Abstract
The structures of virus particles are modelled with new finite periodic functions in spherical space. Two kinds of functions, one with a dodecahedral symmetry code and another with icosahedral, are used to describe several virus capsids. As the functions are periodic we can also forecast the inside of a capsid. In two cases we have been successful.

An accurate polyhedral description of the capsids of the groups of HIV, polioviruses and the adeno-associated virus (AAV-2) is obtained with the snub dodecahedron. While the polio and the HIV viruses are having the same chirality’s, the (AAV-2) virus is having the opposite.

The relationships between stellation and capsid structures are demonstrated by the HIV, (AAV-2) and polio group of viruses having related morphology with the final stellation of the icosahedron.

Capsid structures are accurately and simply related via the ordinary crystallographic rotation and umbrella operations.

Capsid structures seem to be related to the minimal surfaces. Relationships between capsids can be described as isometric transformations.

Icosahedral alloy structures are described with the same mathematical concept with the two kinds of symmetry codes as the capsids.

1 Introduction

Recently we described the stellations of the dodecahedron and the icosahedron as examples of new finite periodicity in a spherical space(1). This was extended also in a recent article with a radial periodicity in form of a new periodic function in order to make complete structures for the dodecahedral space(2).

Another way to say it is that the stellations give a structure on the spherical surface. The radial periodicity as defined below means that we go to concentric spheres on which the radial periodicities give new structures. They are given by the new periodicity and are not related by simple dilatation.

We now also wish to continue with the icosahedral case in spherical space. The background of this is our finding that the structure of a virus particle may be periodic.

2 Background to the radial spherical finite periodicities and symmetry codes

A number of GD (Gauss distribution) terms as added together with a proper constant give the new periodicity. It was first developed to describe the Larsson cubosomes(3,4). One term consists of two infinite planes in space, two terms give four planes that collaborate to form a cylinder, and with three there is a sphere as in eq 2.1. These properties of the GD function in space are the backbone to the 2D periodic properties around the sphere. And the radial periodicity in 3D space completing a finite spherical periodicity, which we will find very useful for structure descriptions. The equations in 2.1 and 2.2 define the periodicities.
Equation 2.1 is of the type used to describe the stellations that give excellent examples of spherical periodicity, as for the final stellation of the icosahedron. With $\delta$ this function in 2.2 is now growing radially in space in a true periodic, and also finite manner. The $\delta$ : $s$ must take the same value in $x$, $y$, $z$ as stepwise increasing radius for the spherical periodicity. So the motion has 3-fold symmetry. In a cube you have four diagonals of such symmetry and in the dodecahedron there are ten. And the motion give now the 3D periodicity as said above. The general 3D radial periodicity is elliptic and we will handle this special case of 3D radial periodicity that is spherical. The elliptic periodicity is easily developed within group theory, and we hope to do so in a forthcoming article.

There are a few simple permutations in space that occur in one form or another in the groups (5), which we call symmetry codes (2). The general positions in the cubic point groups were derived from permutations of variables or the faces from crystals that have been beautifully described in Shubnikov’s book(6). We have shown how to derive exponential functions for these crystal shapes using these general positions(7). And in that way we have calculated the shape of every Shubnikov polyhedron(7).

In analogy we derive the crystal shapes for the dodecahedron and the icosahedron just using the equations for their faces added up on exponential level. Just as we have done with all the cubic point groups(7).

It must be kept in mind that in this study we have only used the simplest polyhedra of five fold symmetry in the symmetry codes. According to Coxeter there are 57 more(16).

The symmetry codes on the exponential scale and used here to make shapes or polyhedra, which after the crystallographic jargon are: cube, rhombic dodecahedron, diamond, octahedron, dodecahedron and the icosahedron. Using GD terms and the new periodicity we shall give detailed examples of the dodecahedral and icosahedral structures here. But we shall first give a short description of the simplest of all, the cube and its spherical periodicity to make you acquainted with this space.

3 Primitive cubic

We start with a simple permutation in space using the position in 6e of for example Pm3m, with the first symmetry code.

$x,0,0; 0,x,0; 0,0,x; -x,0,0; 0,-x,0; 0,0,-x$

And exponentially it becomes

\[ e^x + e^y + e^z + e^{-x} + e^{-y} + e^{-z} = \text{const} \]

Which is a cube as in fig 3.1.
Fig 3.1a. Cube
The equation for the polyhedron in 3.1 is empty, it is just bending planes.
With the GD function the mathematics become rich and we get the hyperbolics or the
stellations, and possibility to periodicity in equation 3.2. The graph is in fig 3.1b.

\[ e^{-x^2} + e^{-y^2} + e^{-z^2} = 2 \]  \hspace{1cm} (3.2)

Fig 3.1b. Hyperbolic octahedron.

