specific $t$-($v$, $k$, 1) design whose symmetries can adequately map polymorphic transformations.

## 2. Origin of the 11-vertex cluster

Amongst the $t$-($v$, $k$, $\lambda$) design it is possible to distinguish the $t$-($v$, $k$, 1) design, or the so-called Steiner systems S($t$, $k$, $v$). The automorphism groups of $S(4, 5, 11)$, $S(5, 6, 12)$, $S(4, 7, 23)$ and $S(5, 8, 24)$ are known as the Mathieu groups $M_{11}$, $M_{12}$, $M_{23}$ and $M_{24}$, respectively (Brown, 2004, p. 98).

The $M_{11}$ group is the supergroup to the $PSL_2(11)$ group, which is the automorphism group for one $t$-($v$, $k$, $\lambda$) design, namely for the so-called biplane 2-(11, 5, 2).

The motivation for a transfer to the structure symmetry description in terms of the groups $PSL_2(p)$, $p = 7, 11$ has been clearly formulated by Konstant (1995) in relation to the problem of representing adequately the symmetry of the $C_{60}$ molecule. There are several sphere tilings (an icosahedron, dodecahedron, truncated icosahedron *etc.*) belonging to the same point group $Y_h$ of the icosahedron. This situation is identical to ordinary crystals where different crystalline structures belong to the same space group (see above and Delgado Friedrichs *et al.*, 1999). The problem of the structure description for $C_{60}$ and three-dimensional carbon networks has been solved (Konstant, 1995; Lijnen *et al.*, 2007) by utilization of the $PSL_2(p)$, $p = 7, 11$ groups; here the rotation group of the icosahedron $Y$ is the subgroup of the $PSL_2(11)$ group. Konstant (1995) notes: 'The 60-element set $PSL_2(11)/Z_{11}$ has a natural structure of the graph of the truncated icosahedron', *i.e.* $C_{60}$ molecule (here $Z_{11}$ is the cyclic group of order 11, 660:11 = 60). Also, Konstant (1995) has defined the 11-element set $PSL_2(11)/A_5$ determining a biplane geometry ($A_5$ is isomorphic to $Y$ with the order of 60). However, the structural interpretation of this 11-element set has not been considered. Our paper is devoted to looking for structural realizations determined by the given 11-element set. One of the authors has carried out a similar search in connection with biopolymers: as it happens, the structures of quite different objects such as $C_{60}$ and an $\alpha$-helix are determined by the same symmetries originating from the $PSL_2(11)$ group (Samoylovich & Talis, 2014). In particular, it was shown in the paper cited that the substructure of a biplane may be identified with a flat development of an identity period for the cylindrical approximation of an $\alpha$-helix, and this identification is in good accordance with the experimental data.

To solve the problem considered in this paper we are using both the $PSL_2(11)$ group and its supergroups, *i.e.* Mathieu groups $M_{11}$ and $M_{12}$.

The 2-(11, 5, 2) biplane used in Konstant (1995) and Lijnen *et al.* (2007) is the constituent part of the Steiner system $S(4, 5, 11)$. The Steiner system $S(4, 5, 11)$ is defined as a subdivision of a collection of 11 positive integers (1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 0) onto 66 five-element blocks (Brown, 2004) and can be constructed from Galois field $p = 11$ as follows. Nonzero squares of GF(11) are numbers 1, 3, 4, 5, 9: $1^2 = 1$, $2^2 = 4$, $3^2 = 9$, $4^2 = 16 - 11 = 5$, $5^2 = 25 - 11 \cdot 2 = 3$, $6^2 = 36 - 11 \cdot 3 = 3$, $7^2 = 49 - 11 \cdot 4 = 5$, $8^2 = 64 - 11 \cdot 5 = 9$, $9^2 = 81 - 11 \cdot 7 = 4$, $10^2 = 100 - 11 \cdot 9 = 1$. These numbers 1, 3, 4, 5 and 9 form an initial block $B_1 = (13459)$ of the biplane 2-(11, 5, 2).

With the definition of the biplane as the 2-(11, 5, 2) design, each element of it belongs to five blocks, and each pair of elements belongs to two blocks. In accordance with Brown (2004), the 4-(11, 5, 1) design, *i.e.* the Steiner system $S(4, 5, 11)$, can be generated by the initial block $B_1 = 13459$:

**Table 2**
The Steiner system $S(4, 5, 11)$.

| | | | | | |
|---|---|---|---|---|---|
| **13459** | 07293 | 03618 | 0412X | 06X59 | 05784 |
| **2456X** | 183X4 | 14729 | 15230 | 1706X | 16895 |
| **35670** | 29405 | 2583X | 26341 | 28170 | 279X6 |
| **46781** | 3X516 | 36940 | 37452 | 39281 | 38X07 |
| **57892** | 40627 | 47X51 | 48563 | 4X392 | 49018 |
| **689X3** | 51738 | 58062 | 59674 | 504X3 | 5X129 |
| **79X04** | 62849 | 69173 | 6X785 | 61504 | 6023X |
| **8X015** | 7395X | 7X284 | 70896 | 72615 | 71340 |
| **90126** | 84X60 | 80395 | 819X7 | 83726 | 82451 |
| **X1237** | 95071 | 914X6 | 92X08 | 94837 | 93562 |
| **02348** | X6182 | X2507 | X3019 | X5948 | X4673 |

$$S(4,5,11) = \{B_1 + k | k \in [0, 1, \ldots X]\} \cup \{\sigma(B_1 - n) + k | n \in B_1, k \in [0, 1, \ldots X]\}. \quad (1)$$

Here all blocks of the biplane state are in the first pair of braces, the second pair of braces corresponds to the rest of the Steiner system $S(4, 5, 11)$, $\sigma$ is the permutation (1X)(25)(37)(48)(69)(0).

