

THE ICOSAHEDRIC SYSTEM AND THE ICOSAHEDRAL SYMMETRY CLASS

ION PETREUȘ¹, TUDOR PETREUȘ²

Al. I. Cuza University, Department of Mineralogy and Geology¹, Iași, Romania

E-mail: opetreus@yahoo.com

Gr. T. Popa University of Medicine and Pharmacy², Iași, Romania

Abstract. Quasicrystals, and particularly icosahedric materials, are of the greatest scientific and technological interest. In this paper we wish to focus on a morphological analysis of some quasicrystal polyhedrons by means of two fundamental laws of crystallography: the law of the constancy of interfacial angles and the law of rational indices. We begin to organize the quasipolyhedrons in crystallographic systems and classes of symmetry. The icosahedric system (or quasicubic system) is defined by its specific axial relation: $a \approx b \approx c$; $\alpha \approx \beta \approx \gamma \approx 90^\circ$. The icosahedral class is defined by its specific symmetry formula, presented in its extended form as: $3L^2 12L^2 10L^3 6L^5 3\pi 12P^2C$. The icosahedron, the regular pentagonal dodecahedron and the rhombic triacontahedron has been analysed: interfacial angle were measured on 3D drawings, stereographic projection and geometrical calculation. We introduced the new principle of corresponding crystal-to-quasicrystal, c-to-qc. A new crystallographic code was necessary to describe corresponding c-to-qc. The other new and important results are the following. Icosahedron is not a simple quasipolyhedron; it is a combination of two simple quasipolyhedrons: the qoctahedron and the qpentagonal dodecahedron.

Its complete notation is $q\{111\}q\{520\}$. The rhombic triacontahedron is a combination of a qcube and a qdiplohedron, being noted by $q\{100\}q\{321\}$. The qcube and the qoctahedron cannot exist as simple quasicrystals. All faces of icosahedron and rhombic triacontahedron were noted with 3 Miller indices (hkl), in agreement with the law of rational indices. It results that the pentagonal quasicrystals structures are 3D.

Key words: quasicrystals, icosahedric system, icosahedral symmetry class, Miller indexing, icosahedron, regular pentagonal dodecahedron, rhombic triacontahedron.

Résumé. Dans le présent ouvrage nous définissons pour la première fois un nouveau système cristallographique, conformément à sa relation axiale spécifique: $a \approx b \approx c$; $\alpha \approx \beta \approx \gamma \approx 90^\circ$; nous allons le nommer système icosaedrique ou quasi cubique. Nous allons encore définir la classe de symétrie icosaedrique selon sa formule de symétrie spécifique: $3L^2 12L^2 10L^3 6L^5 3\pi 12P^2C$. On introduit par là le nouveau principe de la correspondance, cristal-quasicristal, c-qc. Nous avons été obligés d'introduire un nouveau code cristallographique pour pouvoir décrire la transformation c-qc. Nous décrivons en détail les principaux quasicristaux qui appartiennent au système icosaedrique et à la classe de symétrie icosaedrique: l'icosaèdre, le dodécaèdre pentagonal régulier et le triacontaèdre rhombique. Nous présentons aussi les dessins 3D pour ces trois quasicristaux, auxquels nous annexons leurs projections stéréographiques et les indices Miller (hkl). Suite à l'analyse quelques résultats vont surprendre: le q-cube et le q-octaèdre ne sauraient exister en tant que polyèdres individuels, bien au contraire ils peuvent apparaître seulement combinés avec d'autres quasicristaux simples. La notation des facettes de l'icosaèdre, du dodécaèdre pentagonal régulier et du triacontaèdre rhombique avec trois indices Miller (hkl) rationnels, entiers et petits, démontre que la structure de ces quasicristaux est de type 3D.

Mots-clés: quasicristaux, système icosaedrique, classe de symétrie icosaedrique, indices Miller, l'icosaèdre, le dodécaèdre pentagonal régulier, le triacontaèdre rhombique.

INTRODUCTION

The discovery of quasicrystals has actually allowed for the discovery of a new state of condensed matter, quite similar, yet never identical with the crystalline state (Shechtman *et al.* 1984). Considerable progress has been recorded in the synthesis of some metallic quasimaterials obtained by rapid solidification from melts, at cooling rates $>10^6$ K sec⁻¹; formation and growth of metallic

quasicrystals have been explained by nucleation from undercooled melts, due to the icosahedral short-range order already present in liquid alloys (Kelton *et al.* 2003; Sachdev and Nelson 1985). Soft quasicrystalline materials have been largely explored both theoretically and experimentally (Hayashida *et al.* 2007; Lifshitz and Diamant 2007). Colloidal quasicrystals are spontaneously formed by self-assembly in colloidal solutions (Fisher *et al.* 2011; Denton and Löwen 1998); micellar phases can also exist with quasiperiodic structures (Zeng *et al.* 2004; Fischer *et al.* 2011). Colloidal inorganic nanoparticles can self-assemble into binary aperiodic superlattices (Talpin *et al.* 2009). The fullerene materials C_{60} and C_{80} are quasicrystals (Weeks and Harter 1989; Kroto *et al.* 1985; Boo 1992, Fowler and Myrvold 2010). Thousands of proteins have an icosahedric quasicrystalline structure (Branden and Tooze 1999; Marck and Zhou 1992).

The unity of two – structural and morphological – states may be evidenced by a few important observations, such as:

(i) The crystals and quasicrystals have a polyhedral shape, meaning that they have very similar but never identical atomic structures, as some of them are strictly periodic, others are non-periodic. Accordingly, the polyhedrons are also different, namely specific crystalline and specific quasicrystalline, as demonstrated in the present investigation. Example: pentagonal dodecahedron (crystal) and regular pentagonal dodecahedron (quasicrystal). We named them here as corresponding crystal/quasicrystal.

(ii) It is important to know how high or how low is the effect of the five-fold symmetry axes upon both their structure and morphology. In the field of crystal physics the structural transformations of long-range order from quasiperiodic to translational and the mechanism of the quasicrystal-to-crystal phase transition is largely studied (Liu *et al.* 1991; Rochal *et al.* 1996; Rochal 1997; Rochal and Lorman 2003; Stauerer 2000).