We now write periodic functions with the GD function after 2.2, which are finite. As crystals
are of finite periodicity. So we write in eq 3.3 a function with only three terms diagonally that
gives 27 bodies in fig 3.2a.

\[ e^{-x^2} + e^{-y^2} + e^{-z^2} + e^{-(x-2)^2} + e^{-(y-2)^2} + e^{-(z-2)^2} + e^{-(x+2)^2} + e^{-(y+2)^2} + e^{-(z+2)^2} = 2.65 \]  \hspace{1cm} (3.3)

The equation 3.4 contains seven terms, which due to the properties of true periodicity give
343 bodies in fig 3.2b. But the equation itself is a summation and can be written in
Mathematica language as in eq 3.5 below, which of course also gives fig 3.2b.

\[ e^{-x^2} + e^{-y^2} + e^{-z^2} + e^{-(x-2)^2} + e^{-(y-2)^2} + e^{-(z-2)^2} + e^{-(x+2)^2} + e^{-(y+2)^2} + e^{-(z+2)^2} = 2.65 \]  \hspace{1cm} (3.4)

\[ \sum_{i,j,k} a_{ijk} e^{-(x-i)^2} + e^{-(y-j)^2} + e^{-(z-k)^2} = \text{2.65} \]  \hspace{1cm} (3.5)
\[ e^{-x^2} + e^{-y^2} + e^{-z^2} + e^{-(x-2)^2} + e^{-(y-2)^2} + e^{-(z-2)^2} + \\
+ e^{-(x-4)^2} + e^{-(y-4)^2} + e^{-(z-4)^2} + e^{-(x-6)^2} + e^{-(y-6)^2} + e^{-(z-6)^2} + \\
+ e^{-(x+2)^2} + e^{-(y+2)^2} + e^{-(z+2)^2} + e^{-(x+4)^2} + e^{-(y+4)^2} + e^{-(z+4)^2} + \\
+ e^{-(x+6)^2} + e^{-(y+6)^2} + e^{-(z+6)^2} \]

\[ = 2.78 \]

\[ \text{Sum}[e^{-(x-n)^2} + e^{-(y-n)^2} + e^{-(z-n)^2}, \{n, 6, -6, -2\}] = 2.75 \]

3.4

The Mathematica script used follows as below:

\[ \text{Sum}[f, \{n, n_{\text{min}}, n_{\text{max}}, \text{di}\}] \]

the sum with \( n \) increasing in steps of \( \text{di} \), \( n_{\text{min}} \) and \( n_{\text{max}} \)

we often call \( m \) in the text.

This is of course identical with using \( \Sigma \).

3.5

---

**Fig 3.2a** Three terms in eq 3.3 form a small crystal.

**b** Bigger crystal from seven terms in eq 3.4. Or \( m=6 \) in eq 3.5.

With proper choice of constant and terms in summation we can make a ‘virus skin’, and a structure inside as in Figs 3.3. After equation 3.5.

\[ \text{Sum}[e^{-(x-n)^2} + e^{-(y-n)^2} + e^{-(z-n)^2}, \{n, 1.5, -1.5, -1.5\}] = 3.441 = 0 \]

3.5
Duality is established between points and planes, lines and lines(15). The dodecahedron has 12 faces, 20 vertices and 30 lines and the corresponding figures for the icosahedron are 20 faces, 12 vertices and 30 lines. So if you have 12 points at the centres of the faces of a dodecahedron, you have the corner points of an icosahedron. In a way they are identical, which causes some problems of identification. But in this study we have symmetry codes that describe the faces, and in that way the structures of the two polyhedra. Which then are completely different. As the symmetry codes are.

With pentagonal symmetry in spherical space follows whatever size with m in the summation, a structure, or a crystal, or a capsid coming out with one set of points with 5 fold axes, one set of points with 3 fold axes, and one set of points with 2 fold axes. The crystal just grows bigger and bigger, and between the special point positions structure starts to grow. With periodicity comes that structure units are radially repeated with m under the pretext that the new structure is built on the structure for lower m. These special positions always give you a regular dodecahedron, or a regular icosahedron, whatever you like.

