BOX 4.3

BACKGROUND

The triangulation number, T*, and how it is determined*

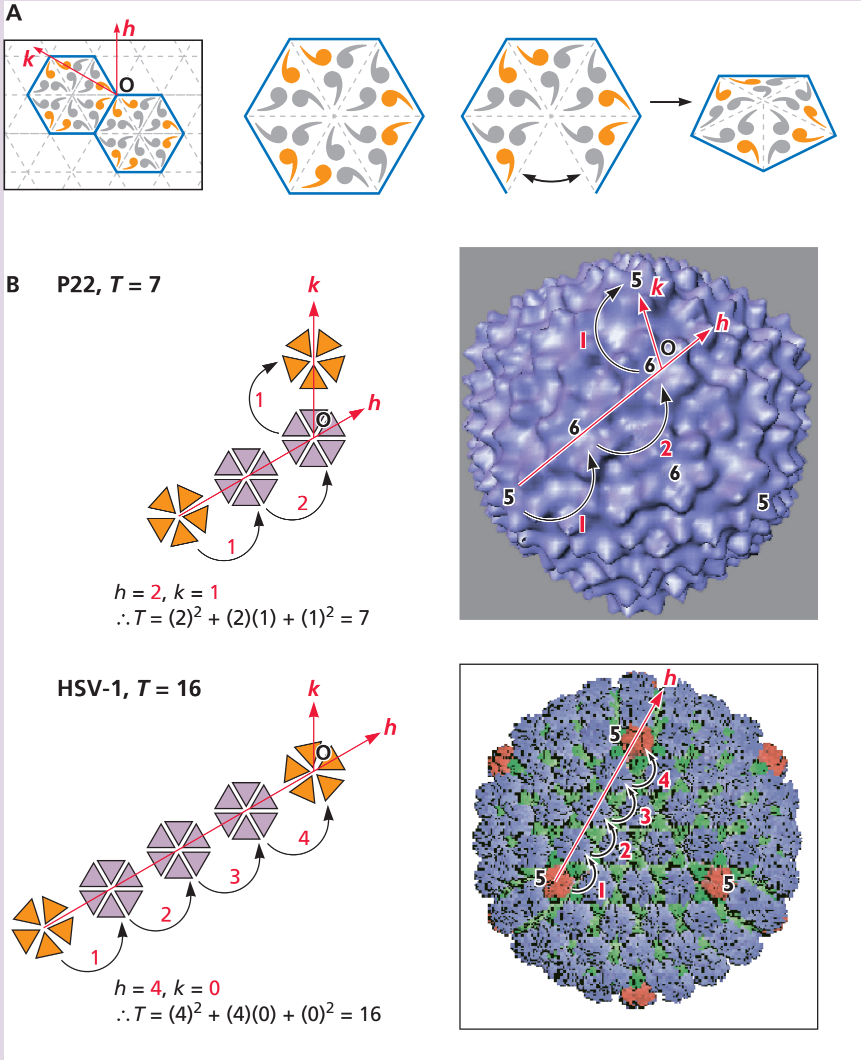
In developing their theories about virus structure, Caspar and Klug used graphic illustrations of capsid subunits, such as the net of flat hexagons shown at the top left of panel A in the figure. Each hexagon represents a hexamer, with identical subunits shown as equilateral triangles. When all subunits assemble into such hexamers, the result is a flat sheet, or lattice, which can never form a closed structure. To introduce curvature, and hence form three-dimensional structures, one triangle is removed from a hexamer to form a pentamer in which the vertex and faces project above the plane of the original lattice (A, far right). As an icosahedron has 12 axes of fivefold symmetry, 12 pentamers must be introduced to form a closed structure with icosahedral symmetry. If 12 adjacent hexamers are converted to pentamers, an icosahedron of the minimal size possible for the net is formed. This structure is built from 60 equilateral-triangle asymmetric units and corresponds to a $T = 1$ icosahedron (Fig. 4.9B). Larger structures with icosahedral symmetry are built by including a larger number of equilateral triangles (subunits) per face (Fig. 4.10). In the hexagonal lattice, this is equivalent to converting 12 **nonadjacent** hexamers to pentamers at precisely spaced and regular intervals.

To illustrate this operation, we use nets in which an origin (O) is fixed and the positions of all other hexamers are defined by the coordinates along the axes labeled h and k, where h and k are any positive integer (A, left). The hexamer (h, k) is therefore defined as that reached from the origin (O) by h steps in the direction of the h axis and k steps in the direction of the k axis. In the $T = 1$ structure, $h = 1$ and $k = 0$ (or $h = 0$ and $k = 1$), and adjacent hexamers are converted to pentamers. When $h = 1$ and $k = 1$, pentamers are separated by one step in the h and one step in the k direction. Similarly, when $h = 2$ and $k = 0$ (or vice versa), two steps in a single direction separate the pentamers.

The triangulation number, T, is the number of asymmetric units per face of the icosahedron constructed in this way. It can be shown, for example by geometry, that

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

Therefore, when both h and k are 1, $T = 3$, and each face of the icosahedron contains three asymmetric units. The total number of units, which must be $60T$, is 180. When $T = 4$, there are four asymmetric units per face and a total of 240 units (Fig. 4.10).



As the integers h and k describe the spacing and spatial relationships of pentamers, that is, of fivefold vertices in the corresponding icosahedra, their values can be determined by inspection of electron micrographs of virus particles or their constituents (B). For example, in the bacteriophage p22 capsid (B, top), one pentamer is separated from another by two steps along the h axis and one step along the k axis, as illustrated for the bottom left pentamer shown. Hence, $h = 2$, $k = 1$, and $T = 7$. In contrast, pentamers of the herpes simplex virus type 1 (HSV-1) nucleocapsid (bottom) are separated by four and zero steps along the directions of the h and k axes, respectively. Therefore, $h = 4$, $k = 0$, and $T = 16$.

Recent application of the principles applied by Caspar and Klug to other uniform lattices that can form icosahedra has generalized the theory of quasiequivalence to account for structures of virus particles that appeared as exception, for example, $T = 2$ protein shells.

Cryo-electron micrographs of bacteriophage p22 and HSV-1 courtesy of B.V.V. Prasad and W. Chiu, Baylor College of Medicine, respectively.