Acta Cryst. (1991). A**47**, 63–70

A Crystal-Chemical Model of Atomic Interactions. 5. Quasicrystal Structures

By L. A. Aslanov

Department of Chemistry, Moscow State University, 119899 *Moscow, USSR*

(*Received* 11 *December* 1989; *accepted* 18 *July* 1990)

Abstract

Experimental data of quasicrystal structures are considered from the point of view of a crystal-chemical model of atomic interactions (CCMAI) developed earlier. It is demonstrated that a quasicrystal consists of adjoining clusters. Each cluster has an icosahedron as the nucleus of the cluster and a few coordination shells. All clusters are truncated except for the central one. The distribution of icosahedral nuclei of clusters is stochastic so that there is orientational order of the icosahedral nuclei without translational symmetry. As a result the atoms are distributed in accordance with a slightly distorted three-dimensional Penrose tiling. This approach explains the very close resemblance of the crystal and quasicrystal structures of substances under consideration and shows the process of quasicrystal formation. The existence of the quasicrystals predicted earlier [Aslanov (1989). *Acta Cryst.* A**45**, 671–678] with the atomic subsystem having translation symmetry is discusseed on the basis of the experimental facts.

Introduction

A crystal-chemical model of atomic interactions (CCMAI) has allowed us to explain on a common basis crystal structures with different chemical compositions, types of chemical bonds, package densities and so on (Aslanov, 1988*a*, *b*, 1989*a*, *b*; Aslanov & Markov, 1989). An attempt was made to test the prognostic ability of CCMAI, and for this purpose the principles of quasicrystal formation were considered and illustrated with a hypothetical example (Aslanov, 1989*a*, *b*). After the manuscripts (Aslanov, 1989*a*, *b*) had been sent to press a few papers appeared (Cahn, Gratias & Mozer, 1988*a*, *b*; Elswijk, De Hosson, Van Smaalen & de Boer, 1988; Gratias, Cahn & Mozer, 1988) in which the results of experimental solutions of quasicrystal structures were described. It was natural to verify whether the predicted principles of the formation of quasicrystal structures (Aslanov, 1989*a*, *b*) agree with the experimental results. Also, some experimental facts (Mai, Tao, Zeng & Zhang, 1988; Mai, Zhang, Hui, Huang & Chen, 1988) can be interpreted in favor of ideas on the existence of quasicrystals with a translationally symmetrical subsystem of atoms (Aslanov, 1989*a*, *b*).

Analysis and discussion

The structure of an icosahedral quasicrystal, with composition close to Ag_6CuLi_3, has been investigated by Elswijk *et al.* (1988) using a single quasicrystal and an Enraf–Nonius CAD-4*F* diffractometer. The structure was solved by the trial-and-error method; atoms were distributed at vertices, midpoints of edges, centers of faces and at some specific points on diagonals of the rhombohedra incorporated in the three-dimensional Penrose tiling (3D PT). One of two versions gave $R = 0{\cdot}41$ and the other $R = 0{\cdot}07$, proving the correctness of the second model, which took into account the isotropic temperature factors of atoms. Later Van Smaalen (1989) confirmed this structure by a solution of the three-dimensional Patterson function.

The analysis of a quasicrystal structure allowed the conclusion that the quasicrystal structure is quite similar to the structure of the Al_5CuLi_3 crystal [space group *Im*3, $a = 13{\cdot}91\,(1)$ Å], which was solved by Cherkashin, Kripyakevich & Oleksiv (1963) and was refined later (Elswijk *et al.*, 1988; De Boissien, Janot, Dubois, Audier & Dubost, 1989). The main result of these two refinements was the interchange of positions of one of the lithium atoms with one of the aluminium atoms. Also, the paper by De Boissien *et al.* (1989) insisted that the twofold position, denoted *A* by Bergman, Waugh & Pauling (1957), was vacant, but, as will be shown below, this fact is not important for the point of view under consideration.

The similarity of the structures of the Al_5CuLi_3 crystal and the Al_6CuLi_3 quasicrystal allows us to restore the shells of a quasicrystal using the atomic coordinates in the Al_5CuLi_3 crystal structure (De Boissen *et al.*, 1989). Taking into account the fact that both aluminium and copper atoms are placed together at the same positions, we designate five independent aluminium and copper atoms distributed at *G*, *A*, *B*, *C* and *F* positions (Bergman, Waugh & Pauling, 1957) by symbols *A*1–*A*5, respectively. For brevity the lithium atoms are marked by symbols *L*1–*L*3; these atoms are distributed at *D*, *E* and *H* positions. So the analysis of the quasicrystal structure Al_6CuLi_3 in this paper is a reinterpretation of the experimental data (Elswijk *et al.*, 1988; De Boissien *et al.*, 1989) in terms of CCMAI.