The formula (1) shows the generation of biplane blocks by a shift of the starting block $B_1$ by $k$, with $k$ belonging to the interval between 1 and 10. For example, by adding numbers from 0 to 10 to each element of $B_1$ we obtain all 11 biplane blocks: $B_1$ = 13459; $B_2$ = 2456X; $B_3$ = 35670; $B_4$ = 46781; $B_5$ = 57892; $B_6$ = 689X3; $B_7$ = 79X04; $B_8$ = 8X015; $B_9$ = 90126; $B_X$ = X1237; $B_0$ = 02348. The rest of the blocks of the Steiner system $S(4, 5, 11)$ are defined by the second pair of braces, so by subtracting a unit from each element of block $B_1$ we obtain five integers 02348; these five integers are transferred into 05784 under the action of the $\sigma$ permutation. After adding $k$ = 2 to each member of 05784 we obtain block 279X6 of the Steiner system $S(4, 5, 11)$ shown in Table 2. The calculated set 279X6 is placed in the third line of the sixth column of Table 2, so it can be labelled as block $B_{36}$. To generate the whole $S(4, 5, 11)$ system this operation is repeated for the rest of the elements of the initial block of the biplane, *i.e.* for 3, 4, 5, 9.

The left column (with bold figures) represents the biplane 2-(11, 5, 2), and biplane blocks $B_{ij}$ now also obtain two subscripts. One must note some properties of the Steiner system $S(4, 5, 11)$ which will be used later on. A triple of integers belongs to four blocks only, while a quadruple of integers belongs to a single block only. These exclusions are determined by the symmetry of the $S(4, 5, 11)$ system.

The $PSL_2(11)$ group consists of permutations of block elements of the biplane, for example permutation $\alpha$ = (1)(3)(459)(27X)(068), $\alpha^3 = 1$, generates the cyclic group of the third order $C_3 = \{\alpha, \alpha^2, 1\}$. Second-order permutations $\delta$ = (13)(42)(57)(9X)(0)(68), $\eta$ = (13)(40)(56)(98)(7)(2X), $\mu$ = (13)(20)(76)(X8)(5)(49) in combination with $C_3$ make up the $D_3$ group. The $PSL_2(11)$ group is the product of the cyclic group $C_{11}$ and rotation group $Y$ of an icosahedron [not a direct product of groups, in accordance with Konstant (1995, p. 965)]; this means that every element $g$ can be uniquely written as $g = cy$ where $c \in C_{11}$ and $y \in Y$.

**Table 3**
The subset of 3 × 3 = 9 blocks of the biplane 2-(11, 5, 2).

| | | |
|---|---|---|
| $B_{91}$ = 16902 | $B_{41}$ = 18467 | $B_{81}$ = 1058X |
| $B_{01}$ = 30482 | $B_{31}$ = 36507 | $B_{61}$ = 3896X |
| $B_{51}$ = 57982 | $b_{71}$ = 9X407 | $B_{21}$ = 4256X |

The set of 11 blocks of the biplane is isomorphic to the coset of 11 classes in the right coset decomposition of $PSL_2(11)$ by the subgroup $Y$:

$$PSL_2(11) = C_{11} \cdot Y = \bigcup_{i=1}^{11} g_i Y, g_1 = 1, \quad g_i \notin Y \supset C_3 = \{\alpha, \alpha^2, 1\}. \quad (2)$$

In decomposing $PSL_2(11)$ onto double cosets, 11 coset classes (2) are divided into five subsets which are $C_3$-invariant:

$$PSL_2(11) = C_{11} \cdot Y = \bigcup_{k=1}^{5} C_3 g_k Y = D_1 \cdot Y \bigcup_{k=3}^{5} C_3 g_k Y = Y \cup \delta Y \bigcup_{k=3}^{5} C_3 g_k Y, \quad \delta C_3 = C_3 \delta, \quad (3)$$

where $\{1, \boldsymbol{\delta}\} = D_1 \not\subset Y$. It means the splitting of the 11-block set of the biplane onto subsets of 2 + 3 × 3 blocks by the action of the permutation $\alpha$. Here two blocks correspond to cosets $Y$ and $\delta$, and 3 × 3 labels three triplets of blocks corresponding to 3 × 3 = 9 cosets $C_3g_3Y$, $C_3g_4Y$, $C_3g_5Y$. The permutation $\delta$ maps the initial $B_{11}$ block into the $B_{X1}$ block. This permutation corresponds to the twofold axis orthogonal to the threefold axis, and the twofold axis transfers the triple 459 into 27X. The permutation $\delta$ belongs to the $D_3$ supergroup of the $C_3$ group; therefore these two blocks $B_{11}$ = 13459 and $B_{X1}$ = 1327X = $\delta B_{11}$ are unchanged under the action of $\alpha$ (the enumeration of blocks is determined by their position in Table 2). The remaining nine blocks decompose into three triples (each triple is positioned in the same line of Table 3), and blocks in each triple are mapped into each other under the action of the permutation $\alpha$.