(iii) There are also morphological transitions from crystal – to – quasicrystal e.g. from pentagonal dodecahedron – to – regular pentagonal dodecahedron.

(iv) The symmetry is the unitary criterion for investigations, systematisation and hierarhisation of both crystals and quasicrystals.

(v) The symmetry controls the structure and the morphology of crystals and quasicrystals. The symmetry of periodic structures and correspondingly the morphology of crystals controls the well known restrictions: there are only 7 crystallographic systems, only 32 symmetry classes, only 14 Bravais lattices and only 230 different space groups.

(vi) The symmetry laws were not applied to quasicrystalline specific polyhedrons: we have no system, nor a symmetry class (not completely identical with point groups). We have no hierarchy and no systematisation of quasicrystals.

(vii) Steinhardt (1996) said: “as an exemple of the application of symmetry principles, the subject of quasicrystals is still in a primitive stage” (p. 14270). Chidambaram (2004) sustains that “Quasicrystals have been studied by using quasiperiodic functions and by a variety of experimental methods – mainly diffraction and electron microscopy – and various tiling-based and other models have been developed, but still the problem of a detailed and satisfactory structural model for quasicrystals remains elusive” (p. 68). Finally, Grimm and Schreiber (2005) consider that: “While there exist sophisticated structure models for various quasicrystals, many important questions remain unanswered...” (p. 95).

In the present study, the law of constance of interfacial angles and the law of rational indices are applied to quasicrystalline polyhedrons. The interfacial angles are determined by three independent methods, namely: (i) 3D drawings; (ii) by means of a stereographic projection on the Wulf net; (iii) by geometrical calculations. The Miller indices (hkl) of all quasicrystal faces were determined by a new principle of corresponding crystal/quasicrystal (c-to-qc). A new crystallographic code was necessary to describe c-to-qc. Examples: cube{100}-to-qcube q{100}; octahedron {111}-to-qoctahedron q{111}; diplohedron {321}-to-qdiplohedron q{321}.

The icosahedric system has been defined by its specific axial relation (and by its specific elementary cell). The icosahedral symmetry class has been defined by its specific symmetry formula. We use the extended symmetry formula (Flint 1971), known as expressing more directly, and more completely the symmetry of a quasipolyhedron. The Hermann-Mauguin notation will be used when all systems and symmetry classes of the quasicrystals will be defined.

The icosahedron, the regular pentagonal dodecahedron and the triacontahedron are only the first three quasicrystals belonging to the icosahedric system and to the icosahedral class. For these three quasipolyhedrons, the 3D drawings, the stereographic projections and the Miller indices of all quasicrystal faces are presented. Indexing ...“proving that a structure is periodic, quasiperiodic or almost periodic” (Cahn *et al.* 1986).

THE ICOSAHEDRIC SYSTEM

A structural and morphological system is entirely defined by its axial relation, namely the relative lengths of the crystallographic axes (a , b , c) and of the angles between them (α , β , γ). In the icosahedric system, the crystallographic axes are three main two-fold symmetry axes. In the non-periodic structures, quite naturally, these three axes are three 1D Fibonacci lattices, in which non-periodicity is expressed through long (L) and short (S) segments. We therefore conclude the axial relation of the icosahedric system is:

$$\begin{aligned} a &\approx b \approx c \\ \alpha &\approx \beta \approx \gamma \approx 90^\circ \end{aligned}$$

This axial relation indicates that the three X Y Z quasicrystallographic axes are only quasiorthogonal to each other, and a , b , c are only quasiequals to each other. Unit cell angles are only approximately 90° (Fry *et al.* 1996, p 337). It results that for quasicrystals we must measure more exactly a , b , c and α , β , γ because the difference between periodic to quasiperiodic is very small. This axial relation fully defines the icosahedric system or quasicubic system.

THE ICOSAHEDRAL CLASS

The icosahedron, regular pentagonal dodecahedron and rhombic-triacontahedron models have been constructed. The three symmetry operations of rotation, reflection and inversion were performed, which led us to the symmetry formula of the icosahedral class, presented in its extended form:

$$\frac{3L^2}{3\pi} \frac{12L^2}{12P^2} \frac{10L^3}{-} \frac{6L^5}{-} C,$$

where:

L = simple symmetry axis

L^n = n-fold symmetry axis

π = main symmetry plan

C = symmetry center

$3L^2$ = three main two-fold symmetry axes

3π = three main symmetry plans

P^2 = symmetry plan perpendicular to a symmetry axis L^2

$-$ = no symmetry plan present

Group $15L^2$ was decomposed into group $3L^2$, representing the main symmetry axes, as they coincide with the three crystallographic axes, while group $12L^2$ stands for the other two-fold symmetry axes. The symmetry planes perpendicular to the three main symmetry axes are noted as 3π .

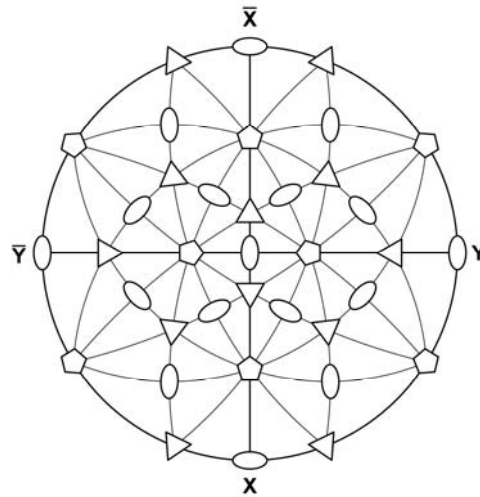


Fig. 1 – Stereographic projection of the icosahedral symmetry class: symmetry axes and planes (identical with the point group $\bar{m}\bar{3}5$).

Figure 1 plots the stereographic projection of the symmetry elements (symmetry axes and symmetry planes) contained in the symmetry formula of the icosahedral class, identical with its corresponding point group $\bar{m}\bar{3}5$, largely presented by Shechtman *et al.*, 1984; Cahn *et al.*, 1986.

