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ORIGINAL PAPER

Models of virus capsids containing 72 pentameric capsomeres

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Abstract A simple model for describing the non-quasi-equivalent icosahedral virus capsid composed of 72 pentameric capsomeres is developed. By means of six-step operations, a new 4-gons polyhedron ***P*** is obtained which contains 72 pentagons, 80 trigons and 210 quadrilaterals. More importantly, it bears icosahedral symmetry. The rationality of the existence of the 4-gons polyhedron ***P*** is further discussed. The results show that this model can be used to represent the capsids of papovaviruses.

Keywords Non-quasi-equivalent icosahedra · Virus capsid · Pentameric capsomere · Polyhedron

1 Introduction

A virus capsid has been considered as a protein shell made up of many protein subunits which protects a virus from being infected. The study of its structure is an important subject of virology. In 1956, Crick and Watson were the first to suggest that the majority of virus capsids are composed of numerous identical protein subunits arranged in either helical or icosahedral symmetry [1]. Some years later, Casper and Klug proposed the notable quasi-equivalence theory to account for the arrangement of proteins on the surface of an icosahedral virus capsid [2]. In their theory, the icosahedral virus capsid is considered as a closed spherical shell that is constructed by combining 60T

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subunits or 12 pentamers and $10(\boldsymbol{T}-1)$ hexamers ($\boldsymbol{T}$ is the triangulation number and it can be 1, 3, 4, 7,...) [2]. Most viruses that have been investigated experimentally abide by these rules, and these rules have been considered as the fundamental framework for understanding the capsids of icosahedral viruses. However, the capsids of papovaviruses [3–6] which are composed of 72 pentameric capsomeres arranged on a $\boldsymbol{T}=7$ icosahedral lattice cannot be explained by the quasi-equivalent theory [7], and a tilting approach was proposed by Twarock to solve the problem mentioned above[8]. This approach provides an excellent interpretation of non-quasi-equivalent subunit arrangements in icosahedral virus capsids that have been observed experimentally but are not covered by the Caspar–Klug approach. This is especially valuable for the structures of polyoma virus, simian virus 40 and papillomaviruses, and so on [3–6].

In the past few years, a large number of theoretical attempts to understand virus capsids appeared, using necessary and simple geometric assumptions, such as discs on a sphere [9,10], simple van der Waals spheres [11], Stock-mayer fluids [12], trapezoidal subunits [13,14], tiles [15] and simple bonding units [7,16,17]. It is noteworthy that Goldberg polyhedra are also good models in the description of icosahedral viral capsids which abide by the quasi-equivalence theory [18]. Nevertheless, Qiu et al. [19,20] recently pointed out that some spherical viral capsids such as herpesvirus capsid [21] and Semliki Forest virus capsid [22] cannot be covered by Goldberg polyhedra. And they have put forward a very useful approach, namely extended Goldberg polyhedra, to model the capsids of these viruses, which has enriched the knowledge of models in realizing virus capsids. Inspired by this idea, we propose another model to characterize the capsids of papovaviruses [3–6] that do not conform to the quasi-equivalence theory in the present work. We hope this method will provide a new insight into the modeling of the non-quasi-equivalence icosahedra virus capsids.

2 Polyhedron model

Geometrically, the non-quasi-equivalent icosahedral virus capsid can be regarded as a geometrical entity formed by 72 identical pentagons, and it has icosahedral symmetry. Therefore, we aim at constructing a polyhedron containing 72 pentagons to depict the capsids of papovaviruses. The construction processes are elucidated as follows.

For a regular pentagon (Fig. 1a), it can be divided into six pentagons (Fig. 1b), and the middle is a regular pentagon, while the others around it are irregular. Then after the transmutation operation, Fig. 1b can be converted into Fig. 1c, in which it possesses six regular pentagons.