0108-7673/91/020063-08$03.00

For clarity we suppose position A to be occupied by an $A2$ atom. The left side of Fig. 1 shows all coordination spheres existing in the Al_5CuLi_3 crystal around the $A2$ atom. Notations of atoms and distances between any atom of a coordination sphere and the central $A2$ atom are depicted below each coordination polyhedron. In Fig. 1 the polyhedra constructed by combination of coordination spheres

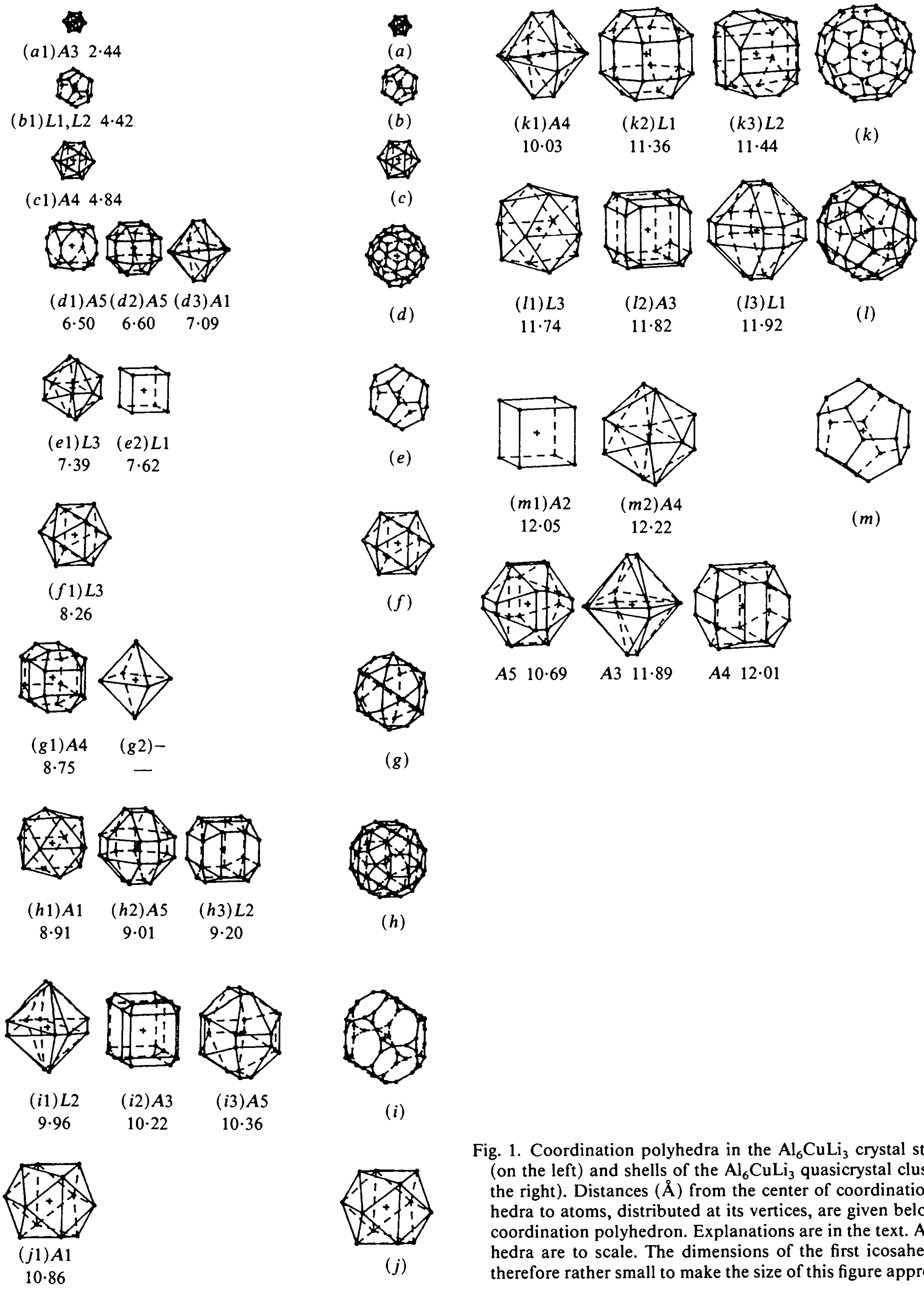

Fig. 1. Coordination polyhedra in the Al_6CuLi_3 crystal structure (on the left) and shells of the Al_6CuLi_3 quasicrystal cluster (on the right). Distances (Å) from the center of coordination polyhedra to atoms, distributed at its vertices, are given below each coordination polyhedron. Explanations are in the text. All polyhedra are to scale. The dimensions of the first icosahedra are therefore rather small to make the size of this figure appropriate.

are summarized in the column at the right-hand side.

The first coordination sphere of the *A*2 atom ($x=y=z=0$) is an icosahedron (Fig. 1*a*1) consisting of the atoms *A*3; it coincides with the first shell of a quasicrystal cluster (Fig. 1*a*). The second coordination sphere is a dodecahedron with lithium atoms at the vertices (Fig. 1*b*), and the third sphere is an icosahedron consisting of the *A*4 atoms (Fig. 1*c*). Thus, the sequence of polyhedra in the icosahedral cluster differs from the very beginning from that which exists in the Mackay (1962) icosahedra, and for this reason each polyhedron in an icosahedral cluster should be considered separately.