In the regions of structure between the special positions for lower m we find simple polyhedra like the icosidodecahedron, the truncated icosahedron, the rhombicosidodecahedron, and the snub dodecahedron(model shown below). Giving structures we can use to describe capsids. The last three can under crystallographic umbrella and rotation operations(11) transform into each other. Of these three the snub dodecahedron seems to be the most common among the groups of virus we have studied. The polyhedron is chiral and both the forms seem to occur among capsids.

When applying this in space with δ, 3D finite periodicity will give a structural content to the calculated inside of the capsid. This is of course of great interest to discuss. We note that for a capsid there is a centre that for some value for the constant has a local icosahedral structure, which with the constant transforms into a small local dodecahedron. And vice versa. This we shall discuss.

With δ we use m in the Sum formula below. For virus m is naturally small, for crystals in metallurgy m is very much higher. And it is true for both that the structures for different m:s are different. And we say they are different crystals. This is obvious and natural for virus, but indeed crystals of this symmetry of different sizes in metallurgy also have different structures. In the way we are used to define the word different.
In order to illuminate structure and symmetry for circular geometry, we show a small pentagon. The equation in 4.1a is from adding lines on the exponential scale. This is the same as given in (10) for the general case of any polygon. Pentagonal structures are derived from lines and symmetry codes as for 3D, and we give the equation for periodicity below in 4.1b. The ten fold rotation symmetry is obvious, with all the radial mirror planes. The m:s are=5, or 10 for crystals in fig 4.1b and in c, and the structure looks exactly like the diffraction pattern of an icosahedral alloy crystal from metallurgy.

\[
\sum \left( e^{(\pi x/2+y/2)^3} + e^{(\pi x/2-y/2)^3} + e^{(\pi x/2+y/2)^3} + e^{(\pi x/2-y/2)^3} + e^{(\pi x/2+y/2)^3} \right) = 10^4
\]

\[
4.1a
\]

We derive the equation for structure in 4.1b:

\[
\sum_{n, m, -m, -}\left( e^{-x^4} + e^{-\left(\pi x/2+y/2\right)^4} + e^{-\left(\pi x/2-y/2\right)^4} + e^{-\left(\pi x/2+y/2\right)^4} + e^{-\left(\pi x/2-y/2\right)^4} \right) = 0
\]

\[
4.1b
\]

And we give two examples below on finite periodic pentagonal structures in circular space.

Fig 4.1a

Fig 4.1b Calculated capsid(m=5). c m=10
The question arises: Where is the similarity? Which we are used to from translation where similarity is obvious - the unit cell is an example. But also the glide and the twist. But not allowed here. We are left with rotation or reflection as similarity.

So the similarity in 2D is kept on by rotating, or reflecting pentagons over the edges exactly as Jacob did to arrive at his model of the quasicrystal(8,9). A Fourier transform of his experiment using 290 pentagons agrees perfectly well with common diffraction patterns of icosahedral alloy crystals (9). Our model as derived from the finite new spherical periodicity and shown in figs 4.b and c agrees perfectly well with Jacob’s transform.

So there are the results in pictures, different in size as well as structure. They look complicated to us but they are not in mathematics, in the rotational manners they are generated. Every position is special as generated by regular pentagons. It is when you get positions inside the pentagons things become more general and complicated. We shall study a couple of cases that occur below for virus structures.

We shall in the following study the inside of a calculated capsid, whenever we find it motivated.

**Motion in calculated capsid structures.**

The first motions are crystallographic and involve one umbrella operation and one rotation operation(11). Both are used to bring a structure into a more regular arrangement, as example a polyhedron. Or to relate or transform two different capsids with or into each other. Examples are the pariacoto and the HIV virus structures as shown below.

In the comparison of an observed capsid and a calculated capsid, and the content, there are two principle motions we see in the calculated case. Sometime the globules of an inner layer have formed catenoids with the capsid – we call that invaginations of the capsid. Or the other way around the globule may have generated from an invagination.

**Dodecahedral virus structures**

We take the dodecahedral case as the first example of this new periodicity in 3D and pentagonal symmetry. First we show the polyhedron and its equation that gives us the symmetry code. The exponential equation 4.1c, contains the planes that build the polyhedron in fig 4.1d.

\[
\begin{align*}
    e^{(x+\tau y)} + e^{(x-\tau y)} + e^{(y+\tau z)} + e^{(y-\tau z)} + e^{(z+\tau x)} + e^{(z-\tau x)} + \\
    e^{-(x+\tau y)} + e^{-(x-\tau y)} + e^{-(y+\tau z)} + e^{-(y-\tau z)} + e^{-(z+\tau x)} + e^{-(z-\tau x)} &= 10^{13}
\end{align*}
\]

4.1c

Fig 4.1d The planes from eq 4.1a bend over and form the dodecahedron.