There are two non-conjugate subgroups $Y$ and $Y'$ in the $PSL_2(11)$ group (Konstant, 1995; Lijnen *et al.*, 2007). The automorphisms group of the Steiner system $S(4, 5, 11)$ is the Mathieu group $M_{11} = \cup_i^{66} m_i C_2 Y$, which contains the automorphisms group $PSL_2(11)$ of the biplane and the $PSL'_2(11)$ group non-conjugate to it, $C_2$ is the cyclic group of order 2. These two subgroups of the $M_{11}$ group (with index 12) have the common subgroup $C_3 = \{\alpha, \alpha^2, 1\}$. By Conway & Sloane (1999, ch. 10, section 1.5) the $2M_{12}2$ group possesses the automorphisms $\theta$, $\theta^2 = 1$, $\theta\, C_3\, \theta^{-1} = C_3$, so, also by Conway & Sloane (1999, ch. 10, section 1.5), the relationships (3) allow us to define

$$PSL'_2(11) = \bigcup_{k=1}^{5} \theta C_3 g_k Y = Y \cup \eta Y \bigcup_{k=3}^{5} C_3 \theta g_k Y, g_1 = 1, \quad C_3 = \{\alpha, \alpha^2, 1\}, \quad (4)$$

**Table 4**
Mapping of nine blocks of the 2-(11, 5, 2) biplane into nine blocks of the Steiner system $S(4, 5, 11)$.

| The initial block of the biplane from the first column of the $S(4, 5, 11)$ | The result of the transformation $\theta$ over the first four elements of the initial block | The block of the $S(4, 5, 11)$, mapped by $\theta$ from the initial block of the biplane |
|---|---|---|
| $B_{91}$ = 16902 | 1694 | $B_{X3}$ = 1694$\underline{\text{X}}$ |
| $B_{41}$ = 18467 | 1845 | $B_{96}$ = 1845$\underline{2}$ |
| $B_{81}$ = 1058X | 1059 | $B_{X2}$ = 1059$\underline{7}$ |
| $B_{01}$ = **30482** | **3045** | $B_{65}$ = **3045$\underline{\text{X}}$** |
| $B_{31}$ = **36507** | **3659** | $B_{X6}$ = **3659$\underline{2}$** |
| $B_{61}$ = **3896X** | **3894** | $B_{X5}$ = **3894$\underline{7}$** |
| $B_{51}$ = *58972* | *5894* | $B_{05}$ = *5894$\underline{X}$* |
| $B_{71}$ = *904X7* | *9045* | $B_{32}$ = *9045$\underline{2}$* |
| $B_{21}$ = *4652X* | *4659* | $B_{64}$ = *4659$\underline{7}$* |

where $\theta\, g_k = m_k$ is the element of the $M_{11}$ group not belonging to the $PSL_2(11)$ group, $\theta\delta = \eta$.

Relationships (3) and (4) define an existence of two 11-block subsets of the $S(4, 5, 11)$ system; these subsets are $C_3$-invariant and can be mapped into each other by the transformation $\theta$. The entity of the $\theta$ transformation is explained below.

The initial block $B_{11}$ intersects with the biplane blocks $B_{n1}$ from Table 2 by two integers, with at least one integer belonging to the subset $A = \{4, 5, 9\}$. At least one integer in each $B_{n1}$ block belongs to the subset $C = \{0, 6, 8\}$, since the $B_{n1}$ block can be represented in the form of $bcaxy$, where $b, c, a$ are integers from $B_{11}$, $C$, $A$; integers $x, y$ belong to $\mathcal{K}$ = [0, ... X], but do not coincide with $b, c, a$. We can show the existence of the $b_1c_1a_1a_2y$ block with $b_1 \in B_{11}, c_1 \in C, a_1, a_2 \in A$ among four $b_1c_1a_1xy$ blocks of the $S(4, 5, 11)$. By definition $a_2 = \alpha(a_1)$, so there exists the transformation $\theta$ mapping the $bca_1xy$ biplane blocks into the $bca_1\alpha(a_1)y$ blocks of the Steiner system $S(4, 5, 11)$. In other words, the transformation $\theta$ complying with relationship (4) leaves invariant the first three columns in nine blocks of the biplane, and allows us to obtain the fourth column from the third one by the permutation (594). The results of that operation are shown in the middle column in Table 4. The left column repeats three triples of blocks from Table 3; here blocks belonging to the same triple are marked by the same type (roman, bold, italic). Since each quadruple is contained only in the single block of the $S(4, 5, 11)$, each quadruple obtained by the transformation $\theta$ is supplemented uniquely by the fifth element, thus forming one of the $S(4, 5, 11)$ blocks. Nine blocks of the $S(4, 5, 11)$ mapped by nine blocks of the biplane are displayed in the right vertical column of Table 4, the supplementing fifth element marked by underlining.

Complying with (4), the block subset of the $S(4, 5, 11)$ system can be mapped into the other subset by the automorphism $\xi$; that other subset is also $C_3$-invariant, and uniquely corresponds to cosets of the $M_{11}$ group:

$$\xi_1 Y \cup \xi_2 \eta Y \bigcup_{k=3}^{5} C_3 \xi_k \alpha_i \theta g_k Y \subset \bigcup_{i}^{66} m_i C_2 Y = M_{11}. \qquad (5)$$

Here $\xi_1$, $\xi_2\eta$ are elements of the $D_3$ group, $\alpha_i \in C_3 = \{\alpha, \alpha^2, 1\}$, $\xi_k\alpha_i\theta g_k = m_k$ are elements of the $M_{11}$ group. Here the considered transformations only change the number of edges meeting in a given vertex, so we will be limited by automorphisms $\xi$ which either preserve the whole block, or preserve three elements.

