Now

$$\begin{aligned}\sin \varphi(\mathbf{0}) &= \sum_{\mathbf{M}} H(\mathbf{0},\mathbf{M}) \\ &= \sum_{\mathbf{M}}{}' H(\mathbf{0},\mathbf{M}) + G(\mathbf{0}) \\ &\le Q + G(\mathbf{0}).\end{aligned} \tag{B.10}$$

Hence a sufficient condition to satisfy equation (B.8) is

$$Q < \alpha[1-4G(\mathbf{0})Q]^{1/2} \tag{B.11}$$

i.e.

$$Q < \alpha[4\alpha^2G^2(\mathbf{0})+1]^{1/2} - 2\alpha^2G(\mathbf{0}). \tag{B.12}$$

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Facetting the Dodecahedron

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Rules are given for the construction of facetted polyhedra which ensure that the reciprocal figures are also polyhedra. The complete set of 22 facetted dodecahedra is enumerated, depicted and correlated with the stellations of the icosahedron.

Introduction and definitions

The name *polyhedron* implies a definition in terms of the flat polygonal faces of the figure. This viewpoint leads naturally to the idea of stellating a polyhedron by extending the planes of the faces to meet again at new edges and vertices. Less obvious is the dual process, *facetting*, in which the vertices are linked together to give new edges and new faces (or *facets*). Coxeter (1963) has given an authoritative account of both constructions but treats only those cases where the derived polyhedra have regular polygonal faces or vertices. This is a severe restriction, satisfied by only five of the 59 stellated icosahedra enumerated by Coxeter, Du Val, Flather & Petrie (1938). It does, however, have the effect of ensuring that the derived polyhedra have well-defined reciprocals, a condition not met by many of the 59 icosahedra.

The operation of reciprocating a polyhedron (P) consists in constructing a set of points reciprocal to the planes of the faces of P; the centre of P is taken as the centre of inversion. The new points are identified with the vertices of the reciprocal (R); they are linked by edges whenever the corresponding faces of P have an edge in common. It follows that the vertices of P are reciprocal to the faces of R and that P and R are topologically dual. Clearly it is possible to define the facetions of P and the stellations of R in such a way as to maintain duality. However, one cannot construct 59 facetted dodecahedra by reciprocating the stellated icosahedra of Coxeter *et al.* (1938), since these were described as *solids* built up from fundamental cells defined by the extended faces of the icosahedron. The reciprocal cells overlap one another and so cannot be used in an analogous way. If, however, one treats a polyhedron as a *surface*, defining precisely how the faces are to be joined together, the construction of the reciprocal follows automatically. This procedure leads to a convenient description of facetting, through the definitions which follow:

1. An *edge* is a straight line connecting two *vertices*.
2. A *polygon* is an endless chain of coplanar edges in which every vertex lies at the end of two and only two edges. The edges may intersect to give star or skew polygons but the intersections are not counted as vertices.
3. A *face* (or *facet*) is a plane surface with a polygonal boundary. If the chain of edges winds round the centre n times the face will have n layers, which may be connected by a winding point.
4. A *polyhedron* is an unbounded surface composed of faces joined together along their edges in such a way that every edge of the polyhedron is the edge of two and only two faces. The faces may intersect but the intersections are not counted as edges.

So far, this follows Coxeter (1963), but does not specify regularity. In order that the reciprocal of a polyhedron should also satisfy rule 4 the dual requirement is introduced:

5. If several vertices lie along the same line, only one edge may be drawn along the line, connecting just two (any two) of the vertices.

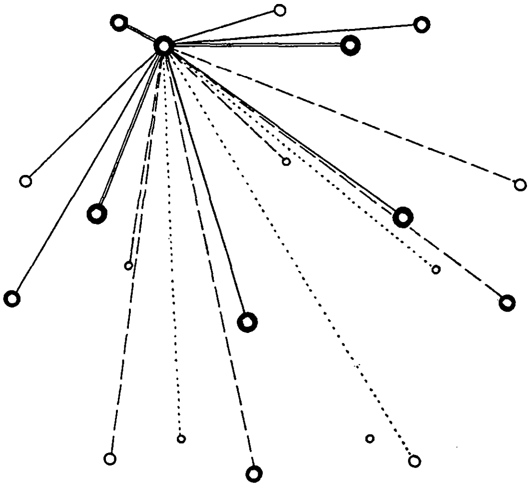

Fig. 1. The edges radiating from one vertex of a dodecahedron. The vertices are ringed and the edges drawn to indicate their type: ═ **a**; ─ **b**; ----- **c**; ······ **d**.