The great stellated dodecahedron has its equation in 4.1d.
\[10^{-(\tau x + y)} + 10^{-(\tau x + y)} + 10^{-(\tau y + z)} + 10^{-(\tau y + z)} + 10^{-(\tau z + x)} + 10^{-(\tau z + x)} = \frac{5}{2}\]

The spherical geometry contains all the symmetry elements with the 2, 3 and 5 fold axes of rotation in the description of structures. And the mirror planes. So we write the symmetry code for the dodecahedron in analogy with the cubic as given before:

\[x, \tau x, 0; \quad 0, x, \tau x; \quad \tau x, 0, x; \quad 0, x, -\tau x; \quad -\tau x, 0, x; \quad -x, -\tau x, 0; \quad 0, -x, -\tau x; \quad -\tau x, 0, -x; \quad 0, -x, \tau x; \quad \tau x, 0, -x;\]

And we move into this space with the summation in 4.1e.

\[
\sum_{e} [e^{-x+\tau y-n)^2} + e^{-(x-\tau y-n)^2} + e^{-(y+\tau z-n)^2} + e^{-(y-\tau z-n)^2} + e^{-(z+\tau x-n)^2} + e^{-(z-\tau x-n)^2}], \quad \text{4.1e}
\]

\{n, m, -m, -n\} - const = 0

There are strong relations between stellations of polyhedra and the capsid structures. They show up for lower constants in the summations below and here we just give one of the most beautiful in form of the great stellated dodecahedron in fig 4.1e(1).

In \(f\) for \(m=1\) as a start we show the dodecahedron, strongly related to the icosidodecahedron. For both, the spherical translation is obvious.

\[\text{Fig 4.1e. The great stellated dodecahedron} \quad f \quad m=1, \text{ const } = 6.55\]

Eq. in 4.1d

Before we continue we reveal the use of a very remarkable database:

\[\text{For all the informations used below we acknowledge the Viper data base(12):}\]

The first virus for us is Bacteriophage alpha3 as shown in fig 4.2a.

**Structural Studies of Bacteriophage alpha3 Assembly**


**Cryo-EM Structure**

T=3

For $m=2$ in equation 4.2, and a constant of 6.5 we have the calculated capsid in fig 4.2b. The morphology between a and b is identical as is obvious by identifying the 5 and 3 fold axes. The polyhedron in b is the icosidodecahedron, which also is found for the capsid.

![Fig 4.2a Bacteriophage alpha3](image1)

![m=2 Icosidodecahedron](image2)

X-ray crystallographic structure of the Norwalk virus capsid


$a = 605.74$, $b = 605.74$, $c = 466.71$, $\alpha = 90$, $\beta = 90$, $\gamma = 90$

T=3

The capsid morphology seems to be close to that of an icosahedral but as there is good general agreement between the Norwalk virus and the calculated dodecahedral picture we include it here. Some umbrella, and rotation operations are needed. For the structure of tomato bushy
stunt virus the similarity with the calculated capsid is even closer.

At the constant there is an icosahedral structure in the centre, which at 6.65 has transformed to a dodecahedron.

![Fig 4.2.c The Norwalk virus](image)

**4.2d** m=3 Const=6.55 Some rotation and umbrella motion is required.

New equation (exponent =4)

\[
\text{Sum} \left[ e^{-(x+\tau y-n)^4} + e^{-(x-\tau y-n)^4} + e^{-(y+\tau z-n)^4} + e^{-(y-\tau z-n)^4} + e^{-(z+\tau x-n)^4} + e^{-(z-\tau x-n)^4} \right]_{\{n, m\tau, -m\tau, -\tau\}} = \text{const} = 0
\]

Host range and variability of calcium binding by surface loops in the capsids of canine and feline paroviruses.


\[
a = 267.563, \ b = 268.446, \ c = 274.328, \ \alpha = 61.946, \ \beta = 62.616, \ \gamma = 60.186
\]

**T=1**

Topologically there is very good agreement, the two structures are relatively simple. Could easily be regarded as the archetype for the rhombicosidodecahedron. With some small rotation the snub dodecahedron is obtained as obvious in fig 4.3a. See below for descriptions of rotations.
The structure of pariacoto virus reveals a dodecahedral cage of duplex RNA.

$$a = 329.332, \ b = 346.944, \ c = 424.893, \ \alpha = 90, \ \beta = 90.83, \ \gamma = 90$$