In order to obtain 72 pentagons, every regular pentagon in the regular dodecahedron (Fig. 2a) has undergone the two-step operation shown in Fig. 1. The resultant structure containing 72 pentagons (Fig. 2b) is now projected onto its circumscribing sphere ***S1*** (Fig. 2c). Next, the surface of the sphere ***S1*** is expanded while keeping the position and size of the polygons unchanged. On the other hand, the cambers of the spherical polygons are allowed to change so as to adapt to the variation of curvature of sphere. Consequently, the stretching-extending sphere ***S2*** (Fig. 2d) enlarges the gaps among

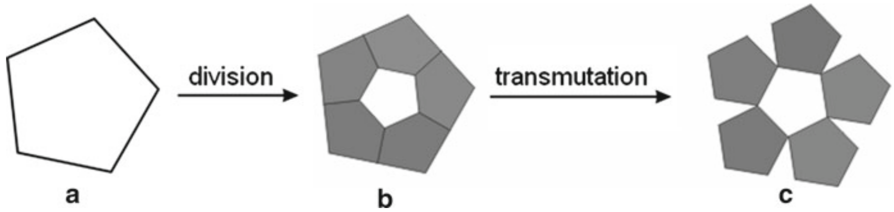

Fig. 1 The division (**a**→**b**) and transmutation (**b**→**c**) processes of a regular pentagon

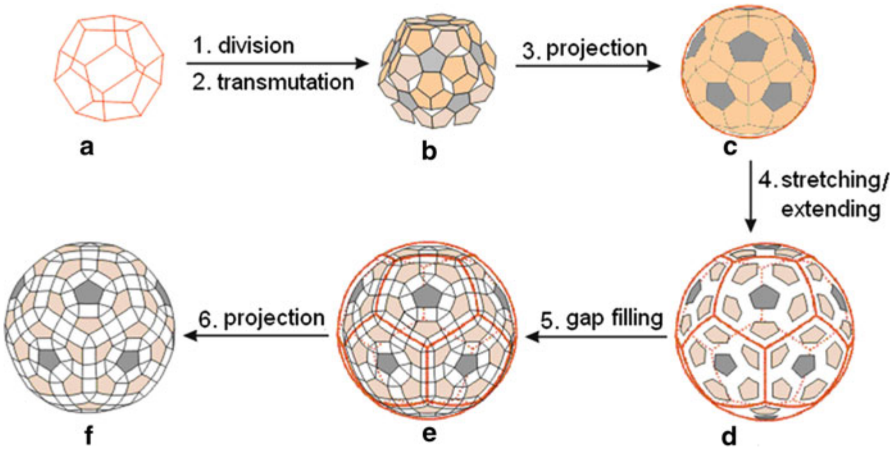

Fig. 2 The construction of polyhedron model for the capsids of papovaviruses. **a** The regular dodecahedron; **b** the structure with 72 pentagons; **c** the circumscribing sphere ***S1***; **d** the stretching-extending sphere ***S2***; **e** the sphere ***S3***; **f** the 4-gons polyhedron ***P***

the arcs as well as those among the vertices of the sphere ***S1***. The stretching-extending operation is stopped when the gaps among the arcs and those among the vertices are extended to the lengths of the arcs. This sphere is denoted as ***S3***, as can be seen from Fig. 2e. It can be observed that the spherical quadrilaterals are derived from the gaps among its arcs, while the spherical trigons are obtained from the gaps among its vertices. Finally, the extended sphere ***S3*** is projected back onto its inscribed polyhedron, thereby forming a new 4-gons polyhedron ***P*** (Fig. 2f), which has icosahedral symmetry. It contains 72 pentagons, 80 trigons and 210 quadrilaterals (Fig. 3). The conversion from the regular dodecahedron to the 4-gons polyhedron ***P*** illustrates that the regular dodecahedron has the feature with scale invariability.

3 Rational 4-gons polyhedron *P*

The Euler's law [23] and the total angular defect [24] by which convex polyhedra must abide have been used here to examine the rationality of the 4-gons polyhedron ***P***.

With respect to the 4-gons polyhedron ***P***, the number of its vertices ***V***, the number of its faces ***F*** and the number of its edges ***E*** are calculated as follows.