The permutation $\alpha$ = (1)(459)(3) determines the possibility to regard the $B_{11}$ = 13459 block as two regular tetrahedra with vertices labelled as 1, 4, 5, 9 and 3, 4, 5, 9 and sharing the common face 459; opposite vertices 1 and 3 are lying on the common threefold symmetry axis of the cluster in Fig. 2(*b*). In the presence of the threefold axis (the $C_3$ group) vertices 1 and 3 are unchanged by cyclic permutations 4→5, 5→9, 9→4 *etc.*

The generation (1) of the Steiner system $S(4, 5, 11)$ from the initial $B_{11}$ block (corresponding to the joining of two tetrahedra), and restrictions imposed on $\xi$, determine the possibility of a tetrahedral–triangular interpretation of block subsets of the $S(4, 5, 11)$ system, *i.e.* the interpretation as equi-edged joins of tetrahedra (triangles) sharing common faces (edges). For example, 15907, 1946X and 14582 blocks mapped from the biplane by the $\theta$ transformation define three tetrahedra attached to the 1459 tetrahedron by common faces ('top' tetrahedra), and blocks 35962, 39487 and 3450X define, respectively, three 'bottom' tetrahedra attached by common faces to the 3459 tetrahedron. All tetrahedra are regular, and all vertices of the cluster in Fig. 2(*b*) get the single-valued enumeration (see Fig. 3). As one can see, each block from the remaining triple particular blocks of the Steiner system ($B_{64}$ = $\underline{59}$476, $B_{32}$ = $\underline{45}$920, $B_{05}$ = 9$\underline{45}$X8, Table 4) defines the join of three regular triangles with the common ('equatorial') edge. Vertices of the equatorial edge are underlined.

Thus, ten cosets of the $M_{11}$ group given by the relationship (5) with the conditions $\xi_1 = \xi_2\eta = \xi_k = 1$, ($\xi_2 = \eta$, $\eta^2 = 1$) determine the initial block and nine blocks in Table 4 having one-to-one correspondence with the 11-vertex tetrahedral cluster in Fig. 3.

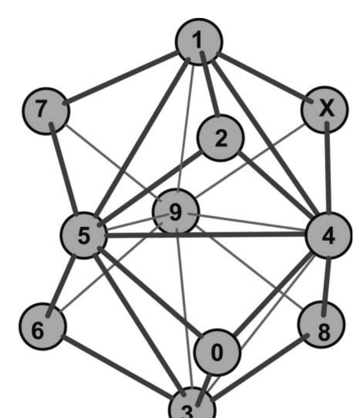


**Figure 3**
The tetrahedral interpretation of the biplane 2-(11, 5, 2) in the Steiner system $S(4, 5, 11)$ coincides with a tetrahedral variant of the 11-vertex cluster in Fig. 2(*b*) and defines uniquely the enumeration of cluster vertices. In accordance with the permutation $\alpha$ = (1)(3)(459)(27X)(068) vertices 1 and 3 are positioned on the threefold axis, while vertices in triplets (4, 5, 9), (2, 7, X) and (0, 6, 8) are connected by the threefold axis.

**Table 5**
Three block pairs in the $S(4, 5, 11)$ system corresponding to transformations of 'top' tetrahedra in Fig. 3.

| Automorphism of the $S(4, 5, 11)$ | Blocks corresponding to 'top' tetrahedra of cluster in Fig. 3 | | |
|---|---|---|---|
| No mapping | 19 570 | 14 9X6 | 15 428 |
| $\xi_3$ | 2X 570 | 72 9X6 | X7 428 |
| $\alpha\xi_3\alpha^{-1}$ | 72 9X6 | X7 428 | 2X 570 |
| $\alpha^2\xi_3\alpha^{-2}$ | X7 428 | 2X 570 | 72 9X6 |

**Table 6**
Three block pairs in the $S(4, 5, 11)$ system corresponding to transformations of 'bottom' tetrahedra in Fig. 3.

| Automorphism of the $S(4, 5, 11)$ | Blocks corresponding to 'bottom' tetrahedra of cluster in Fig. 3 | | |
|---|---|---|---|
| No mapping | 39 562 | 34 987 | 35 40X |
| $\xi_4$ | 08 562 | 60 987 | 86 40X |
| $\alpha\xi_4\alpha^{-1}$ | 60 987 | 86 40X | 08 562 |
| $\alpha^2\xi_4\alpha^{-2}$ | 86 40X | 08 562 | 60 987 |

In our approach physical objects (atomic clusters) are juxtaposed to the block subset of the Steiner system $S(4, 5, 11)$, which in its turn is juxtaposed to the cosets of the decomposition (5). The similar juxtaposition of the graph of the $C_{60}$ molecule to the factorization of the $PSL_2(11)$ group by $Z_{11}$ was fulfilled in the work by Konstant (1995) cited above. Thus, relationships (2)–(5) allow us to select the block subsets of the Steiner system having one-to-one correspondence with 11-vertex equi-edged triangulated clusters (*i.e.* face-to-face tetrahedra joining and/or edge-to-edge triangles joining).

## 3. Symmetry-possible transformations of the 11-vertex cluster

It was suggested that the polymorphic transformation in metals between f.c.c., b.c.c. and h.c.p. modifications should be considered as a transformation of coordination polyhedra by throwing over a minimal quantity of edges (a permutation between the long and short diagonals of a rhombus) (Kraposhin *et al.*, 2002, 2003, 2006). A juxtaposition of the block set of the Steiner system $S(4, 5, 11)$ and corresponding coset classes of the $M_{11}$ group to the 11-vertex cluster allows one to associate the said edge permutations (polymorphic transformations) with automorphisms $\xi_1$, $\xi_2\eta$ and $\alpha_i\xi_k(\alpha_i)^{-1}$, $\alpha_i \in C_3 = \{\alpha, \alpha^2, 1\}$ from relationship (5).