$T=3$

This is an example of a more advanced morphology. If the pikes in fig 4.4 b, marked with white dots, are taken away, figs 4.4a and b show remarkable similarity between observed and calculated morphologies. Remarkable is that the calculated shape deviates from the regular polyhedron(the truncated icosahedron) exactly as the virus capsid does. The pikes are in the 3 fold axes and mark the complete dodecahedron.
Inside the capsid Tang et al found a dodecahedral cage of RNA duplex as shown from electron densities. We strongly recommend our readers to study this very beautiful original work.
‘The capsid exerts reciprocal influences over the three-dimensional arrangement of the viral RNAs’ (directly from Tang et al).
We describe this with the new periodicity below.

4.4a Pariacoto virus

b m=2 const =6.45
Our periodic function forecasts a dodecahedral structure inside the calculated capsid in 4.4b. Which is shown in a split picture in 4.4c. This dodecahedral structure is in fact an icosidodecahedron, which of course is closely related to the dodecahedron. Indeed the whole picture of the structure determination by Tang et al is in remarkable agreement with the calculated capsid with its content.

A simple umbrella distortion operating on the 5 fold axis transforms this morphology into that of the truncated icosahedron.

To this we may add that there are two kinds of invaginations in the calculated capsid. One, which comes from the centres of the 2 fold axes forms an icosidodecahedron, the other comes from the 5 fold centres and form an icosahedron. These are regular polyhedra.

The central dodecahedral structure is stable up to a constant of 6.65, where it starts to transforms to an icosahedral structure.

Structure of poliovirus type 2 Lansing complexed with antiviral agent SCH48973: comparison of the structural and biological properties of three poliovirus serotypes.
a = 345.7, b = 497.2, c = 485.9, α = 90, β = 90, γ = 90
T Number: pT3
Above in 4.4c we show Poliovirus type 2 with only a small angle of rotation away from the truncated icosahedron, or the capsid structure of the pariacoto virus above. The structure is towards the snub dodecahedron type with the same chirality as for HIV below.

Finally we wish to say that with the same formula, equation 4.2, and with increasing m we obtain shapes that look more and more dodecahedral, and are approaching structures in metallurgy. At m=80 τ and fig 4.5 we compare a calculated dodecahedron with one natural made as an aluminium alloy in Professor A.P. Tsai’s laboratory in Sendai(13).

![Icosahedral virus structures](image)

Fig 4.5a m=129.44 or 80τ, Content about 1000 bodies.

b Real dodecahedron Bulk Al65Cu20Fe15 annealed at 845°C for 48hrs. From Prof. A.P. Tsai(13) Tohoku University

### 5 Icosahedral virus structures

The icosahedral planes give the first equation in 5.1a which gives the icosahedron in Fig 5.1a.

\[
e^{(x+y^2)} + e^{(-x+y^2)} + e^{(y+z^2)} + e^{(-y+z^2)} + e^{(z+x^2)} + e^{(-z+x^2)} + e^{((x+y+z)^2)} + e^{((x-y-z)^2)} + e^{((-x+y+z)^2)} + e^{((-x-y-z)^2)} = 10^{13}
\]

\[5.1a\]
Fig 5.1a. Icosahedron after 5.1a.

5.1b The final stellation of the icosahedron, equation in 5.1b. Same morphology as for the HIV virus below.

And the equation for the final stellation of the icosahedron is in 5.1b.

\[
10^{-10(x+\tau^2 y)^2} + 10^{-10(x+\tau^2 y)^2} + 10^{-10(y+\tau^2 z)^2} + 10^{-10(y+\tau^2 z)^2} + 10^{10(z+\tau^2 x)^2} + 10^{10(z+\tau^2 x)^2} + 10^{10(-x+\tau^2 y)^2} + 10^{10(-x+\tau^2 y)^2} + 10^{10(-y+\tau^2 z)^2} + 10^{10(-y+\tau^2 z)^2} + 10^{10(-z+\tau^2 x)^2} + 10^{10(-z+\tau^2 x)^2} + 10^{10(-x-y)^2} + 10^{10(-x-y)^2} + 10^{10(-x-z)^2} + 10^{10(-x-z)^2} = 5/2
\]

We write the symmetry code:

\[
\begin{align*}
&x, \tau^2 x, 0; \quad 0, x, \tau^2 x, 0, x; \quad x, -\tau^2 x, 0, x; \quad 0, x, -\tau^2 x, 0, x; \\
&-\tau x, -\tau x, x; \quad x, -\tau x, -\tau x; \quad -\tau x, -\tau x, x; \quad \tau x, \tau x, \tau x;
\end{align*}
\]