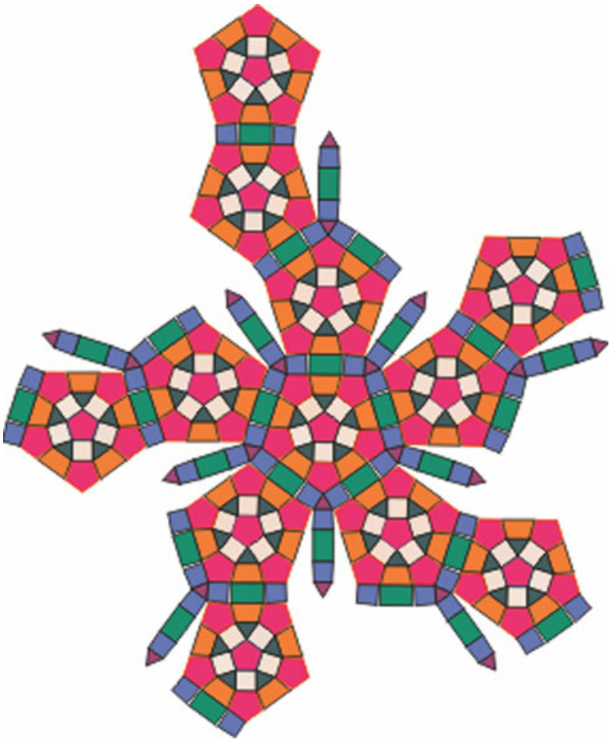

Fig. 3 Schematic representation of the ichnography of the 4-gons polyhedron ***P*** (Fig. 2f)

$$\boldsymbol{V} = (72 * 5 + 80 * 3 + 210 * 4)\,/4 = 360$$
$$\boldsymbol{F} = 72 + 80 + 210 = 362$$
$$\boldsymbol{E} = (72 * 5 + 80 * 3 + 210 * 4)\,/2 = 720$$

It is evident that $\boldsymbol{V} + \boldsymbol{F} = \boldsymbol{E} + 2$, and the 4-gons polyhedron ***P*** strictly conforms to the Euler's law.

For any convex polyhedron, the total angular defect over all its vertices is 720°. Herein, we have obtained two types of convex polyhedra (types ***I*** and ***II***), in which their differences are caused by the constituent polygons with different angles.

With regard to the type ***I***, the total angular defect distributed on each vertex is 2°, so its icosahedral symmetry is preserved. The filled trigons and quadrilaterals in Fig. 3 are analyzed. The equilateral triangles are filled at the positions of 20 threefold axes (Fig. 4a), and the rectangles are filled at the positions of 30 twofold axes (Fig. 4b). At the position of fivefold axis, the combined building block composed of 6 regular pentagons, 5 isoceles triangles, 5 echelons and 5 squares is filled, and it possesses fivefold symmetry, as depicted in Fig. 4c. It can be seen that the angles of the isoceles triangle in Fig. 4c are 70°, 55° and 55°, respectively, while the angles of the echelon are 75°, 75°, 105° and 105°, respectively. In addition, an echelon

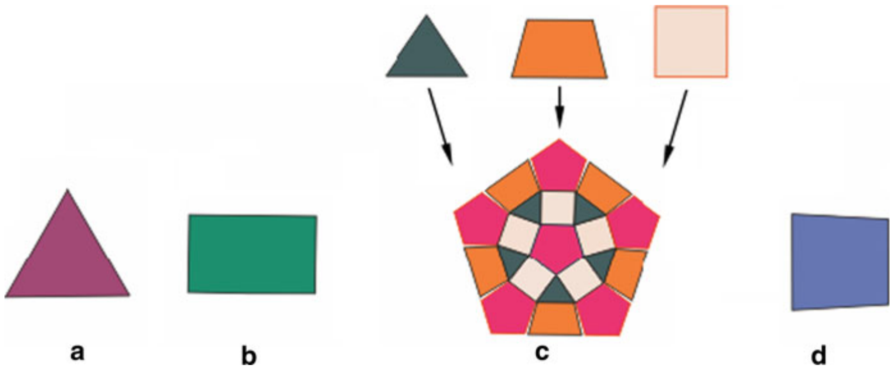

Fig. 4 The components of the ichnography of the 4-gons polyhedron ***P*** (Type ***I***). **a** The equilateral triangle; **b** the rectangle; **c** the combined building block and its components except the regular pentagons (an isoceles triangle with the angles of 70°, 55° and 55°, an echelon with the angles of 75°, 75°, 105° and 105°, and a square); **d** the echelon with the angles of 85°, 85°, 95° and 95°

with the angles of 85°, 85°, 95° and 95° (Fig. 4d) is added on each shorter side of a rectangle.