THE ICOSAHERON

The icosahedron is encountered both in metallic alloys (Stauerer and Deloudi 2009), and in crystallized proteins, especially in the field of animal-viruses (Indelicato *et al.* 2012) and vegetal-viruses (Savithri *et al.* 1989; Matthews 1981).

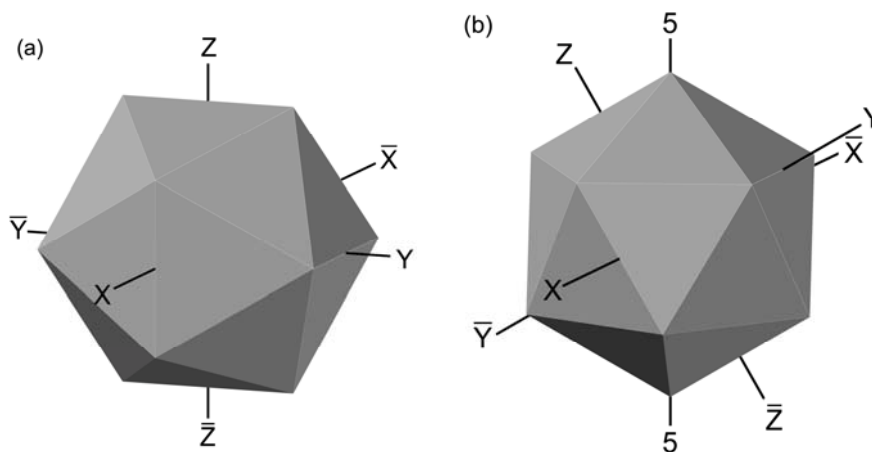


Fig. 2 – Icosahedron in its correct, standard orientation (a), and nonstandard orientation (b).

Figure 2 plots an icosahedron in standard orientation on the crystallographic axes (a) and also in nonstandard orientation, with one of the five-fold axes in vertical position (b). The stereographic projection of all faces of the icosahedron permitted to obtain its stereogram (Fig. 3).

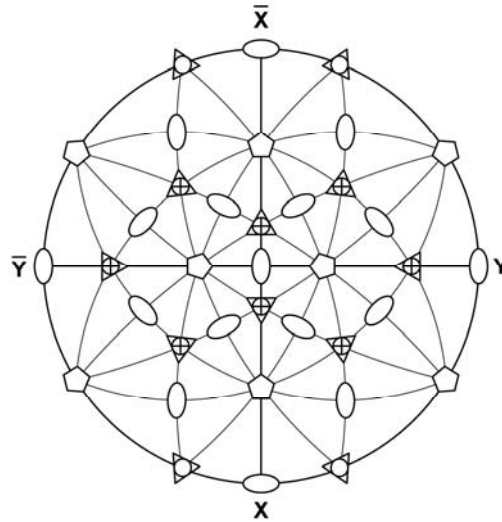


Fig. 3 – Stereogram of the icosahedrons.

Analysis of the stereogram revealed that the icosahedron is not a simple quasicrystal, but a compound one, formed by two simple quasicrystals, namely: a quasioctahedron $q\{111\}$ and a quasipentagonal dodecahedron $q\{hk0\}$. The 8 faces of the icosahedron are stereographically projected exactly in the points representing 8 octahedron faces, which means that these 8 faces of the icosahedron belong to a qoctahedron.

The above observation is confirmed morphologically as well. The 8 faces belonging to the qoctahedron may be easily identified on the icosahedron by simply drawing the octahedron both inside and outside the icosahedron (Fig. 4a, 4b).

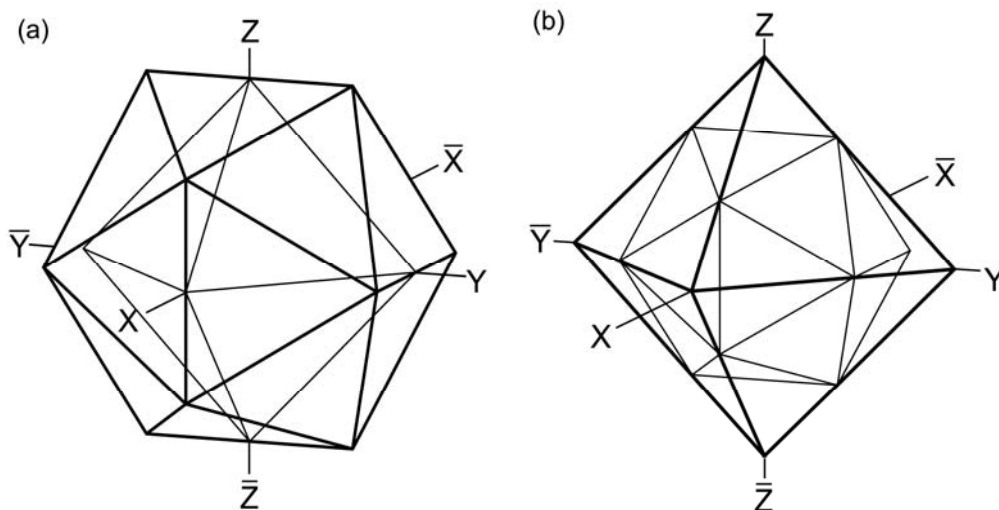


Fig. 4 – (a) Quasioctahedron inside of icosahedrons
(b) Icosahedron inscribed in an octahedron.

Inside the icosahedron, the lines uniting the ends of the XYZ crystallographic axes may be drawn in order to obtain an octahedron; in other words, the octahedron may be inscribed inside the icosahedron, which leads to the following conclusions:

- the crystallographic axes of the icosahedron and of the octahedron are perfectly superposed;
- The 8 faces of the octahedron are parallel to the 8 faces of the icosahedron; consequently, the 8 faces of the icosahedron form 4 families of octahedron reticular planes, namely: family (111) , $(\bar{1}\bar{1}\bar{1})$; family $(\bar{1}11)$, $(1\bar{1}\bar{1})$; family $(\bar{1}\bar{1}1)$, $(11\bar{1})$ and family $(1\bar{1}1)$, $(\bar{1}1\bar{1})$ according to the symmetry centre.