The following polyhedron in a quasicrystal cluster is a truncated icosahedron (Fig. 1*d*), which is a result of the combination of the coordination spheres *d*1–*d*3. The truncated icosahedron is followed by a dodecahedron (Fig. 1*e*) consisting of lithium atoms and an icosahedron with lithium atoms at the vertices (Fig. 1*f*).

Presumably, the coordination sphere *g*1 (Fig. 1) is important for understanding the discrepancies between the Al_5CuLi_3 crystal structure, on the one hand, and the Al_6CuLi_3 quasicrystal structure, on the other hand. After combination of the coordination sphere *g*1 with six points placed at the vertices of an octahedron (Fig. 1*g*2) inscribed into the sphere of the same radius (8·75 Å), the icosidodecahedron (Fig. 1*g*) appears. The octahedron vertices are placed at the 12-fold position of space group *Im*3. The absence of atoms at this position in a crystal explains the discrepancy between chemical compositions of a crystal (Al_5CuLi_3) and a quasicrystal (Al_6CuLi_3). Probably, the transformation of a quasicrystal into a crystal coincides with the change of chemical composition of substance and with an extraction of aluminium atoms out of this position. This hypothesis will be useful hereinafter.

The combination of three subsequent coordination spheres *h*1–*h*3 (Fig. 1) yields a rhombicosidodecahedron (Fig. 1*h*), and the combination of three others (*i*1–*i*3) produces a truncated dodecahedron (Fig. 1*i*). These polyhedra are followed by an icosahedron (Fig. 1*i*). At the periphery of a quasicrystal cluster the polyhedra are distorted. This distortion has two aspects: (i) the lengths of the polyhedra edges are different, as is clearly demonstrated by a truncated icosahedron (Fig. 1*k*); (ii) the atoms of some coordination spheres in a crystal (for example, those depicted in Fig. 1*k*1) 'collapse' into a cluster (compare the 10·03 Å distance in Fig. 1(*k*1) with distances from the cluster center to the polyhedra vertices depicted in neighboring figures). This peculiarity of the crystal structure is a consequence of the fact that the vertices of the *g*2 octahedron (Fig. 1) are vacant. Presumably, the icosidodecahedron 1*g* (Fig. 1) exists in quasicrystals as a whole, rather than partially (Fig. 1*g*1), and the truncated icosahedron (Fig. 1*k*) has no collapses of vertices inside a cluster. In the case of a crystal structure all points forming the polyhedron depicted in Fig. 1*k* had to be projected onto a sphere to obtain a proper illustration.

The last two polyhedra in the cluster under consideration are a rhombicosidodecahedron (Fig. 1*l*) and a dodecahedron (Fig. 1*m*). Eight of twenty vertices in a dodecahedron are filled with aluminium atoms, each of which is surrounded by six aluminium atoms belonging to *i*2 and *l*2 coordination spheres (Fig. 1). These six atoms are placed at icosahedron vertices. Let us suppose now that the complex, consisting of thirteen aluminium atoms, one of which is at the center and twelve others around the central atoms at the icosahedron vertices, is especially stable under conditions of solidification of the melt with composition Al : Cu : Li = 6 : 1 : 3. It is worth supposing that an icosahedral fragment consisting of six atoms will be built up to the whole icosahedron, and the formation of the same cluster shells, as considered above, will again take place around it. However, prior to considering this process one should make two remarks concerning the quasicrystal structure described. First, aluminium atoms placed at the vertices of the coordination sphere *m*2 (Fig. 1) cannot be new centers for multishell clusters, since their inner coordination sphere contains both aluminium (Fig. 1*i*3) and lithium atoms – *i*1, *l*1 and *l*3 in Fig. 1. Because the first coordination sphere differs in chemical composition from the stable complex consisting of thirteen aluminium atoms, one cannot expect these combinations to become the nuclei of new clusters. Finally, it should be noted that the *A*2 atoms can be absent at positions of type *A*, as was pointed out by De Boissien *et al.* (1989). In this case the central body in a multishell cluster should be supposed to be an icosahedron with a vacant center. This supposition has no influence on the analysis made above. Second, the three last coordination spheres of a crystal, depicted in the last row of Fig. 1, seem to be extracted from the sequence of polyhedra with distances from the center to the vertices less than 12·22 Å. This is explained by the fact that for the inclusion of these polyhedra into the analysis it is necessary to build up a few subsequent coordination spheres and combine them with the polyhedra depicted at the end of Fig. 1. But this information would be redundant, as a quasicrystal does not consist of an infinite sequence of shells, but obeys the following rule.

Thirteen aluminium atoms (twelve placed at the icosahedron vertices and one atom at the center of this icosahedron) play the part of the nucleus in a multishell cluster. Just after such nuclei are formed at the cluster periphery, the growth of an initial cluster must inevitably compete with the growth of clusters around new nuclei. The growth of new clusters seems to be preferable, because a total of eight clusters fills the space around an initial cluster faster than the initial cluster only. This process drastically differs from crystallization in the respect that the quasicrystal shells do not penetrate into each other, as was noticed in crystals (Aslanov, 1988*a*, 1989*b*). The fivefold symmetry does not allow the shells to do this. Any shell of an attached cluster represents a fragment of the polyhedra depicted on the right-hand side in Fig. 1. Such fragments adjoin an initial cluster and have new nuclei of clusters at their periphery, so that the growth process starts again.