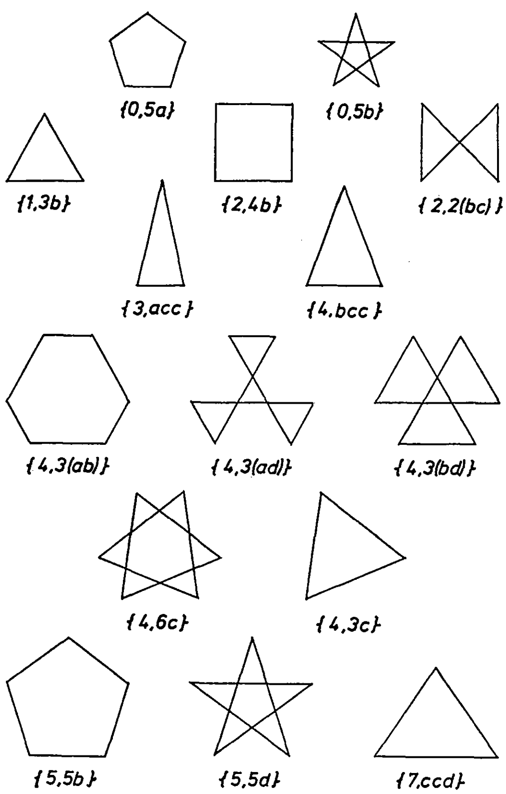

Fig. 2. The facets of the dodecahedron.

6. A *facetion* is a polyhedron of which the vertices coincide with the vertices of a convex polyhedron, or *parent*.

7. We admit only facetions having the same rotational symmetry as the parent. This implies that (*a*) the facetion must include all or none of any set of facets or edges related to one another by rotational symmetry operations of the parent and (*b*) a facet must include all or none of any set of edges in its plane related to one another by those rotational symmetry operations of the parent which transform the plane into itself.

8. Edges or facets passing through the centre of symmetry are not admitted since the reciprocal edge or vertex lies at infinity.

Applications

The facetions of the dodecahedron

There are only four distinct ways of linking two vertices of a regular dodecahedron to form an edge (Fig. 1). Table 1 gives the number of edges of each type (denoted **a**, **b**, **c**, **d**), their lengths and symmetry, *i.e.* the symmetry operations of the dodecahedron which transform the edge into itself. The **c** edges alone can be divided into two mirror-image subsets each having the rotational symmetry of the dodecahedron.

Table 1. *The edges of the dodecahedron*

Symbol	Length	Symmetry	Total number
a	1	$2m$	30
b	τ	m	60
c	$\sqrt{2}$	2	60
d	τ^2	$2m$	30

Note: τ is the positive root of $x^2-x-1=0$.

The planes of the facets are enumerated by taking each type of edge in turn and listing all the planes passing through an edge and another vertex. We define the *index* of the plane as the number of vertices it cuts off from the centre of the polyhedron and the *order* as the number of vertices included in the plane. The planes are denoted by a number pair (index, order); Table 2 lists the complete set.

Table 2. *The planes of the facets*

Index	Order	Edges included	Symmetry	Total number of planes
0	5	**5a**, **5b**	$5m$	12
1	3	**3b**	$3m$	20
2	4	**4b**, **2c**	$2m$	30
3	3	**a**, **2c**	m	60
4	3	**b**, **2c**	m	60
4	6	**3a**, **3b**, **6c**, **3d**	$3m$	20
5	5	**5b**, **5d**	$5m$	12
7	3	**2c**, **d**	m	60

The possible facets are obtained for each type of face-plane, using definitions 2, 3 and 7(*b*). The results are displayed in Fig. 2; the notation indicates the index and the chain of edges. In all cases but one the individual facets are symmetrical with respect to some mirror plane of the dodecahedron; the exception is the triangular facet {4,3**c**} which may be used alone or combined with its mirror image to give the star-hexagonal facet {4,6**c**}. In the (2,4) plane the **b** edges divide into two pairs, not related by any symmetry operation of the facet; either pair may be combined with the **c** edges to give two skew quadrilateral facets, {2,2(**bc**)} and {2,2(**b′c**)}.