5.2

From the symmetry code we formulate the equation for icosahedral periodicity:

\[
\text{Sum}[e^{-10(x+\tau^2 y)^2} + e^{-10(x+\tau^2 y)^2} + e^{-10(y+\tau^2 z)^2} + e^{-10(y+\tau^2 z)^2} + e^{10(z+\tau^2 x)^2} + e^{10(z+\tau^2 x)^2} + e^{10(-x+\tau^2 y)^2} + e^{10(-x+\tau^2 y)^2} + e^{10(-y+\tau^2 z)^2} + e^{10(-y+\tau^2 z)^2} + e^{10(-z+\tau^2 x)^2} + e^{10(-z+\tau^2 x)^2} + e^{10(-x-y)^2} + e^{10(-x-y)^2} + e^{10(-x-z)^2} + e^{10(-x-z)^2}, \\
\{n, m, -m, -n\} - \text{const} = 0
\]

Our first icosahedral virus is an adenovirus:

**The structure of the human adenovirus 2 penton**


\[a = 435.984, \quad b = 300.168, \quad c = 420.621, \quad \alpha = 90, \quad \beta = 104.36, \quad \gamma = 90\]

With this ‘simple virus’ we realize that a small rotation around the 5 fold axis of the yellow-green groups in fig 5.1a makes the structure like the icosahedral in fig 5.1b. Or more advanced-
this is really the archetype for the snub dodecahedron and the chirality is the same as for the adeno-associated virus (AAV-2) below.

Structural fingerprinting: subgrouping of comoviruses by structural studies of red clover mottle virus to 2.4-A resolution and comparisons with other comoviruses

T Number:
pT3

a = 332.07, b = 303.87, c = 314.31, α = 90, β = 90, γ = 90  I 222

Considering what is ‘sticking out’ in the virus is ‘sticking in’ for the calculated capsid the similarity is excellent.
We show the beautiful inside below in 5.2d. At a change of constant the dodecahedron in 5.2d has opened catenoidic contacts with invaginations from the capsid in 5.2c. Which also we describe as a bigger dodecahedron.

5.2d Const =10.84. e Magnification of dodecahedron, Const = 10.86


a = 414.2, b = 414.2, c = 263, α = 90, β = 90, γ = 120

T=1
So far in the calculations with the periodicity for \( m=1 \) we have for the inside one structure, for \( m=2 \) we have two structures. To this we add an example for \( m=3 \), the virus is this bacteriophage G4.

We show a calculated example of the inside for bacteriophage G4 below in 5.3c. The inner dodecahedron is easy to trace, next comes a bigger dodecahedron and the last one is a big icosahedron, marked with white dots, capping the big dodecahedron to one structure.

At slightly higher constant, 10.95, the inner smaller dodecahedron is dissolved and the globules from the big icosahedron have catenoid contacts and form a complex of 32 globules, a complex that is also joint with catenoids to the capsid. This is a beautiful example of duality; the 12 corners of the icosahedron are sitting on the 12 faces of the dodecahedron, to one structure!

![Diagram](image)

**Fig 5.3c** Calculated capsid, \( m=3 \), with periodic content for Bacteriophage G4, \( \text{const} = 10.845 \). Rectangles are an icosahedron which are capping a big dodecahedron to one structure. Note the inner dodecahedron, which is surrounded by a bigger dodecahedron. As in 5.2d and e for \( m=2 \)

**New equation (exponent =4)**

\[
\sum \left[ e^{-\left(x+\tau y-z\right) n} + e^{-\left(-x+\tau y+z\right) n} + e^{-\left(y+\tau z-x\right) n} + e^{-\left(-y+\tau z+x\right) n} + e^{-\left(z+\tau x-y\right) n} + e^{-\left(-z+\tau x+y\right) n} + e^{-\left(x+y+z\right) n} + e^{-\left(-x+y-z\right) n} \right] = 0
\]

\( \{n, m\tau, -m\tau, -\tau\} \) - \( \text{const} = 0 \)

**m=1**

**The crystallographic structure of brome mosaic virus.**


\( a = 269.244 \), \( b = 269.244 \), \( c = 638.136 \), \( \alpha = 90 \), \( \beta = 90 \), \( \gamma = 120 \)

\( T=3 \)

See also Turnip yellow Mosaic Virus

This beautiful structure in fig 5.4a has also been given a simple calculated capsid in 5.4b.
Fig 5.4a Brome mosaic virus

b m=1 const =10.45. The polyhedron is the first stellation of the icosahedron called the triakis icosahedron and is related to the rhombic triacontrahedron.