The general idea of the structure of the initial multishell cluster is depicted in Fig. 2. The icosahedral nucleus corresponding to the icosahedron in Fig. 1(*a*) is situated at the center of the cluster. It is shaded by dots to show that it consists of the aluminium atoms only. The intermediate shells (Figs. 1*b*–*h*, *j*, *k*) are omitted for clarity. The combination of the shells indicated by indices *i* and *l* in Fig. 1 gives twenty semiicosahedra which can be built up to form the whole icosahedron, as is demonstrated in Fig. 2. The centers of these icosahedra are distributed at the vertices of a dodecahedron (Fig. 1*m*). But this is the geometry of a cluster. The chemical composition of the icosahedra ought to be taken into consideration. Only eight icosahedra consisting of the aluminium atoms exist in reality as explained above. They are distributed at the vertices of the cube and shaded with dots. All other positions are possible if a cube is chosen inside the dodecahedron in the other orientation, but not as it is shown in Fig. 2.

All icosahedra including the central one are oriented uniformly with respect to each other. This precise orientation of the icosahedra is valid throughout the quasicrystal because of the coincidence of the elements of symmetry of all shells of the cluster including shells *a*, *i*, *l* (Fig. 1).

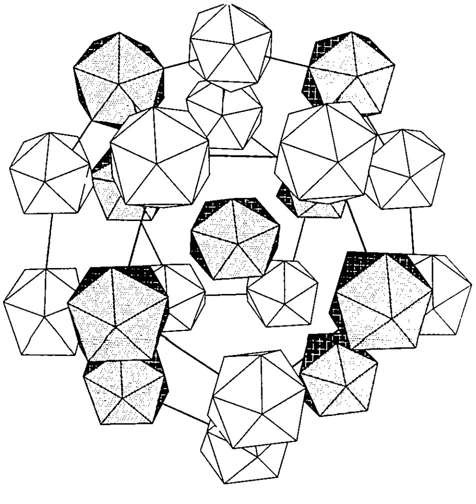

Fig. 2. The distribution of the icosahedral nuclei of the initial cluster in the icosahedral quasicrystals. The dotted icosahedra consist of the aluminium atoms only (the nuclei of the clusters). The blank icosahedra are the alternative places of the icosahedral nuclei of the clusters. All icosahedra have an orientational order. The solid lines between the icosahedra are the edges of a dodecahedron.

The adjoining fragments of clusters have only some of the symmetry elements of the initial cluster, and small fragments can have no symmetry elements at all. But if any adjoining cluster fragment is built up mentally to give the whole cluster, all its symmetry elements will be either parallel to or coincide with symmetry elements of an initial cluster. This situation takes place because the icosahedral nuclei of all clusters are oriented uniformly with respect to the initial cluster and, therefore, with respect to each other. This important point of quasicrystal formation should be discussed in detail.

It is worth paying attention to the fact that eight triangular faces of a truncated dodecahedron (Fig. 1*i*) are shared with icosahedra (Fig. 1*a*) which are the nuclei of adjoining clusters. If a shell depicted at Fig. 1(*i*) is a real Archimedean semiregular solid and adjoining icosahedra (Fig. 1*a*) are the real Platonic regular solids all symmetry elements of these solids are parallel or coincident provided these polyhedra share the triangular faces.

It is necessary to point out the fact that only eight of the twenty dodecahedron vertices are centers of adjoining clusters (they are arranged as a cube). There are a few combinations of eight dodecahedron vertices giving a cube. At the quasicrystal formation the choice of combination is a stochastic one. Each combination has an individual distribution of the icosahedral nuclei of adjoining clusters around the initial cluster, but the icosahedral nuclei are oriented perfectly with respect to the initial cluster in any position. So the quasicrystal has no translational symmetry, but has a perfect orientation of all icosahedral nuclei. The previous analysis (Aslanov, 1989*a*, *b*) did not take into account the stochastic distribution of the icosahedral nuclei and a model contained the translational symmetry for the first coordination shell. This problem of the quasicrystal structures will be discussed at the end of this paper, and it is now worth considering one more example of a quasicrystal structure.

The structure of the $Al_{100}Mn_{24}Si_{14}$ quasicrystal was solved by Cahn, Gratias & Mozer (1988*a*, *b*) (see also Gratias, Cahn & Mozer, 1988). The crystal compound of the same composition has essentially the same structure (Cooper & Robinson, 1966) as a quasicrystal. The $Al_{100}Mn_{24}Si_{14}$ crystals have space group *Pm*3, $a = 12{\cdot}68\ (2)$ Å. Their structure differs only slightly from b.c.c., and because of these differences two types of clusters should be considered, namely (i) the center is at point 0, 0, 0, and (ii) the center coincides with point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. We will repeat below just the same procedure which was performed for the quasicrystal structure Al_6CuLi_3: the reinterpretation of the experimental data for the quasicrystal structure $Al_{100}Mn_{24}Si_{14}$ (Cahn, Gratias & Mozer, 1988*a*, *b*; Gratias, Cahn & Mozer, 1988; Cooper & Robinson, 1966) will be fulfilled in terns of CCMAI.