The facetions are constructed from sets of facets, following rules 4 and 7(*a*). Where **a**, **c**, or **d** edges are present each edge must be common to two facets, related by a half-turn about the twofold axis of symmetry bisecting the edge, unless the facet is itself symmetrical about this axis. Thus each of the sets of facets containing **a**, **c** or **d** edges only constitutes a facetion. So also does the set {2,4**b**}, but in the remaining sets the **b** edges are unshared ({2,4**b**} is exceptional just because each facet contains two sets of **b** edges). The sets with unshared **b** edges can be combined in pairs to give a further 14 facetions, not counting the combination of {4,3(**ab**)} with {4,3(**bd**)} which is equivalent to {4,3(**ad**)}. There are no more, since the facets {2,2(**bc**)} and {2,2(**b′c**)} have both **b** and **c** edges unshared and can only be combined together, to give {2,4**b**}. (But if we set aside rule 8 and allow the rectangular facet with **b** and **c** edges which passes through the centre of symmetry, this can be combined with either {2,2(**bc**)} or {2,2(**b′c**)} to give two more 'improper' facetions.)

In all, there are 22 facetions; they are depicted in Fig. 3, though it must be remembered that only a part of each surface is in fact visible. The notation indicates the facets used. Five of the facetions are fully regular and are listed by Coxeter (1963): the dodecahedron itself [0,5**a**], the great stellated dodecahedron [5,5**d**], the 'five cubes' [2,4**b**], the 'five tetrahedra' [4,3**c**], and the 'ten tetrahedra' [4,6**c**]. The last three, as implied by their familiar names, are composed of several interpenetrating but distinct polyhedra of lower symmetry. There is one other such facetion: [1,3**b**; 4,**acc**] is composed of ten triangular antiprisms. (The two improper facetions are also compounds, both comprising five improperly facetted cubes. These are one-sided, or non-orientable, surfaces, owing to the use of the diagonal facets.)

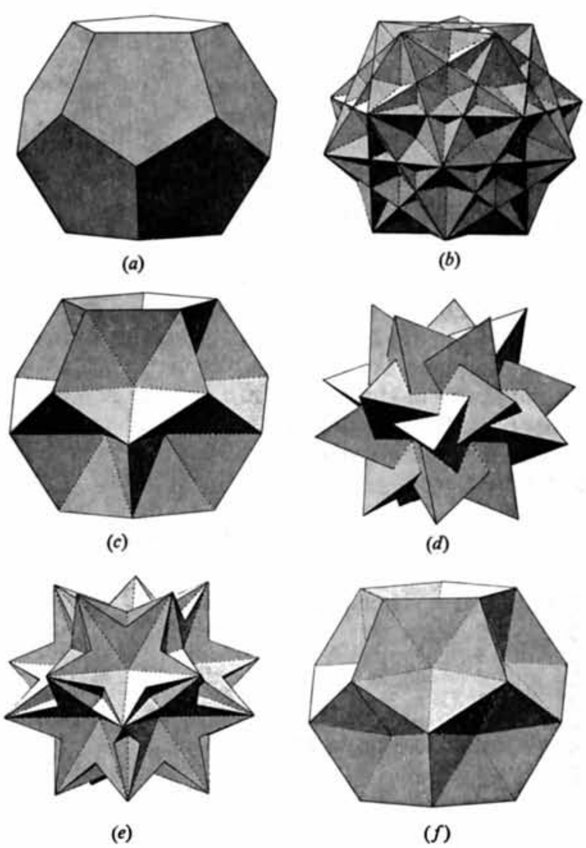

Fig. 3. Facetions of the dodecahedron. (*a*) [0, 5**a**], (*b*) [2, 4**b**], (*c*) [4, 3(**ad**)], (*d*) [4, 3**c**], (*e*) [4, 6**c**], (*f*) [3, **acc**].

