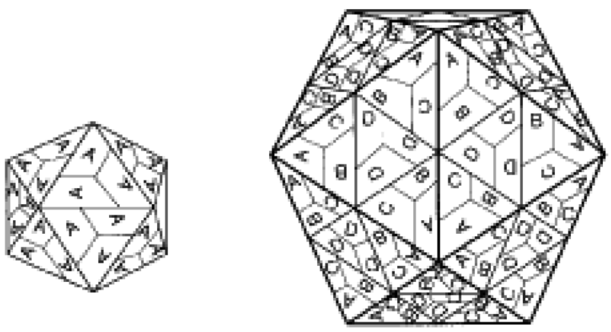
Virus Capsid Model

Most of the spherical viruses have an icosahedral symmetry and the number and arrangement of subunits are determined by “T-number”, which is derived from the “quasi-equivalence theory” developed by Caspar and Klug (1962).

Quasi-Equivalence theory

When three subunits which are intrinsically asymmetric are placed in a triangular surface of an icosahedron with three-fold symmetry, one could place 60 subunits on the surface of the icosahedron in equivalent manner (Figure 1 (a)). This structure can be regarded as being built with twelve pentamers. There are a number of viruses which consist of 60 subunits. However, most viruses are larger, and in these cases, they consist of more than 60 subunits so that not all the subunits can be placed in equivalent positions. Furthermore, their capsids are made of only one kind of polypeptide chain. How can the subunits be arranged in icosahedral symmetry? In answer to the question, Caspar & Klug (1962) presented the concept of “quasi-equivalence”.



(a) $T=1$ (b) $T=4$

Figure 1. Structure of spherical shells and the theory of quasi-equivalence

A, B, C and D in (b) are the same subunits, but placed in non-equivalent positions. In the case of T=1, all the 60 subunits can be placed in equivalent positions, but when T > 1, not all of the subunits can be arranged in equivalent positions.

According to the theory, the icosahedral virus capsid consists of pentamers and hexamers. Hexamers are basically flat, whereas pentamers have a convex shape forming the twelve apexes of the icosahedron. Generally, the same protein molecule forms both pentamer and hexamer[1)]. The bonding relation and their environment in the icosahedron are not identical. It is thought that the subunits retain the relationship to the neighboring subunits with some distortion or “quasi-equivalent” relation. This theory is called the “quasi-equivalence theory”.

What is the T-number?

Pentamers occupy the twelve apexes and, therefore, there are always twelve pentamers present, but the number of hexamers depends on the size of the virus.