Outside the icosahedron, an octahedron may be easily drawn, by inscribing the icosahedron inside the octahedron (Loreto *et al.*, 1990, p. 163). It results:

- 8 icosahedron faces coincide exactly with 8 octahedron faces;
- again, 8 icosahedron faces represent 8 octahedron faces. The notation in Miller indices is the same for the octahedron faces and for the 8 faces of the icosahedron;
- the five-fold axes of the icosahedron modify in no way the 8 faces of the octahedron. The whole structure corresponding to the families of octahedric planes is not modified by pentasymmetry.

The 8 faces of the icosahedron have been precisely identified. There follows the identification of the other 12. Obviously, these 12 faces should belong to a dodecahedron. The five-fold axis suggests a pentagonal dodecahedron.

A family of pentagonal dodecahedrons therefore exists (Table 1); each pentagonal dodecahedron may be specifically determined, according to the interfacial angles.

Table 1

A family of pentagonal dodecahedrons

Positive	Negative
{410}	{140}
{310}	{130}
{520}	{250}
{210}	{120}
{530}	{350}
{320}	{230}
{430}	{340}
{540}	{450}

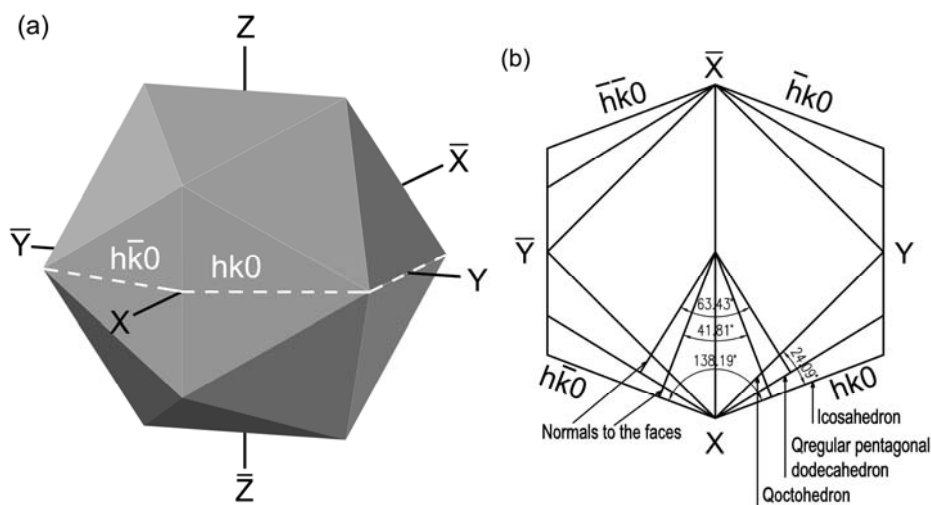


Fig. 5 – Ecuatorial section in the plane of XY axes of the icosahedron (a), and interfacial angles (b)

The interfacial angles between 2 faces of a pentagonal dodecahedron (more precisely, others than the previously identified octahedron ones), intersecting according to a common edge, namely angle $(hk0)\wedge(\bar{h}\bar{k}0)$ of Figure 5a, were measured on a 3D icosahedron (Fig. 5b). The value obtained was $(hk0)\wedge(\bar{h}\bar{k}0)=41.81^\circ$. This angle was calculated geometrically, the value obtained being 41.50° , namely very similar to that of the interfacial angle $(520)\wedge(5\bar{2}0)$ of 43.36° , corresponding to the pentagonal dodecahedron $\{520\}$. Stereographic projection of the 12 faces of the pentagonal dodecahedron $\{520\}$ (Fig. 6) evidenced that the poles of the 12 icosahedron faces are stereographically projected quite close to the stereographic poles of the pentagonal dodecahedron $\{520\}$.

The difference of the interfacial angle between quasicrystal $q\{520\}$ and crystal $\{520\}$ is of $43.36^\circ - 41.50^\circ = 1.86^\circ$. Pentasymmetry modified the structure of the pentagonal dodecahedron $\{520\}$ with a very low angular value, of only 1.86, for obtaining the quasicrystal $q\{520\}$.

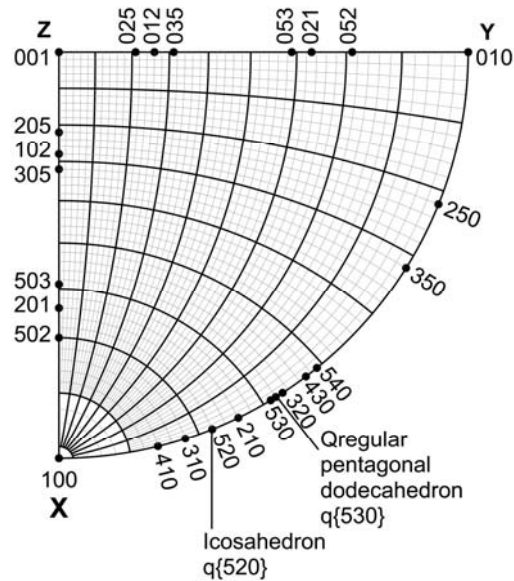


Fig. 6 – Stereogram of the pentagonal dodecahedrons

Consequently, there exists a pair of corresponding polyhedrons: the pentagonal dodecahedron crystal $\{520\}$ and the qpentagonal dodecahedron quasicrystal $q\{520\}$. It shows that:

- (i) the icosahedron is composed of a quasioctahedron $q\{111\}$ and a qpentagonal dodecahedron $q\{520\}$;
- (ii) the notation of the icosahedron is $q\{111\}q\{520\}$;
- (iii) the quasioctahedron cannot exist as an individual quasicrystal, but only in combination with the qpentagonal dodecahedron $q\{520\}$, thus forming together the quasicrystal known as icosahedron.