For the type ***II***, similar to Goldberg polyhedra, the total angular defect is distributed to the 60 vertices of 12 pentagons which located at the position of fivefold axis, so it is 12° for each vertex. The total angular defect of the other vertices (except the 60 vertices) is 0°, which means that the sum of all the angles at the other vertices is 360°. Similarly, its icosahedral symmetry is kept. The equilateral triangles filled at the positions of 20 threefold axes (Fig. 5a) and the rectangles filled at the positions of 30 twofold axes (Fig. 5b) are as same as those of type ***I***. But the combined building block having fivefold symmetry at the position of fivefold axis is different from that of type ***I***. It includes 6 regular pentagons, 5 equilateral triangles, 5 echelons and 5 squares, as displayed in Fig. 5c. Furthermore, the angles of the echelon are 78°, 78°, 102° and 102°, respectively. Additionally, on each shorter side of a rectangle, an echelon with the angles of 84°, 84°, 96° and 96° (Fig. 5d) is added.

4 Conclusions

In summary, a theoretical model to represent the capsids of papovaviruses containing 72 pentameric capsomeres has been proposed. A new 4-gons polyhedron ***P*** is obtained via six-step operations (division, transmutation, projection, stretching-extending, gap filling and back projection), and it contains 72 pentagons, 80 trigons and 210 quadrilaterals. The pentagons, trigons and quadrilaterals are used to model the pentamers of virus capsids as well as the interactions of the pentamers at the positions of both threefold and twofold axes. The rationality of the existence of the 4-gons polyhedron ***P*** has been confirmed by the Euler's law. Moreover, two types of convex polyhedra composed of polygons with different angles have been obtained by analyzing the total angular defect. This approach overcomes the limitations of the number of pentagons, thereby providing new ideas in modeling the virus capsids. At the same time, the other

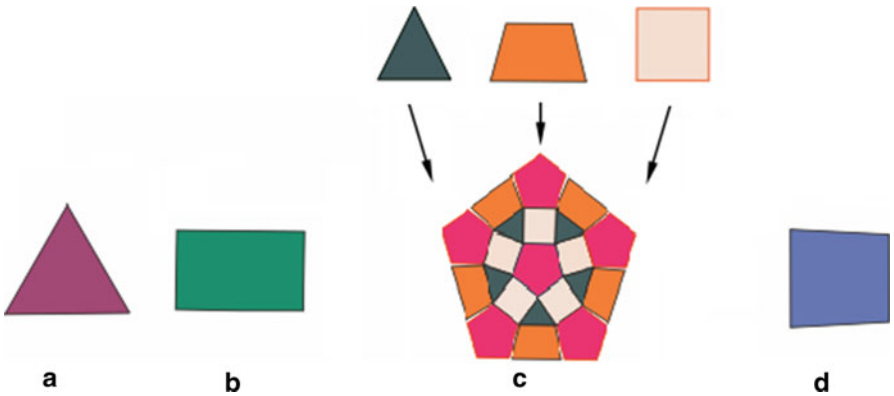

Fig. 5 The components of the ichnography of the 4-gons polyhedron ***P*** (Type ***II***). **a** The equilateral triangle; **b** the rectangle; **c** the combined building block and its components except the regular pentagons (an equilateral triangle, an echelon with the angles of 78°, 78°, 102° and 102°, and a square); **d** the echelon with the angles of 84°, 84°, 96° and 96°

methods like "polyhedral links model" have also been developed [25,26], as reviewed by Jablan and coworkers [27], and we are attempting to apply them to the constructions of other virus capsids, which are underway.

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