All shells of both clusters with the coordination polyhedra in a crystal are depicted in Fig. 3. They were built in accordance with the atomic positional parameters published by Cooper & Robinson (1966). The centers of both clusters are vacant. The aluminium and silicon atoms (roentgenographically undistinguishable) are designated by indices *A*1-*A*9, the manganese atoms have indices *M*1 and *M*2. Fig. 3 needs a minimum of comment after analysis of the Al_6CuLi_3 structure. To be brief, the *a, c, e, h, k, l, s* polyhedra are icosahedra, *p* is a cuboctahedron, *b, f, m, q* are icosidodecahedra, *d, j, n, u* are distorted rhombicosidodecahedra, *g, r* are distorted truncated icosahedra, *i, t* are distorted truncated dodecahedra. The more the distance between the cluster center and the coordination shell atoms, the greater the deformation of polyhedra. This is due to the deformations of clusters appearing in a transition from a quasicrystal to a crystal state. The two last polyhedra in each cluster (Figs. 3*i, j, t, u*) are deformed so much that their pictures had to be obtained by the projection of the vertices of respective coordination polyhedra *i*1-*i*3, *j*1-*j*3, *t*1-*t*3, *u*1-*u*3 (Fig. 3) on the sphere. Perhaps the coordination polyhedra *i*3 and *j*1 (as well as *i*3 and *u*1) should be interchanged. This allows one to lower the scattering of distances from the cluster center to the vertices of coordination polyhedra in a crystal combined in one shell of a quasicrystal. But in this case the trigonal and pentagonal faces of the *i, j, t, u* polyhedra in Fig. 3 will be deformed more strongly. In fact, this rearrangement changes nothing, so that one can consider the variant depicted in Fig. 3 only.

Atoms *A*5 (Figs. 3*i*1, *j*3) and *A*4 (Figs. 3*t*1, *u*3) arrange halves of the icosahedra with centers of these icosahedra at the vertices of a cube. Let us assume that the icosahedral cluster with aluminium atoms at the vertices of an icosahedron is the most stable complex appeared during the solidification of a melt with composition $Al:Mn:Si = 1000:24:14$. One can assume that any of eight halves of an icosahedron at the cluster periphery is built up to the whole icosahedra, and all of them become nuclei of new clusters. The other twelve atomic groups with six atoms in each group (*i*2, *i*3, *j*1, *j*2 in a cluster with center at point 0, 0, 0 and *t*2, *t*3, *u*1, *u*2 in a cluster with center at point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ in Fig. 3) cannot arrange icosahedra, because they include manganese atoms (*i*3 and *t*3) together with aluminium atoms, and this is why these groups of atoms are most strongly deformed during the transformation to a crystal. In a quasicrystal these groups of atoms do not arrange the nuclei of new clusters because of the presence of manganese atoms.

Presumably, clusters with centers at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ have no difference in a quasicrystal. The transposition of *b, c* polyhedra (Fig. 3) in the first cluster in comparison with *l, m* polyhedra (Fig. 3) in the second is a formality, as a small change in distance from the centers of clusters to atoms due to the transformation of a quasicrystal into a crystal is quite permissible.

Analyzing Figs. 1 and 3 one can conclude that the idea of the quasicrystal structure demonstrated in Fig. 2 is valid for $Al_{100}Mn_{24}Si_{14}$ as much as for Al_6CuLi_3. The peripheral shells in both quasicrystals are a truncated dodecahedron (Fig. 1*i*, Figs. 3*i, t*) followed by a rhombicosidodecahedron (Fig. 1*l*, Figs. 3*j, u*) and the symmetry elements coincide with those of the icosahedral nuclei (the first shell of the cluster - Fig. 1*a* and Figs. 3*a, k*).

So, the quasicrystal has the only center in an initial multishell cluster, and all other clusters are the fragments of an initial one adjoining each other as demonstrated in Fig. 4(*a*). The initial cluster is schematically shown in Fig. 4(*a*) as three concentric circles (shells) with center at point *O*. The adjoining fragments of clusters with centers at points M_m and N_n are equivalent within the rows M_m or N_n, but any of the M_m fragments is not equivalent to any of the N_n fragments.

To make clearer the description of a quasicrystal structure, Fig. 4(*b*) shows schematically the crystal structure as proposed by CCMAI. All multispherical complexes are identical and interpenetrate each other, so that all centers of complexes are identical too. As a result, translational symmetry arises throughout the crystal.

The proposed model of a quasicrystal structure does not contradict a widely used concept based on the 3D PT. The statement of the problem discussed above shows that the quasicrystal structure formation principles proposed earlier (Aslanov, 1989*a*, *b*) and developed here are confirmed by experimental facts, and proves once again the correctness of CCMAI which gives the only explanation for the very tight resemblance of the crystal and quasicrystal structures of the substances under consideration.