5.4c m=1, const=11.53.

The dodecahedron of small globules inside from 5.4b collaborates with the skin of capsid and give the polyhedron, the icosidodecahedron, with an interesting double hull in fig 5.4c. The holes in 3 fold axes have a correspondence in the real virus in 5.4.a

Next we describe the important HIV and AAV-2 viruses

Crystal Structure of a Human Rhinovirus that Displays Part of the HIV-1 V3 Loop and Induces Neutralizing Antibodies against HIV-1
\(a = 318.9, b = 349.3, c = 368.4, \alpha = 90, \beta = 90, \gamma = 90\)

T Number: \(pT3\)

Shown in fig 5a.

**Morphogenesis and morphology of HIV, Structure-function relations,**
**Gelderblom et al.**

Shown in fig 5.5g

The atomic structure of adeno-associated virus (AAV-2), a vector for human gene therapy.

Xie, Q., Bu, W., Bhatia, S., Hare, J., Somasundaram, T., Azzi, A. & Chapman, M.S.  

\(a = 249.69, b = 249.69, c = 644.76, \alpha = 90, \beta = 101.16, \gamma = 120\)

T=I

Shown in fig 5.5c

Again we realize we need to carry out a crystallographic operation to make the calculated capsid in fig 5.5b look like the calculated structure (close to the rhombicosidodecahedron). This is shown with white rectangles in figs 5.5a and b.

![Fig 5.5a.HIV virus.](image)

Rotations around two 5 fold axes give the distribution of squares as in b.  

5.5b m=2, const =10.9

However the HIV capsid is very similar as it is to the snub dodecahedron, which is shown in fig 5.5c and d. Clockwise-rotation of the pentagons brings you over to the other chiral form seen in fig 5.5f. In practice you perform this operation by cutting out the triangles, do the rotations and put the triangles back into their new positions. This manipulation is also needed for the rotations discussed below.
Fig 5.5c HIV capsid somewhat rotated.

The mirror form of the snub dodecahedron is shown in fig 5.5.f and it is in excellent agreement with the AAV-2 virus capsid in fig 5.5.e.

Anti-clockwise and clockwise rotations in the capsid of the AAV virus in fig 5.5e of a few degrees around the 5 fold axis with five small yellow bodies give morphologies as in the rhombicosidodecahedron and the truncated icosahedron. And relations with the pariacoto virus as discussed above.

Fig 5.5 e The adeno-associated virus (AAV-2). The agreement with the snub dodecahedron in f is excellent.

Fig 5.5f The snub dodecahedron.
5.5 g The rotation operations are easily realized in this picture of the HIV virus.

The groups of three rings inside each triangle in the HIV picture in fig 5.5g (Russell Kightley Media, see above) correspond to the 60 pikes in the final stellation of the icosahedron in fig 5.1b.

We now wish to show a part of the inside of the calculated capsid from fig 5.5b. There is a dodecahedron in fig 5.5h connected to globules at a constant of 11.3, which is decomposed to an icosahedral structure at 10.8, in fig 5.5i.

This is an example of higher periodicity and according to this we have inside the capsid two different structures. This we compare with our last example, which is about an AAV virus in a report from Bettina Böttcher (14). There are two kinds of globules in 5.5j, which is an open view of fig 5.5b. We have localized some of them with squares to form an icosahedron(m=1), and the rest, close to or in contact with the capsid(m=2), form an icosidodecahedron, a polyhedron we have given in fig 5.4 c. Böttcher says there is ‘an intimate contact between globules and genome’(Figure 2 in her article).
In fig 5.5k at higher const the bodies from the icosidodahedron have opened catenoids with the capsid, and also with the bodies from the icosahedron. The centre is becoming dodecahedral as also was shown in fig 5.5h. We propose that this describes what is related to an exposure of PL (phospholipids domain), as said by Böttcher, which also according to her is linked to the disappearance of the globules at inside of the capsid.

Fig 5.5j const 10.75
Fig 5.5k const 11.0

The same morphology is also present in the bacteriophage P2 virus.

Finally we wish to say that with the same formula, equation 5.3, and with increasing m we obtain shapes that look more and more icosahedral as shown in fig 5.6a. This is compared with an aluminium alloy from Professor A.P. Tsai’s laboratory in Sendai (13). Tsai’s etch picture is about 10 microns.