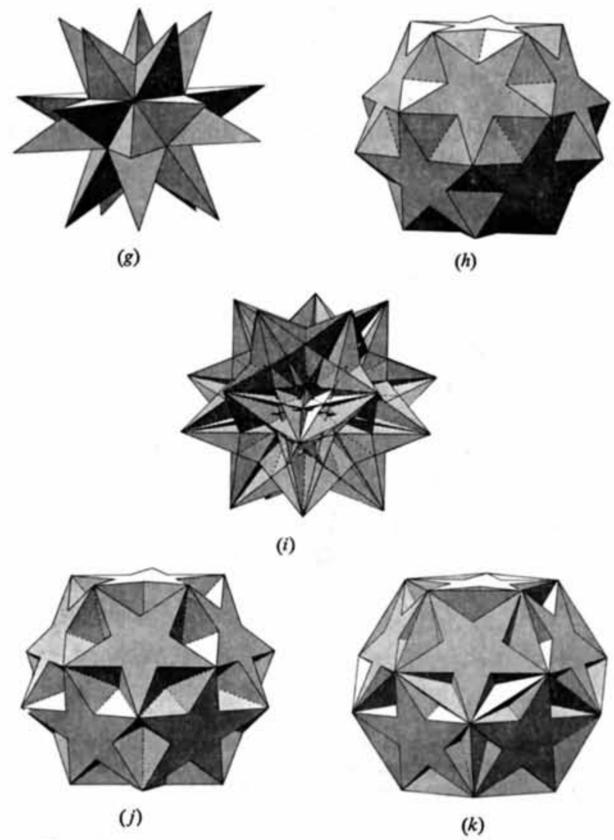

Fig. 3 (*cont.*). (*g*) [5, 5**d**], (*h*) [0, 5**b**; 1, 3**b**], (*i*) [7, **ccd**], (*j*) [0, 5**b**; 4, 3(**bd**)], (*k*) [0, 5**b**; 4, 3(**ab**)].

The stellations of the icosahedron

Each of the facetions of the dodecahedron has a characteristic *vertex polygon*, all of which may be derived from a single diagram (Fig. 4). This represents the intersection of the edges radiating from a vertex with the (1,3) plane between it and the centre. For each point we can construct a reciprocal line (inverting with respect to the centre of the diagram), representing an edge in a face-plane of the icosahedron. The vertex polygon for any facetted dodecahedron is constructed by linking the points to show the lines of intersection of the facets with the plane; the face of the reciprocal stellated icosahedron is obtained by a corresponding traverse of edges. The construction shows that the facetions [4,3**c**], [4,6**c**] and [4,3(**ad**)] are self-reciprocal and thus also stellations of the icosahedron. Table 3 shows the relation between our surfaces and the solid stellations of Coxeter *et al.* (1938). These authors did not distinguish between stellations which look alike from the outside, so that four of their solids correspond to two or more surfaces.

Table 3. *Facetted dodecahedra and stellated icosahedra*

Solids*	Surfaces†	Density	Genus
A	[0, 5**a**]	1	0
B	[0, 5**b**; 1, 3**b**]	2	5
C	[2, 4**b**]	5	0
D	[3, **acc**]	5	6
E	[4, **bcc**; 4, 3(**ab**)]	15	26
G	[5, 5**d**]	7	0
H	[7, **ccd**]	25	6
$\mathbf{De}_1$	[0, 5**b**; 4, 3(**ab**)]	7	0
$\mathbf{De}_1$	[1, 3**b**; 4, 3(**ab**)]	5	16
$\mathbf{De}_2$	[0, 5**b**; 4, **bcc**]	8	15
$\mathbf{De}_2$	[1, 3**b**; 4, **bcc**]	10	0
$\mathbf{D}+\mathbf{f}_2$	[4, **bcc**; 5, 5**b**]	4	15
$\mathbf{De}_2\mathbf{f}_2$	[0, 5**b**; 5, 5**b**]	4	9
$\mathbf{De}_2\mathbf{f}_2$	[1, 3**b**; 5, 5**b**]	6	5
$\mathbf{Ef}_1$	[4, 6**c**]	10	0
$\mathbf{E}f_1$	[4, 3**c**]	5	0
$\mathbf{Ef}_2$	[4, 3(**ab**); 5, 5**b**]	11	20
$\mathbf{Ef}_1\mathbf{g}_1$	[4, 3(**ad**)]	0	11
$\mathbf{Ef}_1\mathbf{g}_1$	[0, 5**b**; 4, 3(**bd**)]	7	20
$\mathbf{Ef}_1\mathbf{g}_1$	[1, 3**b**; 4, 3(**bd**)]	5	16
$\mathbf{Ef}_1\mathbf{g}_1$	[4, **bcc**; 4, 3(**bd**)]	15	26
$\mathbf{Fg}_1$	[4, 3(**bd**); 5, 5**b**]	11	0

* After Coxeter *et al.* (1938), who do not list $\mathbf{D}+\mathbf{f}_2$.
† This work.