While block-to-block mapping, the automorphisms $\xi_k$, $3 \le k \le 5$ preserve not less than three elements. The choice of the retained three elements is determined by the requirement to compose it from elements representing triples entering into the permutation $\boldsymbol{\alpha}$. The choice of concrete $\xi_k$ (*i.e.* the choice of the element of the $M_{11}$ group) is defined by an affiliation of the retained triple elements only to three more blocks. For example, for three elements 570 of the block $B_{X2}$ = 15907 = 19570 [5 belongs to (459), 7 to (27X) and 0 to (068)] such blocks will be $B_{31}$ = 36570, $B_{16}$ = 84570 and $B_{03}$ = 2X570. Transformations of the initial cluster (Fig. 3) are hypothetically possible by the substitution of edge 19 by edges 36, 48 and 2X. Edges 36 and 48 exist already in the initial cluster; hence transfer from the initial 19570 block to 36570 and 48570 blocks corresponds simply to the removal of the 19 edge in the initial cluster. There is no 2X edge in the starting cluster, since the transfer from the 19570 to 2X570 block (determined by $\xi_3$) can define such a cluster transformation when its vertex, edge and face numbers are unchanged.

By using the permutations $\alpha$ and $\alpha^2$ to the initial $B_{X2}$ = 19570 and mapped block $B_{03}$ = 2X570 one can obtain two block subsets with three blocks in each subset (the first and second lines in Table 5), which are $C_3$-invariant and mapped into each other in one column (*i.e.* from one line to the other) by the $\xi_3$ automorphism. Blocks in the first line correspond to three 'top' tetrahedra of the 11-vertex cluster in Fig. 3 and should be mapped into the blocks of the second line; however by mapping blocks in one column, in the general case we cannot preserve a maximal quantity of edges. In fact, the $\xi_3$ mapping of the 19570 block transfers it into the 2X570 block and ensures the preservation of edges at three vertices 5, 7 and 0 while substituting the 19 edge by the 2X edge. While mapping the 19570 block into the 729X6 block the $\alpha\xi_3\alpha^{-1}$ automorphism ensures the preservation of edges at four vertices 5, 0, X and 6 by changing the 19 edge by the 72 edge. While mapping the 19570 block into the X7428 block the $\alpha^2\xi_3\alpha^{-2}$ automorphism ensures the preservation of edges at five vertices 5, 0, 4, 2 and 8 by changing the 19 edge by the X7 edge. The edges belonging to these five vertices are not edges of the 197X 'rhombus' (Fig. 3), so while mapping the 19570 block onto the X7428 block, the $\alpha^2\xi_3\alpha^{-2}$ automorphism will correspond to change the 19 rhombus diagonal by the 2X diagonal, *i.e.* a $2\pi$-disclination. By using three such $2\pi$-disclinations ($C_3$-invariant) one can map the first line in Table 5 into the fourth line of the same column; this mapping corresponds to the transformation of each tetrahedron belonging to the triple of 'top' tetrahedra in Fig. 3. In Tables 5–9 two integers corresponding to the flipped edge are distinguished in a block by spacing.

Similarly, for the three 'bottom' tetrahedra we obtain three other pairs of blocks (Table 6).

The transfer from the upper to the lower lines of blocks (Tables 5 and 6) is effected by the substitution of non-coincident elements; this substitution corresponds to skipping of the 19 edge and inserting the 2X edge, skipping the 14 edge and inserting the 72 edge, skipping the 15 edge and inserting the X7 edge and so ion. Fig. 4 shows this edge-skipping–inserting process as two snapshots of the ball-and-stick model. The skipped edges 19, 14 or 15 are designated by the black magnetic stick. One can easily see the transfer from three tetrahedra sharing the black common edge (Fig. 4*a*) into an octahedron (Fig. 4*b*).

The last three blocks corresponding to triples of triangles with a common edge are unchanged; the angle is only changed between triangle planes not coincident to the common 459 face.

The above-considered permutations of edges reconstruct the starting cluster. These permutations correspond to mapping of nine blocks in the relationship (5). Since the

**Table 7**
Block permutations in the Steiner system $S(4, 5, 11)$ transforming the tetrahedral cluster (Fig. 3) into two one-capped octahedra (Fig. 5).

| | |
|---|---|
| 13459 → | 1327X |
| 149X6 → | 2X570 |
| 15428 → | 729X6 |
| 19570 → | X7428 |
| 39562 → | 8640X |
| 34987 → | 08562 |
| 3540X → | 60987 |
| 13459 → | 13068 |
| 45920 → | 45920 |
| 59476 → | 59476 |
| 945X8 → | 945X8 |

**Table 8**
Block permutations in the Steiner system $S(4, 5, 11)$ for transforming the tetrahedral cluster (Fig. 3) into the 60°-rhombohedron with three additional caps (Fig. 6).

| | |
|---|---|
| 13459 → | 13459 |
| 19570 → | 19570 |
| 149X6 → | 149X6 |
| 15428 → | 15428 |
| 13459 → | 13068 |
| 39562 → | 8640X |
| 34987 → | 08562 |
| 3540X → | 60987 |
| 45920 → | 45920 |
| 59476 → | 59476 |
| 945X8 → | 945X8 |

mapped nine blocks from Table 4 intersect with the initial block, thus by (5) there must be mapping of the initial block into blocks of the $S(4, 5, 11)$ intersecting with the mapped blocks in Tables 5 and 6. At $\xi_1 = \delta$, $\xi_2 = 1$ one obtains mapping of the initial block 13459 onto the $C_3$-invariant 1327X and 13068 blocks which intersect with the blocks in the lower lines of Tables 5 and 6 by the triples 27X and 068. Thus, the above-considered edge permutation corresponds to mapping of 13459 onto 1327X and 13068, *i.e.* two tetrahedra 127X and 3068 arise as the tetrahedral caps for emerged octahedra. Then the permutation of blocks shown in Table 7 corresponds to the reconstruction of the 11-vertex tetrahedral cluster (Fig. 3) into two one-capped octahedra (Fig. 5).