MILLER INDICES OF THE ICOSAHEDRON FACES

The octahedron and the qoctahedron have similar Miller (hkl) symbols, once the orientation of faces (111) of the qoctahedron on the reference axes remained unmodified as an effect of icosahedron's pentasymmetry. The 8 faces of the icosahedron are identical with the 8 faces of the octahedron. The Miller indices of these 8 icosahedron faces are the following (Fig. 7a):

$$(111); (\bar{1}\bar{1}\bar{1}); (\bar{1}\bar{1}1); (\bar{1}\bar{1}\bar{1}); (1\bar{1}\bar{1}); (11\bar{1}); (\bar{1}\bar{1}1); (1\bar{1}\bar{1}).$$

Consequently, octahedron $\{111\}$ is identical with octahedron $q\{111\}$. These two corresponding polyhedrons, namely octahedron $\{111\}$ and octahedron $q\{111\}$, have identical stereograms (Fig. 7b).

The 8 octahedric faces of the icosahedron alternate with the 12 faces belonging to the pentagonal dodecahedron $q\{520\}$. The Miller indices of the faces of the pentagonal dodecahedron $q\{520\}$ are the following:

$$(520); (\bar{5}20); (\bar{5}\bar{2}0); (\bar{5}\bar{2}\bar{0}); (205); (\bar{2}05); (20\bar{5}); (\bar{2}0\bar{5}); (052); (05\bar{2}); (0\bar{5}2); (0\bar{5}\bar{2}).$$

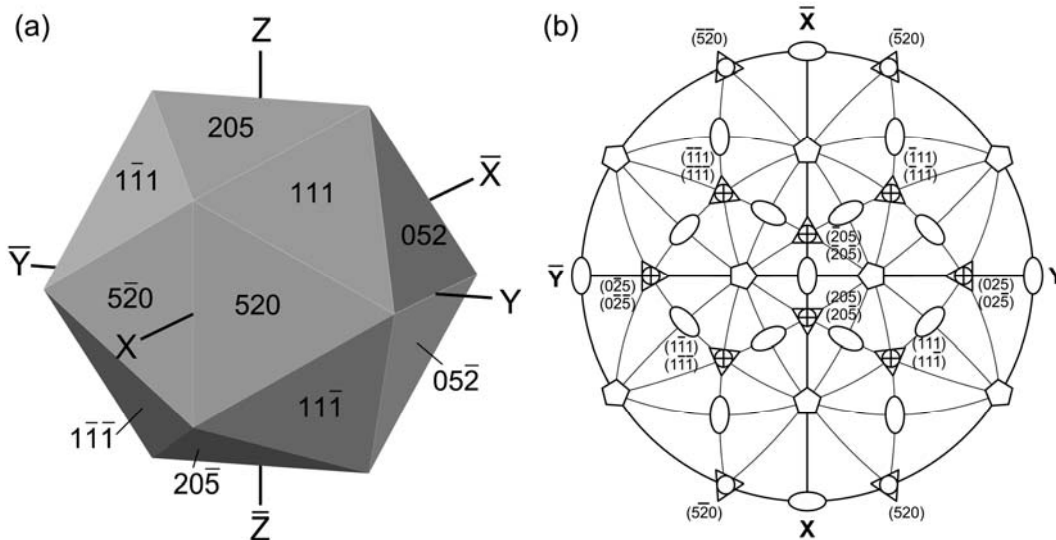


Fig. 7 – Miller indices of the icosahedron faces: on the icosahedron (a), and on the stereogram (b).

THE REGULAR PENTAGONAL DODECAHEDRON

The world of crystals registers no regular pentagonal dodecahedron; it is specific to the quasicrystalline, aperiodic and pentasymmetric substances. Identification of the corresponding crystal of this quasicrystal in the family of pentagonal dodecahedrons is essential. The same methods were applied, namely: interfacial angles, stereograms and geometrical calculations.

The interfacial angles specific to the corresponding pentagonal dodecahedrons, namely crystals and quasicrystals, are presented in Table 2. Geometrical calculations of the interfacial angle $(hk0)\Delta(h\bar{k}0)$ for the regular pentagonal dodecahedron gave a value of 63.42° . Further on, this angle was measured on a 3D section through the regular pentagonal dodecahedron, the result obtained was 63.43° . The angle was compared with the interfacial angles $(hk0)\Delta(h\bar{k}0)$ specific to irregular pentagonal dodecahedrons (crystals, Table 2). The closest value obtained, of 61.55° , is specific to the irregular pentagonal dodecahedron $\{530\}$ (crystal). The difference of the interfacial angle between the quasicrystal called regular pentagonal dodecahedron and the one called irregular pentagonal dodecahedron is 1.87° . Such a difference expresses the effect of the five-fold symmetry axis upon the structure of the irregular pentagonal dodecahedron $\{530\}$, which transforms it into its corresponding quasicrystal $q\{530\}$, defined as a regular pentagonal dodecahedron.

All faces of the positively and negatively regular pentagonal dodecahedron (Figs. 8a and b) were noted in Miller indices, according to the principle of the corresponding polyhedrons. Figure 9 renders the stereographic projection of these two polyhedrons – $q\{530\}$ and $q\{350\}$.

Table 2

Interfacial angles of the pentagonal dodecahedrons, qpentagonal dodecahedrons and the difference between the crystal-quasicrystal corresponding polyhedrons

Crystals (according to Ford 1958, p. 82)	
$100\Lambda hk0$	$hk0\Lambda \bar{h}\bar{k}0$
$100\Lambda 410 = 14^\circ 02$	$410\Lambda 4\bar{1}0 = 28^\circ 04$
$100\Lambda 310 = 18^\circ 26$	$310\Lambda 3\bar{1}0 = 36^\circ 52$
$100\Lambda 520 = 21^\circ 48$	$520\Lambda 5\bar{2}0 = 43^\circ 35$
$100\Lambda 210 = 26^\circ 34$	$210\Lambda 2\bar{1}0 = 53^\circ 07$
$100\Lambda 530 = 30^\circ 57$	$530\Lambda 5\bar{3}0 = 61^\circ 55$
$100\Lambda 320 = 33^\circ 41$	$320\Lambda 3\bar{2}0 = 67^\circ 22$
$100\Lambda 430 = 36^\circ 52$	$430\Lambda 4\bar{3}0 = 73^\circ 44$
$100\Lambda 540 = 38^\circ 39$	$540\Lambda 5\bar{4}0 = 77^\circ 19$
Quasicrystals	
$q100\Lambda q520 = 20^\circ 75$	$q520\Lambda q5\bar{2}0 = 41^\circ 50$
$q100\Lambda q530 = 31^\circ 71$	$q530\Lambda q5\bar{3}0 = 63^\circ 40$
Difference between crystal/quasicrystal	
$100\Lambda 520 = 1^\circ 13$	$520\Lambda 5\bar{2}0 = 1^\circ 86$
$100\Lambda 530 = 1^\circ 14$	$530\Lambda 5\bar{3}0 = 1^\circ 85$