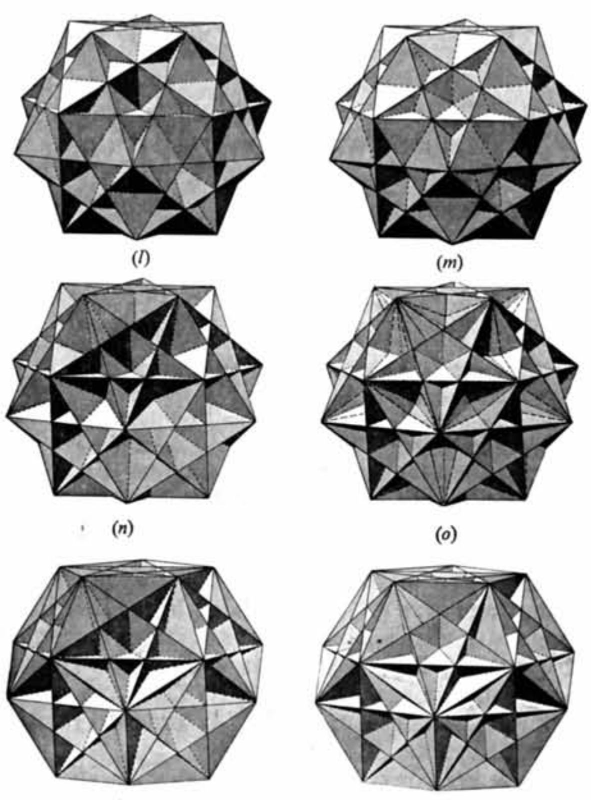

Fig. 3 (*cont.*) (*l*) [1, 3**b**; 5, 5**b**], (*m*) [1, 3**b**; 4, **bcc**], (*n*) [4, 3(**bd**); 5, 5**b**], (*o*) [4, **bcc**; 4, 3(**bd**)], (*p*) [4, 3(**ab**); 5, 5**b**], (*q*) [4, **bcc**; 4, 3(**ab**)].

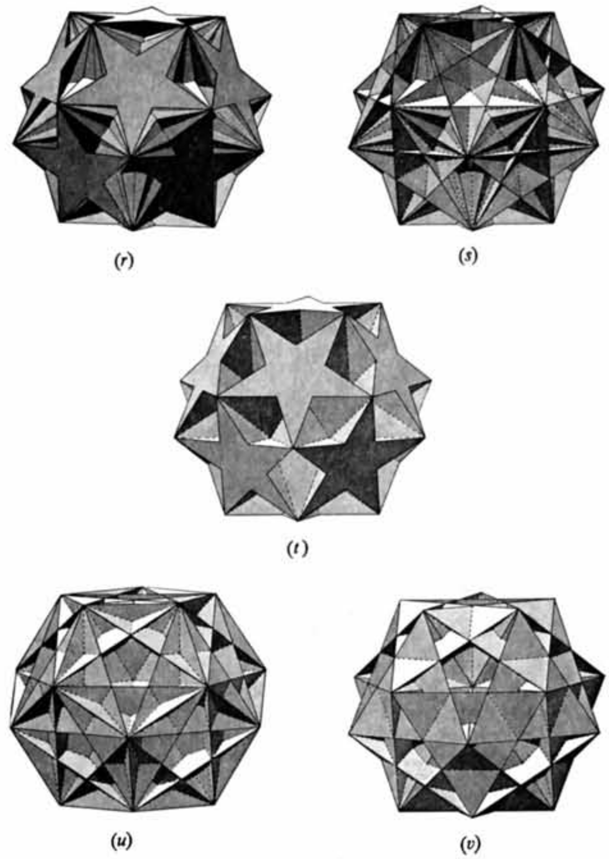

Fig. 3 (*cont.*) (*r*) [0, 5**b**; 4, **bcc**], (*s*) [4, **bcc**; 5, 5**b**], (*t*) [0, 5**b**; 5, 5**b**], (*u*) [1, 3**b**; 4, 3(**ab**)], (*v*) [1, 3**b**; 4, 3(**bd**)].