The special sort of quasicrystals which is intermediate between the real quasicrystal and the crystal was predicted (Aslanov, 1989*a*, *b*). In Fig. 4(*a*) none of M_m fragments coincides with any of the N_n fragments; but there is a fraction of fragments (Fig. 4*c*) which is common for M_m and N_n. Hence, the translational symmetry, for a row, depicted in Fig. 4(*a*) exists only for icosahedral nuclei (the first shells), and for fragments of other shells depicted in Fig. 4(*c*). Let us imagine that at the periphery of an initial cluster with center at point *O* (Fig. 4*a*) there are both icosahedral nuclei with centers at points M_1, N_1 in the horizontal direction and two more icosahedral nuclei in directions inclined at 70, 53° (the angles between the threefold axes in the cube and

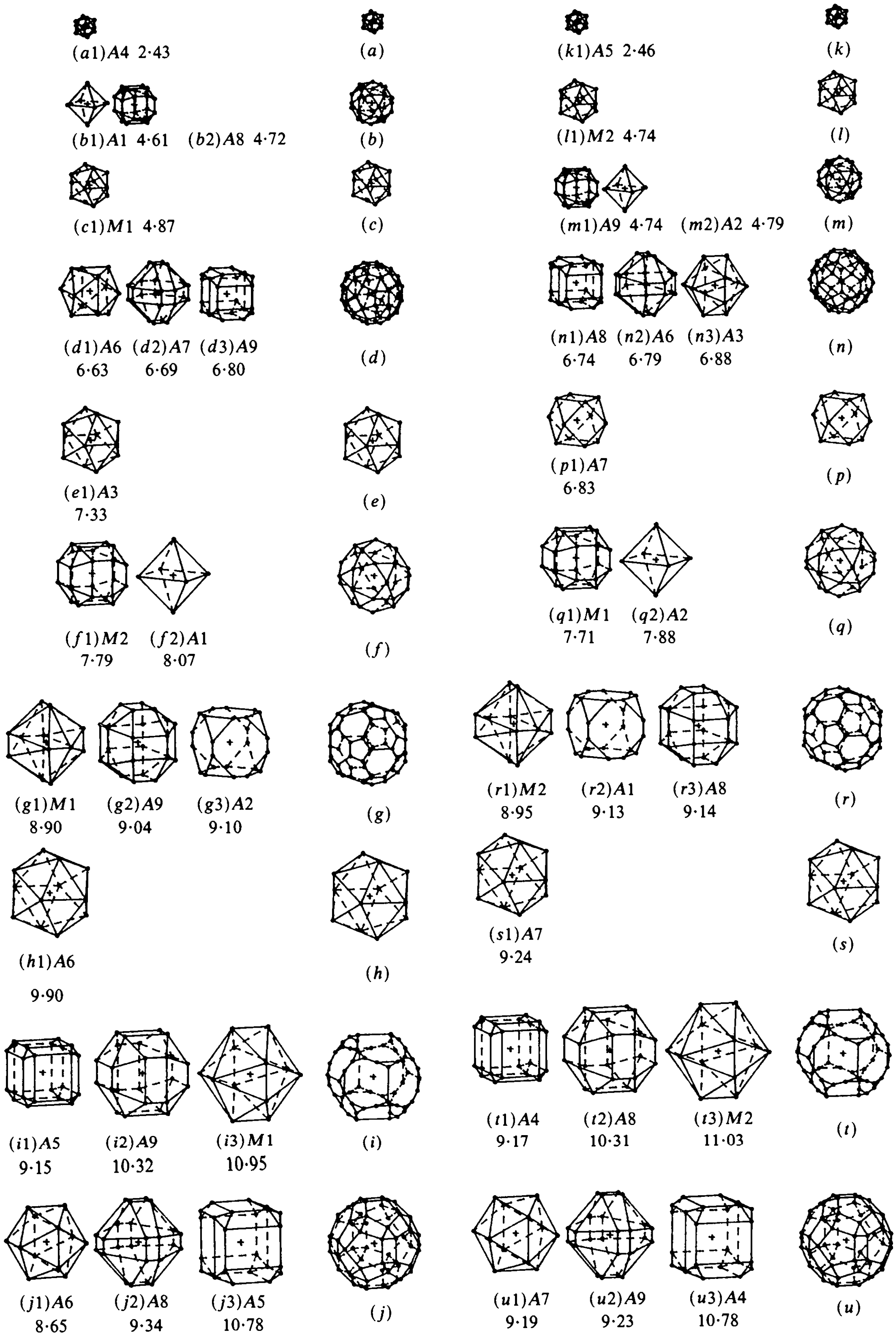

Fig. 3. Coordination polyhedra in the $Al_{100}Mn_{24}Si_{14}$ crystal structure (on the left) and shells of the quasicrystal cluster of the same composition (on the right). Distances (Å) from center of coordination polyhedra to atoms, distributed at its vertices, are given below each coordination polyhedron. Polyhedra (a)-(j) belong to the cluster with center at point 0, 0, 0; polyhedra (k)-(u) belong to the cluster with center at point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. Explanations are in the text. All polyhedra are to scale. The dimensions of the first icosahedra are therefore rather small to make the size of this figure appropriate.