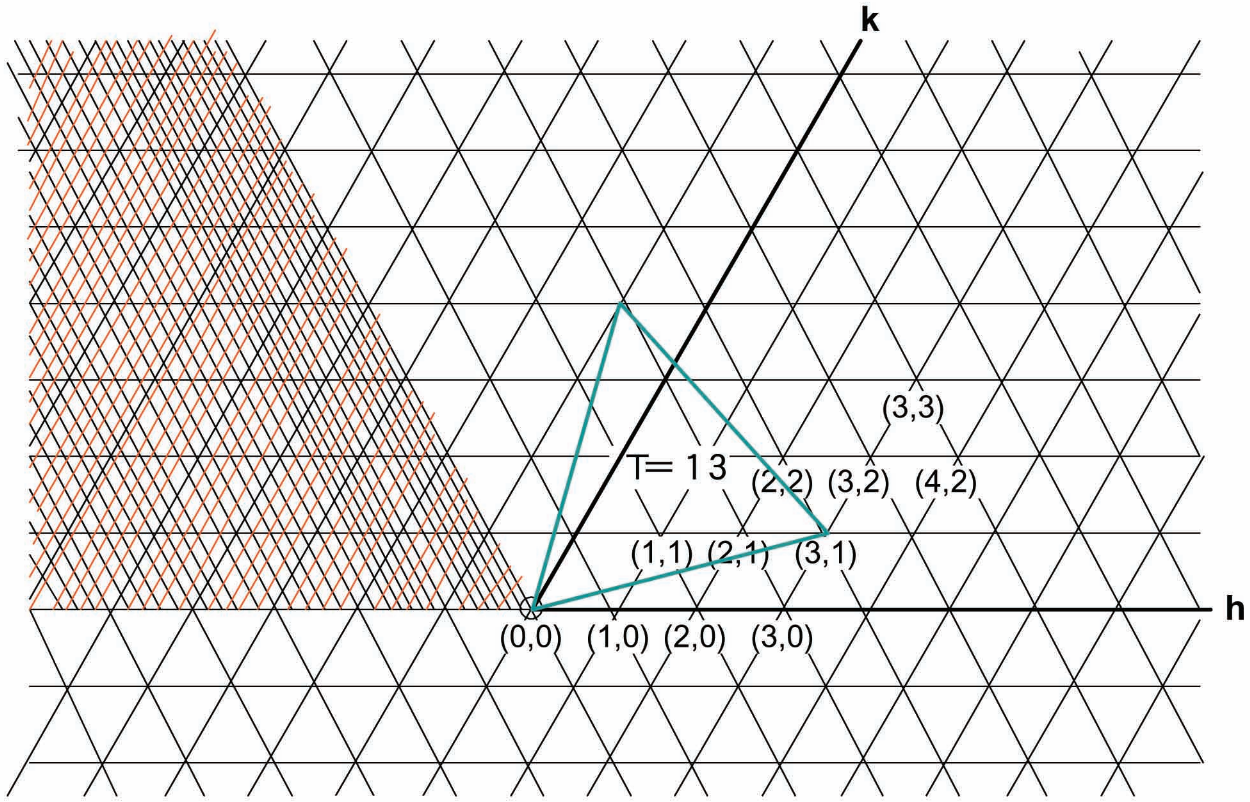


Figure 2. p6 net.

Choosing an arbitrary lattice point in the p6 net as the origin and placing a pentamer, T-number is defined as $T=h^2+hk+k^2$, where (h, k) is the closest pentamer from the origin. T signifies the number of small unit triangles in a facet of the icosahedron. The green triangle indicates the case of T=13.

First, draw a net consisting of regular triangles and take an arbitrary lattice point as the origin. Two straight lines that are crossing at the angle of 60° are taken as h-axis and k-axis. Now, in order to make the origin a five-fold symmetry, cut out one sixth (the shaded area in the figure) and join the two edges. A convex pentamer is thus made. The next question is which lattice point to choose as the closest pentamer. The chosen position uniquely determines the size of the icosahedron. For example, denote the intersection points as (h, k) and if the closest pentamer to the origin is placed (1,0), an icosahedron consisting solely of pentamers is formed (Figure 1(a)). T-number or the triangulation number which determines the size of an icosahedron is defined as:

$$T=h^2+hk+k^2$$

where h and k are 0 or positive integers. T-number can take only some discrete values such as 1, 3, 4, 7, 9, 12, 13 etc. In Figure 3, an area which is delimited by h- and k-axis is shown. It can be readily shown that T-number corresponds to the number of the small unit regular triangles and that $S=\sqrt{T}$ is the length of each edge of the regular surface triangles of an icosahedron.

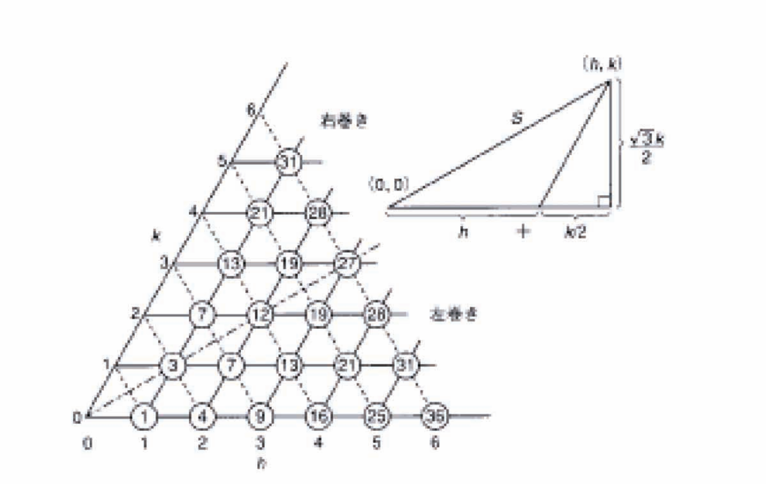


Figure 3. T-number, right-handed and left-handed icosahedron, and the relationship between the T-number and the length of each edge of the regular triangular surface