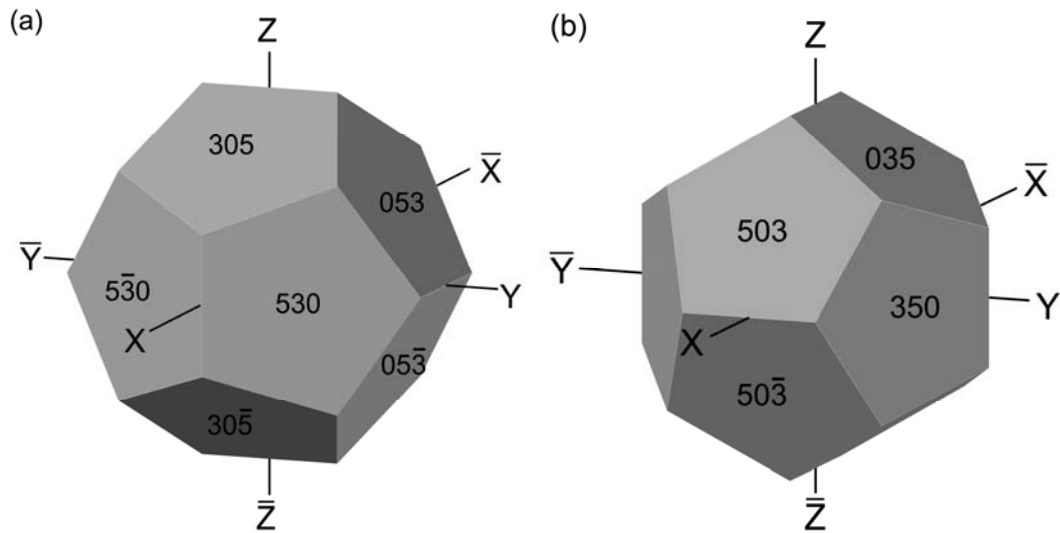


Fig. 8 – Miller indices of the faces of the qpositive $q\{530\}$ (a), and qnegative regular pentagonal dodecahedron $q\{350\}$ (b).

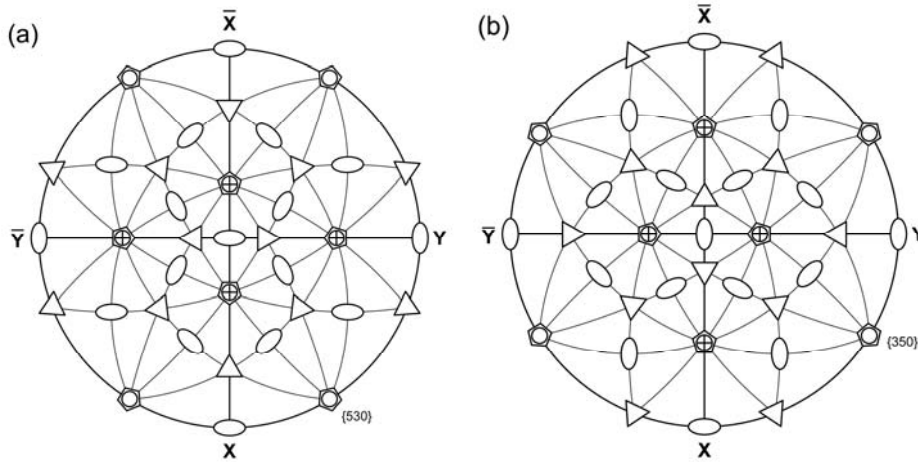


Fig. 9 – Stereograms of qpositive $q\{530\}$ (a) and qnegative $q\{350\}$ (b) regular pentagonal dodecahedrons

The following results were obtained:

(i) the existence of the corresponding crystal/quasicrystal polyhedrons in the family of pentagonal dodecahedrons is once more demonstrated;

(ii) the structural difference, in terms of interfacial angles, between a crystal and its corresponding quasicrystalline is very small (1.87°);

(iii) the corresponding polyhedrons: pentagonal dodecahedrons $\{530\}$ and qpentagonal dodecahedron, $q\{530\}$ are quasiidentical.

THE RHOMBIC-TRIACONTAHEDRON

The rhombic-triacontahedron is a polyhedron composed of 30 faces: 6 belong to the qcube: (100) ; $(\bar{1}00)$; (010) ; $(0\bar{1}0)$; (001) and $(00\bar{1})$, and 24 faces, respectively, belong to a quasicrystal $q\{hkl\}$ (Fig. 10).

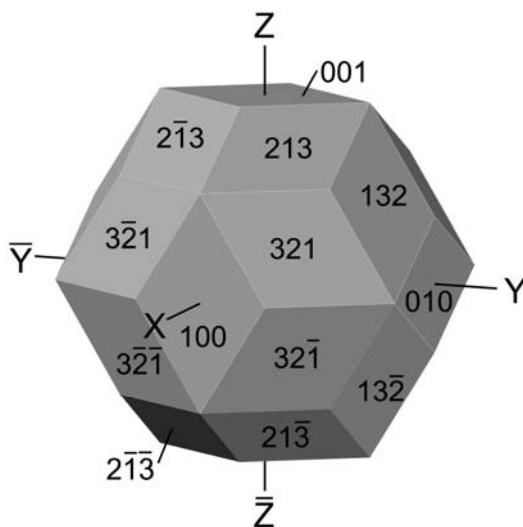


Fig. 10 – Miller indices of the rhombic triacontahedron faces.