dodecahedron) with respect to the horizontal direction. Then in the inclined row of cluster fragments there will be the same translational symmetry, as in the horizontal row (Fig. 4*a*), but Fig. 4(*c*) should be turned at 70, 53° around point *O*. It can easily be shown that both rows have translational symmetry for the first (icosahedral) shells only, because the other shells have no common atoms. This aggregate of atoms consists of two subsystems of atoms. One of them consists of central atoms and atoms of the first icosahedral shell of clusters. This subsystem has translational symmetry over all of a quasicrystal. The other subsystem of atoms consists of fractions of the second and subsequent shells of clusters. These fractions have different orientations in space, so that there is no translational symmetry in this subsystem of atoms, generally, in spite of the fact that inside separate parts of this atomic subsystem there exists a local translational symmetry coinciding with the symmetry of the first subsystem of atoms, as was shown above. Now there are experimental data which support this prediction.

Mai, Zhang, Hui, Huang & Chen (1988) and Mai, Tao, Zeng & Zhang (1988) found that an alloy with composition Al_6CuLi_3 annealed 1 h at 888 K and quenched in water has a very peculiar structure which combines both crystal and quasicrystal properties. There are six important experimental results in favor of this point of view.

First, a single quasicrystal with dimensions 4× 4 mm was investigated with a narrow X-ray beam and the same diffraction pictures were received at every point of this single quasicrystal. This proved that there was a single quasicrystal but not an alloy consisting of a mixture of crystals and quasicrystals.

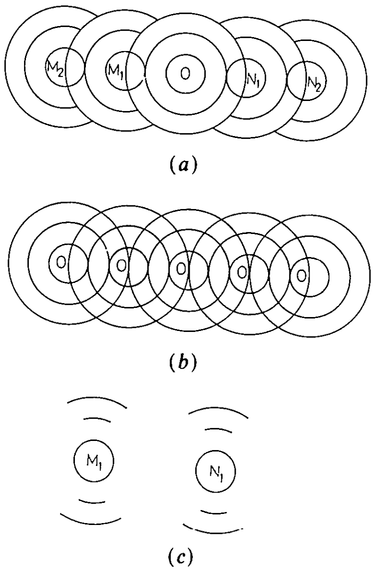

Fig. 4. (*a*) Schematic drawing of a quasicrystal; (*b*) schematic drawing of a crystal; (*c*) fractions of clusters with translation symmetry.

Second, all precession photographs contained reflections of two types: one set of reflections corresponded to the reciprocal lattice of a crystal, but the other set belonged to a quasicrystal.

Third, the precession photographs along the fivefold axis have mirror planes. One can draw two sets of lines through the diffraction spots and parallel to a mirror plane and in the perpendicular direction. The spacing between the lines in the first set is not variable. It corresponds to a crystal cell dimension of 13·9 Å. But the spacing of the lines in the second set is like an incommensurate phase with a golden ratio. In accordance with the model described earlier (Aslanov, 1989*a*, *b*) three of fifteen planes of an icosahedron coincide with three of nine planes of a cube. These planes are perpendicular to a fourfold axis of a cube. All fivefold axes of an icosahedron belong to these planes. As an edge of the cubic elementary cell is perpendicular to these planes the precession photographs along a fivefold axis contain rows of reflections perpendicular to a mirror plane and spacing between reflections inside these rows corresponds to 13·9 Å. The fivefold axes of an icosahedron do not coincide with any rational direction of the cube situated in indicated mirror planes so the distribution of the reflections on the precession photographs corresponds to a quasicrystal.

Fourth, there are two groups of precession photographs taken along the threefold axis of an icosahedron (Mai, Tao, Zeng & Zhang, 1988). The first group contains four photographs taken along a threefold axis of an icosahedron which correspond to a threefold axis of a cube. The symmetry of these photographs contains a threefold axis. But six photographs of the other threefold axis of an icosahedron have no threefold symmetry. These experimental results can be explained by the fact that all four threefold axes of the cube can be matched with four threefold axes of an icosahedron. The first group of precession photographs contains the reflections generated by a translationally symmetrical atomic subsystem with cell dimension 9·8 Å (Mai, Zhang, Hui, Huang & Chen, 1988). This value is equal to half of the face diagonal of the cube if the edge of this cube is 13·9 Å. This means that a Bravais cell is b.c.c., which corresponds to the crystal structure Al_5CuLi_3 and the quasicrystal structure Al_6CuLi_3 described above.

Fifth, fifteen precession photographs along the twofold axis (Mai, Tao, Zeng, & Zhang, 1988) were divided into two groups - three of them have two mutally normal mirror planes, the others do not. For an explanation of this fact it should be mentioned that no one twofold axis of an icosahedron (there are 15 such axes) coincides with the six twofold axes of a cube, but three twofold axis of these 15 coincide with a fourfold axis of a cube. Any of these three axes should give a precession photograph with two mirror planes normal to each other, but all other twofold axes of the quasicrystal should give photographs with no plane at all.