In case the permutation is fulfilled only for three top tetrahedra or for three bottom tetrahedra (Table 8), the octahedron with two tetrahedral caps will be formed as shown in Fig. 6 (here there are three more tetrahedra attached to one cap). In the present case edges 19, 14 and 15 of the invariable blocks 19 570, 14 9X6 and 15 428 are parts of the 13459 block, and this block retains the upper inner tetrahedron 1459.

It is clear that the configuration of the cluster in Fig. 5 coincides with hexagonal close packing and/or with the stacking fault (twin) by the {111} plane of the face-centred cubic packing. Without three additional tetrahedra (vertices 2, 7, X) the configuration in Fig. 6 corresponds to the 60° rhombohedron for both close packings, *i.e.* to f.c.c. and h.c.p.

To obtain one more configuration – three-capped trigonal prism (a Bernal polyhedron with nine vertices, *Z*9) and two vertical tetrahedral caps – one must take the block set {1327X, 13068; 2X570, 729X6, X7428; 08562, 60987, 8640X; 45920, 59476, 945X8} as the initial blocks. That set defines the configuration of two one-capped octahedra (Fig. 5). The triple 420 is selected in the 45920 block which maps three regular triangles 459, 425 and 405 with the common edge 45. The triple 420 is also contained in the 38420, 76420 and 1X 420 blocks. Similarly to the derivation of the preceding configuration,

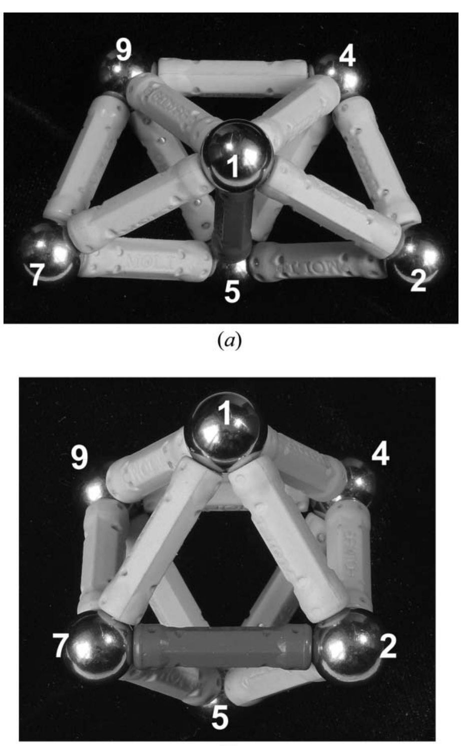


**Figure 4**
A ball-and-stick model illustrating the transfer from the face-to-face join of three tetrahedra (*a*) into an octahedron (*b*) by the diagonal flipping (see Fig. 1). The common edge of three tetrahedra (1–5) is shown in black. The numbering of vertices corresponds to Fig. 3.

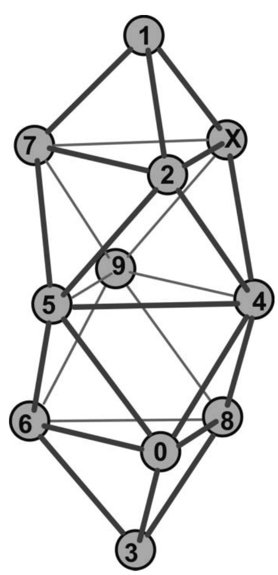


**Figure 5**
Two one-capped octahedra are the result of the transformation of the 11-vertex cluster in Fig. 2(*b*) by the substitution of blocks in the Steiner system $S(4, 5, 11)$ in accordance with Table 7.

**Table 9**
The transfer from the upper three blocks to lower triple generates a nine-vertex trigonal prism (Bernal polyhedron) with two tetrahedral vertical caps (Fig. 7).

| | | |
|---|---|---|
| 59 420 | 94 576 | 45 9X8 |
| 76 420 | X8 576 | 20 9X8 |

blocks 1X420 and 38420 must be deleted because edges 1X and 38 are present but not edge 76. By action of the permutation $\alpha$ one obtains two more pairs of blocks from the 45920 and 76420 pair (Table 9).

This set defines the substitution of edges 59, 49 and 45 by edges 76, X8, 20. The obtained set of blocks {1327X, 13068, 2X570, 729X6, X7428; 08562, 60987, 8640X; 76420, X8576, 209X8} defines the Bernal polyhedron *Z*9 of liquid metal with two vertical tetrahedra 1327X and 13068 (Fig. 7). The *Z*9-polyhedron is also a building unit for the crystal structure of many compounds: carbides, borides, silicides, phosphides of transition metals, for examples $Fe_3C$, $Cr_7C_3$, $Fe_3P$, $Pd_3Si$ (Schubert, 1964). It was shown by Hyde *et al.* (1979) that three-capped trigonal prism *Z*9 is also the structural unit of twin planes {112} for h.c.p. and {113} for f.c.c. packings. This relationship between twin and $Fe_3C$ carbide structures became a foundation for the model of eutectoid and martensitic transformations in steels by Kraposhin *et al.* (2013).