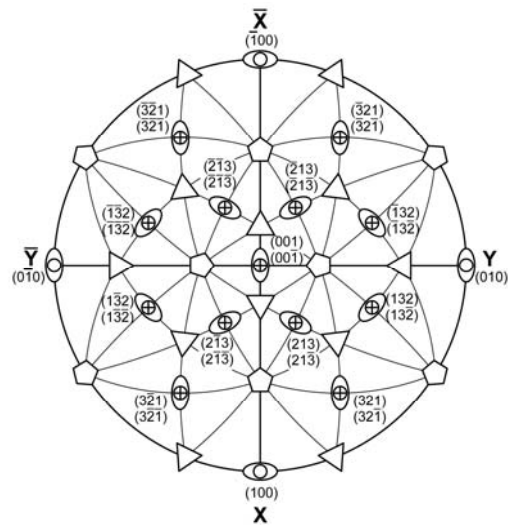


Fig. 11 – Stereogram of the rhombic triacontahedron.

The five-fold axis affects the cube in no way. However, this cube cannot exist as an independent polyhedron, but only in combination with another qcrystal. In the case of the triacontahedron, the qcube is combined with a qcrystal $\{hkl\}$ from the icosahedric system, which has 24 faces. The normals to these 24 faces coincide exactly with the two-fold symmetry axes. Two complementary methods are available for finding out the polyhedron to which these 24 faces belong, namely:

- (i) stereographic projection
- (ii) 3D drawing of the triacontahedron.

Figure 11 illustrates the stereographic projection of the triacontahedron; its 24 faces are stereographically projected in the very vicinity of the corresponding crystal, called diplohedron $\{321\}$, (at distances of only 1 degree). It results that the 24 faces of the triacontahedron belong to the diplohedron $\{321\}$.

The angle between the normals to the faces $(321)\wedge(3\bar{2}1) = 64.37^\circ$ was measured on the 3D drawing of the triacontahedron. In the case of the diplohedron $\{321\}$ crystal, this angle is 63.26° . The difference between the diplohedron crystal and the diplohedron quasicrystal is $64.37^\circ - 63.26^\circ = 1.11^\circ$. For the interfacial angle $(100)\wedge(321)$, the difference is only 0.43° . This method confirms once more that the 24 faces of the triacontahedron belong to the diplohedron $\{321\}$. The triacontahedron is a quasicrystal composed of a qcube $q\{100\}$ and a qdiplohedron $q\{321\}$. The triacontahedron is noted as $q\{100\}q\{321\}$. The difference registered between the diplohedron crystal $\{321\}$ and its corresponding form, quasicrystal $q\{321\}$ is 1 degree.

IMPLICATIONS

We have defined the icosahedric system (or quasicubic system) by its specific axial relation: $a \approx b \approx c$; $\alpha \approx \beta \approx \gamma \approx 90^\circ$. We have now the elementary cell of the icosahedric quasicrystals, named qc cell. The first implication is a more accurate determination of lattice parameters of icosahedric quasicrystals, avoiding to confuse them with a cubic one. The icosahedric system is a fundamental reference for all icosahedric materials, inorganic (metallic alloys) and organic (proteins and polymers).

Our new principle of corresponding crystal – to – quasicrystal introduces a new philosophy in these structural and morphologic transitions, from quasiperiodicity to periodicity and from polyhedron to quasipolyhedron. We can describe them by the new code: crystal – to – quasicrystal introduced in the present paper. Examples: cube – to – qcube; octahedron – to – qoctahedron; pentagonal dodecahedron – to – qregular pentagonal dodecahedron; diplohedron – to – qdiplohedron. Stereographic projection is a good instrument to evaluate morphological transition that means to express quantitatively the deformation of crystal – to – quasicrystal. The morphological transformations, in terms of interfacial angles, are:

- In the corresponding cube – to – qcube and octahedron – to – qoctahedron the deformation is zero;
- The irregular pentagonal dodecahedron $\{520\}$ is transformed into a regular pentagonal dodecahedron by a deformation of only 1.86° interfacial angle;
- The diplohedron $\{321\}$ is transformed into qdiplohedron $q\{321\}$ by a deformation of only 1.11° interfacial angle.

Furthermore, a quasicrystal seems to be the result of structural coexistence of periodic – to – quasiperiodic. Example: icosahedron is a coexistence between a qoctahedron (periodic) and a qpentagonal dodecahedron (quasiperiodic).

The icosahedral symmetry class has been defined by its specific symmetry formula $3L^2 12L^2 10L^3 6L^5 3P^2C$. The icosahedron, the regular pentagonal dodecahedron and the rhombic triacontahedron have been analysed: interfacial angles were measured on 3D drawing and stereographic projection along with geometrical calculation were performed. Surprising results and implications are of the following:

- cube and octahedron cannot exist alone as a simple quasicrystals
- icosahedron is not a simple quasipolyhedron; it is a combination of two simple quasipolyhedrons: the octahedron and the pentagonal dodecahedron;

- rhombic triacontahedron is a combination of a cube and a dodecahedron.

Miller indexing of quasicrystals is not satisfyingly solved at present. “Exact mathematical indexing of the faces of icosahedral convex polyhedra necessarily involves irrational numbers” (Loreto *et al.* 1990 p.176). The results of our investigation suggest the following new solutions:

- pentagonal quasicrystal structure and morphology are 3D;
- the standard scheme with six icosahedral base vectors seems to be not necessary, at least for pentagonal quasicrystals. The principle of corresponding crystal – to – quasicrystal allow us to note all the quasicrystal faces with only three Miller indices (hkl), in total agreement with the law of rational indices.

The validity of fundamental laws of crystallography for quasicrystals was proved.

Finally, we are going to ask the question “what is the relation between an icosahedral virus capsid and the orientation of Watson-Crick’s double helical DNA model inside a virus capsid?” Today we can only speculate that the angle of 36° between two adjacent two-fold axes of the icosahedron is exactly the angle of 36° of the right-handed rotation between base pairs that produces a double helix with 10 base pairs per turn. Moreover, $2 \times 36^\circ = 72^\circ$, the normal interfacial angle between the normals of two octahedron faces of the icosahedron.

ACKNOWLEDGMENTS

The authors thank Prof. Dr. Haino Uwe Kasper for his contribution to this paper and for useful discussions.