The real difference between these 'look-alike' stellations is brought out by comparing the density and the genus of the polyhedra (see Table 3); these numbers characterize the surface and so are the same for each of a pair of duals. The density is the number of times the centre is 'wrapped up' by the surface and can be calculated from the solid angles subtended by individual facets at the centre of the dodecahedron, remembering that some regions of the facets must be given double or negative weights. One interesting result is that [4,3(**ad**)] has zero density, *i.e.* that the centre is not enclosed. This is because the centre point of each of the pentagonal 'dimples' constitutes an infinitesimally narrow tunnel giving access to a central icosahedral cavity.

The topological concept of genus is most simply appreciated as a generalization of Euler's rule (Ball, 1959): if F, V and E are the numbers of faces, vertices and edges of the polyhedron then its surface is of genus $\frac{1}{2}(2+E-F-V)$. If the genus is zero the surface is simply connected, *i.e.* deformable into a sphere. For compound facetions the formula must be applied to the component polyhedra individually. A face of which the edges form n distinct chains must be counted n times, as must a vertex with n distinct chains of edges in its vertex polygon.

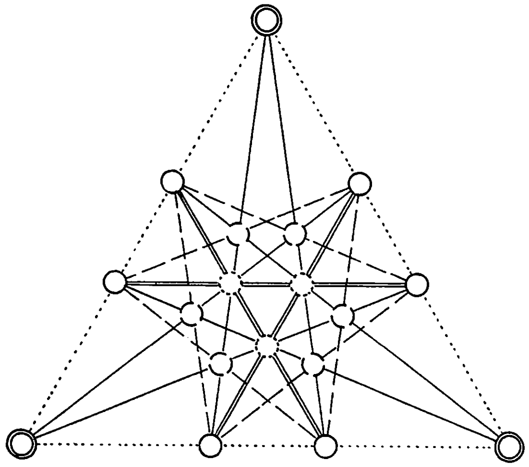

Fig. 4. The vertex figure. The points of intersection of the dodecahedral edges with the plane are circled to indicate the type of edge, as in Fig. 1. Also shown are the corresponding reciprocal lines, which form the edges in the face-plane of the icosahedron.

Thus it appears that 44 of the '59 icosahedra' (Coxeter *et al.*, 1938) have no reciprocals. In all of these it is impossible to describe the face by a polygon which satisfies rule 5, so that any attempt at reciprocation gives a figure with more than two faces meeting along some edges. It is interesting that of the dual pair of rules 4 and 5, 5 is trivial for facetted dodecahedra while 4 is intuitively obvious but in stellating the icosahedron it is 4 which is trivial while 5 is not obvious at all.

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Interpretation of the 10Å Rotation Function of the Satellite Tobacco Necrosis Virus

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The rotation function calculated with 10 Å three-dimensional data from monoclinic crystals of the satellite tobacco necrosis virus was fitted numerically to an icosahedral axis set. The r.m.s. angular deviation of the observed peak maxima from the calculated model axis set was 0·67° and the largest deviation was 1·4°. Thus, there is no significant deviation from icosahedral symmetry at 10 Å resolution. An investigation of the effects of the data inclusion limits and the radius of integration on the resolution of neighboring peaks in the rotation function showed that the best resolution was obtained by using only a thin shell of the highest-resolution data available and a radius of integration no larger than the estimated diameter of the virus protein subunit.

Introduction

The crystallization of a virus, the tobacco mosaic virus, was first reported by Stanley (1935). Soon thereafter a number of small spherical plant viruses were crystallized and in 1944 X-ray diffraction patterns were obtained from dried crystals of a very small virus-like particle then called 'derivative' or 'protein' of the tobacco necrosis virus (TNV; Crowfoot & Schmidt, 1945). The particle was about one-third the molecular weight of TNV with which it was associated during infection and was thought to be a byproduct of infection rather than a separate virus. It is now recognized as the satellite tobacco necrosis virus (STNV) which, although antigenically unrelated to TNV, requires simultaneous co-infection by TNV in order to produce progeny (Kassanis & Nixon, 1961).

Crick & Watson (1956) proposed that the structural protein coat of small spherical viruses was made up of a number of identical subunits packed with cubic point symmetry to form the virus surface. This theory was formalized and extended by Caspar & Klug (1962)