One needs to be convinced that the Steiner system also contains a transition between two 11-vertex configurations shown in Fig. 2, *i.e.* the transformation of eight regular tetrahedra into three octahedra sharing a common edge. One can

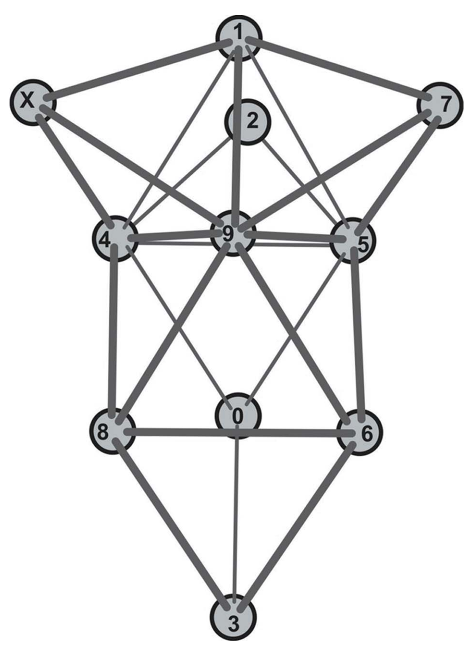


**Figure 6**
The octahedron with five tetrahedral caps (60°-rhombohedron in the closest crystalline packing with three additional tetrahedral caps) is the result of the transformation of the 11-vertex in Fig. 2(*b*) by the substitution of blocks in the Steiner system *S*(4, 5, 11) in accordance with Table 8.

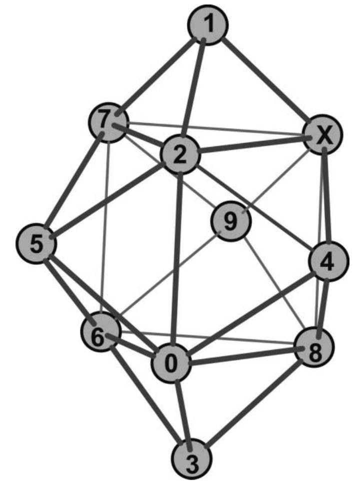


**Figure 7**
The five-capped trigonal prism is the result of the transformation of the 11-vertex in Fig. 2(*b*) by the substitution of blocks in the Steiner system *S*(4, 5, 11) in accordance with Table 9. Without vertices 1 and 3 it coincides with the nine-vertex Bernal polyhedron.

take blocks {13459, 19570, 149X6, 15428, 39562, 34987, 3540X, 45920, 59476 and 945X8} as an initial collection that is the cluster in Fig. 2. Similarly to the preceding derivation in the block 45920 (which maps three regular triangles 459, 425 and 405) the triple 420 is selected and so on. As a result one obtains the collection {13459, 19570, 149X6, 15428, 39562, 34987, 3540X, 76420, X8576 and 209X8}, but now we consider the block 13459 as a mapping of the join of three triangles 134, 135 and 139 sharing the common edge 13. In the outcome three octahedra sharing the common edge 13 are obtained (Fig. 8). The join of three regular octahedra about a common edge is possible only in the four-dimensional {3, 4, 3} polytope; hence three-dimensional projection in Figs. 2(*a*) and 8 inevitably has non-equal edges.

The summary of mutual mapping between blocks of the Steiner *S*(4, 5, 11) system corresponding to the above-considered reconstructions of the 11-vetex cluster is shown in Table 10.

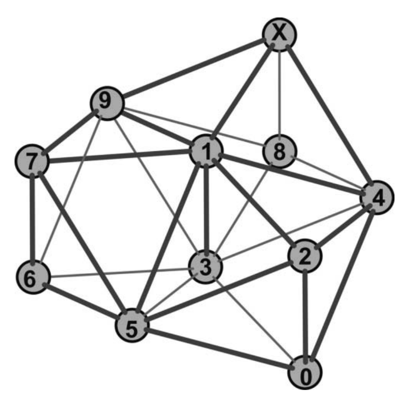


**Figure 8**
The substitution of blocks in the Steiner system *S*(4, 5, 11) in accordance with the ultimate left column in Table 10 ensures the transfer from the tetrahedral to octahedral interpretation of the Steiner system *S*(4, 5, 11).

**Table 10**
Summary of the mutual mapping between blocks of the $S(4, 5, 11)$ system giving receiving different crystalline structures in metals.

| Three octahedra with a common edge | Eight regular tetrahedra | Two seven-vertex clusters | Trigonal prism with five caps | 60°-rhombohedron with three caps |
|---|---|---|---|---|
| 13459 | ←**13459**→ | 1327X→ | 1327X→ | 13459 |
| 19570 | ←**19570**→ | X7428→ | X7428→ | 19570 |
| 149X6 | ←**149X6**→ | 2X570→ | 2X570→ | 149X6 |
| 15428 | ←**15428**→ | 729X6 → | 729X6→ | 15428 |
| 13459 | ←**13459**→ | 13068→ | 13068→ | 13068 |
| 39562 | ←**39562**→ | 8640X → | 8640X → | 8640X |
| 34987 | ←**34987**→ | 08562→ | 08562→ | 08562 |
| 3540X | ←**3540X**→ | 60987→ | 60987→ | 60987 |
| 76420 | ←**59420**→ | 59420→ | 76420→ | 59420 |
| X8576 | ←**94576**→ | 94576→ | X8576→ | 94576 |
| 209X8 | ←**459X8**→ | 459X8→ | 209X8→ | 459X8 |

## 4. Discussion

The abundance of 11-vertex clusters (both in tetrahedral and octahedral conformations) in the observed crystalline structures (see §1) can be considered as a physical realization of the abstract symmetry constructions analysed here. The basic symmetry construction used by us is the factorization of the $M_{11}$ group [supergroup of the $PSL_2(11)$ group] by the icosahedral subgroup $Y$. The results presented in the paper show the possibility of describing the physical phenomenon of polymorphic (martensitic) transformations by the symmetries determined by the $M_{11}$ group.