5.6a From equation 5.3, with m=40 tau, const=10.8.

b Etch picture from surface of 5-fold plane of an AlPdMn single quasicrystal. From Prof. A.P. Tsai (13) Tohoku University
6. Some final remarks. The snub dodecahedron and the minimal surfaces.

We have described the relations of the viruses’ pariacoto, HIV and AAV-2, and their relations to other virus morphologies via the crystallographic rotation and umbrella motions(11). We wish to conclude describing these motions in spherical geometry. Take an icosahedron and mark the centres of each of the 20 triangles. These centres are now the corners of the dual dodecahedron. Still on the icosahedron you make new five rings, smaller, by marking their corners halfway to the five fold corner of the icosahedron. The polyhedron is the rhombicosidodecahedron. And the small five rings in each dual dodecahedral face form the sixty pikes in the final stellation of the icosahedron in fig 5.1.

Next construction is to rotate the inner, smaller pentagon 30 degrees so that its corners sit on the icosahedral edges. The polyhedron created is the truncated icosahedron. We realize we have produced the morphologies of the capsids of the HIV, AAV-2 and pariacoto viruses. And all the related viruses are obtained by various degrees of rotation and umbrella distortions. This is all simply realized from the description of HIV given in fig 5.5.g.

Another way to this is to consider that these transformations are contained in the rotation of pentagons in the snub dodecahedron in order to go from one of its chiral forms to the other. An important aspect is to consider the curvature of the surface of a capsid and to the belonging calculated surface. A polyhedron like a dodecahedron has positive Gaussian curvature, while its calculated capsid with their bodies in a sort of stellated positions has mainly negative Gaussian curvature. We give an example from fig 5.a, the human adenovirus, with its calculated capsid, which consists of 12 spheres fused together in fig 6.1a.

Fig 6.1a m=1

b Adenovirus 2 again.

Fig 6.1c The FRD minimal surface
We realize that the surface in 6.1a is formed from catenoids between the spheres when they approach each other. The surface is close to a minimal surface, and as the geometry is close to that of the virus capsid, the blue region 6.1b must also be close to a minimal surface. The spheres in 6.1a are really pentagonal, which is even clearer for the buttons that form the boundaries for the capsid. If the pentagonal spheres are slightly rotated we see that the pentagonal corners form triangles between themselves. And we clearly have the case for the adenovirus; the whole capsid has become a snub dodecahedron in fig 6.1b. We have obtained a chiral geometry for the capsid, and the blue surface must also be chiral due to this rotation. Physically this is very similar to a real minimal surface we show in fig 6.1c, which is called the FRD(17). Which is periodic and corresponds to cubic close packing of spheres in Euclidean space. Which has 12 catenoids or openings. This is also the case for the capsid or the structure in 6.1a, but in a pentagonal space. And in that way occupy a smaller volume. With unit edge the volume for the cubeoctahedron is 2.36, and for the icosahedron it is 2.18.

In differential geometry surfaces related via Bonnet transitions are isometric which physically means no cost of energy. Indeed it is tempting to assume that the rotations here are isometric. But in these cases we merely see this as a geometrical method to discuss similarities between capsid structures. As no such transformations have been reported.

It seems to us that most of the capsids discussed in this article can be described with surfaces having negative Gaussian curvature, and be related to minimal surfaces. We shall continue this part of the study.

We finally wish to say that already at m=5 we clearly see two cases of crystals, the icosahedral structure for m=5, and the dodecahedral also for m=5 in fig 6.2. Instead of unit cells, we say we have crystals, one for each m in the new periodicity. The building principles are planes that keep on adding to each other, which we described in ref 2. It is here easy to realize that the shapes now are coming like in metallurgy for much higher m. In fig 6.2a you see the corners of 5 fold symmetry in a regular icosahedron, while in b the corners have 3 fold symmetry in a regular dodecahedron. On the other hand, peeling off these layers, one by one, or going down in m and crystal size, we come to the virus structures. In this exercise in spherical geometry.

Fig 6.2a m=5 Icosahedral structure                     b m=5 Dodecahedral structure

Acknowledgement

I thank professor Kåre Larsson for excellent discussions.
References

1 S. Andersson [www.sandforsk.se](http://www.sandforsk.se), Stellations, compounds, periodicity and the exponential scale, November, 2004.


7 S. Andersson [www.sandforsk.se](http://www.sandforsk.se), Group and Structure, chap 8, Living book.


12 **Viper data base**