REFERENCES

- Boo, W. (1992), *An introduction to fullerene structures. Geometry and symmetry. Journal of Chemical Education*, **69**, 605–609.
- Branden, C., Tooze, J. (1991), *Introduction to protein structure*. 2nd ed., 410 p. Garland, New York.
- Cahn, J.W., Shechtman, D., Gratias, D. (1986), *Indexing of icosahedral quasiperiodic crystals. Journal of Materials Research*, **1**, 13–26.
- Chidambaram, R. (2004), *Cluster-disordered glue' model for icosahedral quasicrystals. Journal of Non-Crystalline Solids*, **334–335**, 68–70.
- Denton, A., Löwen, H. (1998), *Stability of colloidal quasicrystals. Physical Review Letters*, **81**, 469–472.
- Fischer, S., Exner, A., Zielske, K., Perlich, J., Deloudi, S., Steurer, W., Lindner, P., and Förster, S. (2011), *Colloidal quasicrystals with 12-fold and 18-fold diffraction symmetry. Proceedings of the National Academy of Science*, **108**, 1810–1814.
- Flint, E. (1971), *Essentials of crystallography*, 232 p. Mir Publishers, Moscow.
- Ford, W., E. (1958), *DANA'S Textbook of Mineralogy*, 4th ed., 851p. John Wiley and Sons, New York.
- Fowler, P.W., Myrvold, W. (2010), *Non-IPR fullerenes with properly closed shells. Physical Chemistry Chemical Physics*, **12**, 14822–14826.
- Fry, E., Logan, D., Stuart, D. (1996), *Virus crystallography*. In: C. Jones, B. Molloy, and M. Sanderson Eds., *Methods in Molecular Biology*, **56**, Crystallographic Methods and Protocols, 319–363. Humana Press Inc. Totowa, NJ.
- Grimm, U., Schreiber, M. (2005), *Electronic structure of quasicrystals*. In: G. Bassani, G. Liedl & P. Wyder (Eds.), *Encyclopedia of Condensed Matter Physics*. p. 95–100. Academic Press.
- Hayashida, K., Dotera, T., Takano, A., Matsushita, Y. (2007), *Polymeric quasicrystal: Mesoscopic quasicrystalline tiling in ABC star polymers. Physical Review Letters*, **98**, 195502–195505.
- Indelicato, G., Cermelli, P., Salthouse, D.G., Racca, S., Zanzotto, G., Twarock, R. (2012), *A crystallographic approach to structural transitions in icosahedral viruses. Journal of Mathematical Biology*, **64**, 745–773.
- Kelton, K.F., Lee, G.W., Gangopadhyay, A.K., Hyers, R.W., Rathz, T.J., Rogers, J.R., Robinson, M.B., Robinson, D.S. (2003), *First X-ray scattering studies on electrostatically levitated metallic liquids: demonstrated influence of local icosahedral order on the nucleation barrier. Physical Review Letters*, **90**, 195504–195507.
- Kroto, H.W., Heath, J.R., O'Brien, S.C., Curl, R.F., Smalley, R.E. (1985), *C 60: buckminsterfullerene. Nature*. **318**, 162–163.
- Lifshitz, R., Diamant, H. (2007), *Soft quasicrystals – Why are they stable? Philosophical Magazine*, **87**, 3021–3030.

- Liu, W., Köster, U., Zaluska, A. (1991), *Continues decomposition of icosahedral quasicrystals in Al-Cu-Fe alloys*. Physica Status Solidi (a), **126**, K9-K14
- Loreto, L., Farinato, R., Pappalardo, F. (1990), *Icosahedral symmetry, icosahedral polyhedra, and indexing methods*. In: L. Loreto & M. Ronchetti (Eds.), *Topics on contemporary crystallography and quasicrystals*. Special Issue of "Periodico di Mineralogia", **LIX**, 157–196.
- Mak, T.C., Zhou, G.D. (1993), *Crystallography in modern chemistry*. 1323 p. John Wiley and Sons, Inc., New York.
- Matthews, R.E.F. (1981), *Plant Virology*. 2nd ed., 1020 p. Academic Press, London.
- Rochal, S. (1997), *Theory of the crystal-quasicrystal phase transition and its applications to particular structures*. Crystallography Reports, **42**, 714–723.
- Rochal, S., Dmitriev, V., Lorman, V., Toledano, P. (1996), *Local mechanism for crystal-quasicrystal transformations*. Physics Letters A., **220**, 111–116.
- Rochal, S., Lorman, V. (2003), *Continuous defect-free structural transformation of long-range order from quasiperiodic to translational*. Physical Review B., **68**, 144203–144208.
- Sachdev, S., Nelson, D.R. (1985), *Order in metallic glasses and icosahedral crystals*. Physical Review B. **32**, 4592–4606.
- Savithri, H., Suryanarayana, S., Murthy, M. (1989), *Structure-function relationships of icosahedral plant viruses*. Archives of Virology, **109**, 153–172.
- Shechtman, D., Blech, I., Gratias, D., Cahn, J.W. (1984), *Metallic phase with long-range orientational order and no translational symmetry*. Physical Review Letters, **53**, 1951–1954.
- Steurer, W. (2000), *Geometry of quasicrystal-to-crystal transformations*. Materials Science and Engineering: A. **294**, 268–271.
- Steurer, W., Deloudi, S. (2009) *Crystallography of Quasicrystals*. 384 p. Springer-Verlag Berlin Heidelberg.
- Steinhardt, P.J. (1996), *New perspectives on forbidden symmetries, quasicrystals, and Penrose tilings*. Proceedings of the National Academy of Science, **93**, 14267–14270.
- Talapin, D.V., Shevchenko, E.V., Bodnarchuk, M.I., Ye, X., Chen, J., Murray, C.B. (2009), *Quasicrystalline order in self-assembled binary nanoparticle superlattices*. Nature, **461**, 964–967.
- Weeks, D.E., Harter, W.G. (1989), *Rotation–vibration spectra of icosahedral molecules. II. Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene*. The Journal of Chemical Physics, **90**, 4744–4771.
- Zeng, X., Ungar, G., Liu, Y., Percec, V., Dulcey, A.E., Hobbs, J.K. (2004), *Supramolecular dendritic liquid quasicrystals*. Nature, **428**, 157–160.