Without condition of equal edges in the starting 11-vertex cluster (Fig. 2*b*) one can draw all configurations shown in Figs. 3–8 without any edge permutations. By imposing the equal-edge condition onto initial and end configurations of the 11-vertex cluster, one can use the triangular–tetrahedral interpretation of the block subset of the Steiner $S(4, 5, 11)$ system to determine the symmetry-possible transformations of that cluster, and, therefore to determine trajectories of mutual reconstructions of metallic f.c.c., b.c.c. and h.c.p. structures. In the framework of the approach used here, the generating clusters for the structures of carbides (and borides, silicides, phosphides) formed by transition metals can be determined as well (the nine-vertex Bernal polyhedron). Also, it can be shown that by the same approach the other triangulated $N$-vertex equi-edged Bernal polyhedra $ZN$, $N$ = 8, 9 and 10 ($Z8$-trigondodecahedron, $Z10$ two-capped twisted cube), and 11-vertex fragment of the irrational Coxeter–Bordijk helix (Boerdijk, 1952; Coxeter, 1985) can be derived.

As a matter of fact, the tetrahedral variant of the 11-vertex cluster in Figs. 2 and 3 represents three seven-vertex fragments of the Coxeter–Bordijk tetrahedral helix with the length of four tetrahedra each and intersecting between each other by two tetrahedra: $11 = 3 \times 7 - 2 \times 5$. As can be shown, there is the automorphism $\xi$ complying with (5) and mapping blocks 68907, 45920 and 94X58 of the right column in Table 6 onto blocks 68951, 4598X and 94X70, and leaving blocks 1327X, 13068, X7428, 08562 and 59476 intact. The obtained eight-block set defines the face-to-face join of two such seven-vertex clusters from the tetrahedral helix: $11 = 2 \times 7 - 3$.

Both the 11-vertex tetrahedral cluster in Fig. 2(*b*) and the 11-vertex fragment of the Coxeter–Bordijk tetrahedral helix embed into the {3, 3, 5} polytope, which is a tiling of the three-dimensional sphere (determined in four-dimensional space) onto 600 regular tetrahedra (Coxeter, 1973). Symmetries of that tiling permit (Nelson, 1983) us to derive all known building units for metallic structures having $Z$ vertices: Bernal polyhedra ($Z8$, $Z9$, $Z10$), Frank–Kasper polyhedra ($Z14$, $Z15$, $Z16$) and two non-canonical polyhedra $Z11$ and $Z13$. In particular, the $Z11$ polyhedron has been derived by Nelson from the symmetries of the {3, 3, 5} polytope as the net result of a disclination action. In the framework of our approach $Z11$ can be derived from $Z9$ with two tetrahedral caps. One feature of the $Z11$ polyhedron is the presence of one sixfold vertex with two fourfold vertices. Undoubtedly, this $Z11$ and similar polyhedra are significant in the structure and structural transformation of metallic phases, but this topic is beyond the scope of our paper.

The case of the non-canonical $Z11$ polyhedron (an irregular 11-vertex triangulation of a sphere) illustrates one of our results: the one-to-one mapping of two certain blocks of the Steiner system $S(4, 5, 11)$ corresponds to the $2\pi$-disclination, fulfilling the diagonal flipping in a rhombus.

Enumeration of all mapped blocks complying with the relationship (5) in the Steiner system $S(4, 5, 11)$ determines a specific class of 11-vertex equi-edged triangulated clusters. The mutual transformations between members of this class provide the transfer from close-packed tetrahedral fragments of the {3, 3, 5} polytope up to 11-vertex triangulated irregular sphere tilings and determine local reconstructions during polymorph transformations in metals.

So, the derivation of this class of clusters is ensured by one-to-one correspondence between cosets of Mathieu group $M_{11}$, a block set of the Steiner system $S(4, 5, 11)$ and 11-vertex equi-edged triangulated clusters. This correspondence was realized only in the framework of generalized crystallography.

## 5. Conclusions

This paper proposed a structural interpretation of the Steiner system $S(4, 5, 11)$. The interpretation is based on the revealed one-to-one correspondence between cosets of the Mathieu group $M_{11}$, a block set of the Steiner system $S(4, 5, 11)$ and 11-vertex equi-edged triangulated clusters.

The special class of triangulated equi-edged 11-vertex clusters complying with structural interpretation of the Steiner system $S(4, 5, 11)$ has been defined. Mutual transformations of clusters belonging to this special class ensure the transition from close-packed tetrahedral fragments of the {3, 3, 5} polytope to 11-vertex irregular triangulations of a sphere. The $2\pi$-disclination (diagonal flipping in a rhombus) corresponds to the mutual mapping of certain blocks of the $S(4, 5, 11)$.

Automorphisms of the Steiner system $S(4, 5, 11)$ determine uniquely mutual transformations of 11-vertex clusters belonging to the defining class; the said transformations correspond to local reconstructions in the polymorphic transformations in metals.

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