Sixth, the stereographic projection of the symmetry elements observed in this quasicrystal by Mai, Tao, Zeng & Zhang (1988) clearly indicates the consistency of the threefold and twofold axes with the threefold and fourfold axes of a cube respectively.

So a model of a quasicrystal structure including the hypothesis of the special sort of quasicrystal containing the translationally symmetrical subgroup of atoms was supported by experimental facts.

Attention has been concentrated in this paper on an explanation of quasicrystal structures taking into consideration the principles of CCMAI. But as a result one can make a conclusion about the efficiency of the CCMAI as a common theoretical background for both crystals and quasicrystals.

References

ASLANOV, L. A. (1988*a*). *Acta Cryst.* B**44**, 449-458.
ASLANOV, L. A. (1988*b*). *Acta Cryst.* B**44**, 458-462.
ASLANOV, L. A. (1989*a*). *Acta Cryst.* A**45**, 671-678.
ASLANOV, L. A. (1989*b*). *Structures of Substances* (in Russian). Moscow Univ. Press.
ASLANOV, L. A. & MARKOV, V. T. (1989). *Acta Cryst.* A**45**, 662-671.
BERGMAN, G., WAUGH, J. L. T. & PAULING, L. (1957). *Acta Cryst.* **10**, 254-258.
CAHN, J. W., GRATIAS, D. & MOZER, B. (1988*a*). *Phys. Rev. B*, **38**, 1638-1642.
CAHN, J. W., GRATIAS, D. & MOZER, B. (1988*b*). *J. Phys. (Paris)*, **49**, 1225-1233.
CHERKASHIN, E. E., KRIPYAKEVICH, P. I. & OLEKSIV, G. I. (1963). *Kristallografiya*, **8**, 846-851.
COOPER, M. & ROBINSON, K. (1966). *Acta Cryst.* **20**, 614-617.
DE BOISSIEN, M., JANOT, CH., DUBOIS, J. M., AUDIER, M. & DUBOST, M. (1989). *J. Phys. (Paris)*, **50**, 1689-1709.
ELSWIJK, H. B., DE HOSSON, J. TH. M., VAN SMAALEN, S. & DE BOER, J. L. (1988). *Phys. Rev. B*, **38**, 1681-1685.
GRATIAS, D., CAHN, J. W. & MOZER, B. (1988). *Phys. Rev. B*, **38**, 1643-1652.
MACKAY, A. L. (1962). *Acta Cryst.* **15**, 916-918.
MAI, Z., TAO, S., ZENG, L. & ZHANG, B. (1988). *Phys. Rev. B*, **38**, 12913-12916.
MAI, Z., ZHANG, B., HUI, M., HUANG, Z. & CHEN, X. (1988). *Phys. Lett. A*, **130**, 376-380.
VAN SMAALEN, S. (1989). *Phys. Rev. B*, **39**, 5850-5856.

Acta Cryst. (1991). A**47**, 70-73

The Icosahedral Point Groups

BY DANIEL B. LITVIN

Department of Physics, The Pennsylvania State University, The Berks Campus,
PO Box 7009, *Reading, PA* 19610-6009, *USA*

(*Received* 19 *January* 1990; *accepted* 4 *September* 1990)

Abstract

Basic group-theoretical properties of the icosahedral point groups are derived. Here are given the permutations of the vertices of an icosahedron under the action of the elements of the icosahedral point groups, the icosahedral point groups' multiplication tables, subgroups, sets of conjugate subgroups, centralizers and normalizers of arbitrary subsets and coset and double coset decompositions.

1. Introduction

Basic group-theoretical properties of the 32 crystallographic point groups have been tabulated by Janovec, Dvorakova, Wike & Litvin (1989). Here, we extend that work to the icosahedral point groups. Icosahedral point groups have been of interest in connection with the vibrational (Boyle & Parker, 1980) and electronic properties (Boyle, 1972) of icosahedral molecules. Much work has been done on the coupling coefficients of the icosahedral groups, see for example Golding (1973), Boyle & Ozgo (1973), Pooler (1980) and Fowler & Ceulemans (1985). The representations of the icosahedral group have been studied by Backhouse & Gard (1974) and polynomial invariants by Cummins & Patera (1988). Additional interest in the icosahedral groups stems from the icosahedral symmetry of biological macromolecules (Litvin, 1975) and the discovery of quasicrystals (Shechtman, Blech, Gratias & Cahn, 1984; see also Nelson, 1986).

In § 2 we define the icosahedral groups in terms of the symmetry of an icosahedron inscribed in a cube. In § 3 we give the permutations of the vertices of the icosahedron under the action of the elements of the icosahedral point groups, the icosahedral point groups' multiplication tables, subgroups, sets of conjugate subgroups, centralizers and normalizers of arbitrary subsets, and coset and double coset decompositions.

0108-7673/91/020070-04$03.00