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Discrete groups and internal symmetries of icosahedral capsids.

The Caspar-Klug classification of icosahedral capsids [1] takes into account only their size, given by the triangular number T = p + pq + q. It can also note the difference between chiral and non-chiral capsids. But it does not take into account more subtle differences resulting from the differentiation of coat proteins serving as elementary blocks from which capsids are assembled by agglomeration. [2], [3]. We develop further the classification of icosahedral capsids introduced a few years ago [4], [5], using the symmetry group action on the elementary triangles

We analyze the differentiation of coat proteins forming an icosahedral viral capsid with a given triangular number T. A typical icosahedral capsid can be subdivided into twelve pentagons and 10(T-1) hexagons, which can be realized either as genuine hexamers, or as a combination of dimers or trimers.We assume that the pentamers, which are found in twelve vertices of the capsid, display five identical sides. This is usually the case, except for the Papovaviridae family in which all pentamers are maximally differentiated, displaying five different sides (abcde) instead of five identical ones (aaaaa).

Hexamers can display various degrees of differentiation. The symmetry imposes that their sides can be either of two types, or three types, or six different types: (abababab), (abcabc) or (abcdef), respectively, because 6 is divisible by 2, 3 and 6. These cases have been discussed in our previous work, and enabled us to introduce four internal symmetry classes in capsid viruses, according to the presence or absence of the aforementioned hexamer types. The full information about a given icosahedral capsid structure can be read from one of the twenty identical triangular faces. The first hexamer type, (abababab) is fouund only in triangles's centers, because of its three-fold symmetry; the type (abcabc) can be found at the edges of the triangular face, and maximally differentiated hexamers (abcdef) can be found in any position.

However, a more subtle analysis can be made if other hexamer types are taken into account. The partition into 2, 3 or 6 different sides must be maintained, but the two (ab) and three (abc) proteins can be placed differently in a hexamer, e.g. like (aaabbb) instead of (abababab), or (aabbabab); the three different proteins (abc) can be displayed as (abccba) instead of (abcabc), generating even instead of chiral symmetry around the edge. With these new configurations included, the classification of icosahedral capsids becomes more complete.

We also show how the capsids agglomerate in a way that always minimizes the number of different proteins needed for the construction. This is being illustrated on the examples provided by the herpesvirus (T=16) and human adenovirus (T=25). Our classification gives some extra hints concerning genetic proximity of viruses displaying similar classes of capsid symmetries.

References

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