In (a) and (b) of Figure 1, examples of the head shell with T=1 and T=4 are shown. When either h or k is zero, or h=k, the structure is uniquely determined. However, when neither h nor k is zero and h≠k, right-handed (d) and left-handed (l) icosahedra can be distinguished. For example, the T-number of phagel and phage T4 is T=7l and T=13l, respectively, but that of the polyoma virus is 7d.

Some viruses like bacteriophage T4 have a prolate-shaped head which is an icosahedron elongated along the five-fold axis. Let us consider how the prolate icosahedron can be constructed. An icosahedron is made of three parts; namely a top and bottom cap and a cylinder that connects the two (Figure 4).

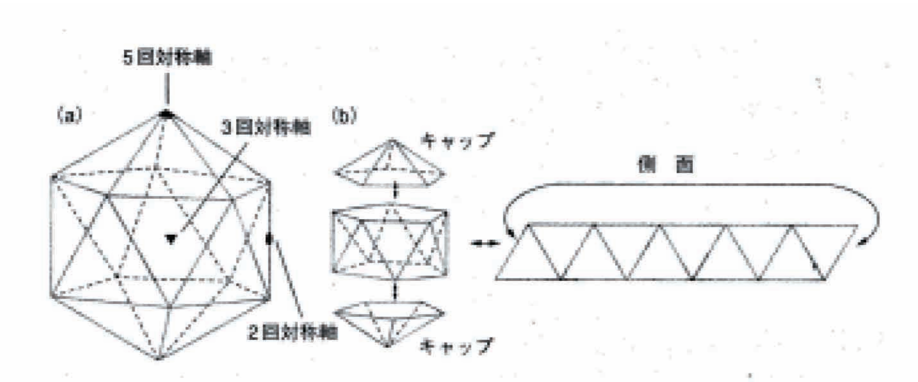


Figure 4. Caps and a cylinder that constitute an icosahedron.

The cylinder part is made of ten triangles and the triangles can be characterized by a Q-number. The Q-number also specifies the number of the unit triangles like the T-number, but can take the value of any positive integers. In the case of phage T4, T=13[1] and Q=21[2]. In figure 5, the normal Q=21[2] as well as the rare case of Q=13 (isometric) and Q=17 (intermediate) are shown.

wild type   intermediate   isometric

Figure 5. Examples of prolate icosahedrons. T=13 cap and Q=21(wild type), 17 (intermediate) and 13(isometric).

Quasi-equivalent theory and the determined high resolution structure of the head shell

Since the appearance of the quasi-equivalence theory, a number of high resolution structures of some spherical plant viruses have been reported. As a result, some change in the concept of quasi-equivalence became necessary. Originally, the concept of "quasi-equivalence" assumed that the intersubunit interactions are basically identical in pentamers and hexamers, but accommodated in slightly different environments (See positions A through D in Figure 1) by "distortion". However, looking at the high resolution structure of SBMV (Southern Bean Mosaic Virus), the three-dimensional structures of each subunit in non-equivalent positions are almost identical, but instead, a number of "non-equivalent" bonds are present. In other words, subunits are accommodated not by distortion, but by different bonds in the icosahedron. Furthermore, in adenovirus (T=25), not a pentamer, but a subunit which has a pseudo-fivefold symmetry is placed in each five fold symmetrical position. Another unexpected finding was the polyoma virus structure, where all the 72 capsomers were pentamers. However, aside from the exception, almost all the structures of spherical viral capsids are still found to be made of pentamers and hexamers, namely based on the "quasi-equivalent theory".

Notes:
1) There are some exceptional cases such as in phage T4, where pentamers and hexamers are made of different polypeptide chains.
2) Recently, the correct number of Q was found to be 20 instead of 21 as previously reported.

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