Generalization of Euler’s formula for adjacent polyhedra

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Abstract

Euler's formula for polyhedra is one of the most famous mathematical results. It is also widely used outside mathematics. In particular, it is used in the analysis of molecular structures, many of which have a polyhedral shape. Generalizations of Euler's formula for non-simply connected and multidimensional polyhedra are well known. This article presents a generalization of Euler's formula for adjacent polyhedra. Various cases of adjacency are considered: face-sharing, edge-sharing and vertex-sharing connections. For a system of adjacent polyhedra, a single formula relates the number of vertices, edges and faces in the form V – E + F = N + 1, where N is the number of polyhedra.

Keywords *Convex Polyhedra · Euler’s formula · Adjacency matrix*

1 Introduction

Euler's formula for polyhedra is one of the most famous mathematical formulas. It reflects the most fundamental topological properties of three-dimensional bodies [1]. Naturally, this formula is widely used in the study of molecular structures that have a polyhedral shape. In chemistry, the most famous examples of polyhedral structures are fullerenes with pentagonal and hexagonal faces. Euler's formula characterizes the shape of the cavities of clathrate frameworks, as well as their polyhedral fragments. In one way or another, this formula can also be used to describe the structure of several adjacent polyhedra, which may be of interest for describing various processes of structure formation.

Euler's formula relates the number of vertices, edges, and faces of a single polyhedron by a simple ratio. Spatial structures in the form of several adjacent polyhedra are rather difficult to perceive. The most natural approach to the analysis of such molecular structures is based on the use of an adjacency matrix. The total number of particles (vertices) is usually known. The total number of bonds (edges) is easy to calculate. No distinction is made here between internal and external edges. Elementary cycles are conveniently considered as faces of complex structures. There are explicit formulas that allow one to calculate the number of cycles of different lengths using the adjacency matrix [2–4]. This approach requires caution, since it is necessary to check the elementary nature of the cycles. In tetrahedrally coordinated systems, problems with the number of square and pentagonal cycles usually do not arise when calculating using the adjacency matrix. In real systems, it is also difficult to confuse adjacent squares with a hexagonal ring. Therefore, using the total number of elementary cycles significantly simplifies the analysis. In this article we will analyze purely mathematical relationships between the total numbers of vertices, edges and faces of spatial structures formed by adjacent polyhedra.

The impetus for writing this paper was a recently obtained formula that relates the number of vertices, edges, and faces for water clusters in the form of edge-sharing prisms [5]. Analysis of geometric examples showed the presence of very general relationships similar to Euler's formula. This article is devoted to demonstrating these examples, as well as proving general formulas.

2 Description of the problem

To depict the structure of polyhedra, their flat images (planar graph) are often used, called Schlegel diagrams (Fig. 1a). These diagrams take also into account the framing face. Euler's formula for convex polyhedra has the following form

$$V - E + F = 2 \tag{1}$$

Where V, E and F are the number of vertices, edges and faces. The simplest consequence of equation (1) is the following relation for a flat meshwork without taking into account the “back” face (Fig. 1b)

$$V - E + F = 1 \tag{2}$$

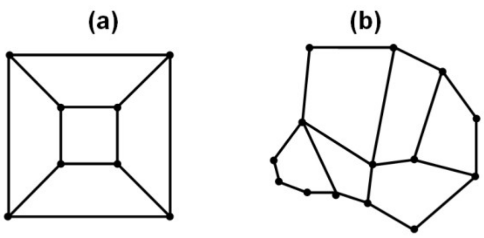

Fig. 1 (a) Schlegel diagrams of cube, (b) Meshwork of adjacent polygons.

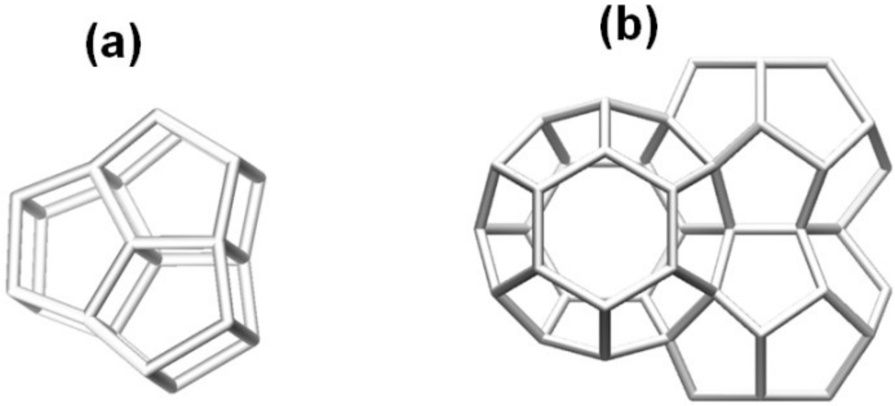

Fig. 2 (a) Edge-sharing pentagonal prisms, (b) four vertex-sharing polyhedra (two superimposed polyhedra on the left)

We will use both of these relations. Note that equation (2) is valid for any simply connected set of adjacent polygons, since the perimeter of such a region can be considered the "back" face, which, if taken into account, we obtain (1). And if we do not take it into account, we obtain (2). The shape of the enclosing polygon is not important, since we are talking about topological properties. A widely known generalization of Euler's formula for non-simply connected polyhedra has the following form.

$$V-E+F=2-2g \tag{3}$$

Here, g is the genus of a surface which is equal to the number of "holes" of a surface.

The right side of equation (3) is called the Euler characteristic of a surface. Its maximum value is 2. A relation similar to formula (1) was obtained by us for various combinations of three edge-sharing prisms (Fig. 2a) [5].

$$V-E+F=4 \tag{4}$$

The question arises whether it is possible to obtain a general formula for an arbitrary number of edge-sharing prisms and an arbitrary number of any polyhedra. No less interesting is the case of vertex-sharing polyhedra, i.e. a set of polyhedra with a common vertex. As an example of such a structure, Fig. 2b shows a fragment of the clathrate frameworks consisting of four 24-vertex polyhedra with one common vertex.

3 Results and discussion

3.1 Face sharing

First, let us consider an example of the simplest union of two polyhedra of arbitrary shape: when they have an n-gonal common face. For the total number of vertices, edges and faces, the following obvious relationships are true: $V = \sum v - n$, $E = \sum e - n$, $F = \sum f - 1$. Here the summation is over two polyhedra. Taking into account (1), we get

$$V - E + F = 3 \tag{5}$$

3.2 Edge sharing

Let us now consider a set of N polyhedra that have one common edge. We consider the case when their adjacent dihedral angles add up to 2π. Usually their number is small, but we are considering the general case. Let such a structure have N adjacent faces, which are polygons with the number of sides n_k, where k varies from 1 to N (Fig. 3). When calculating the number of vertices of the general structure, it is necessary to eliminate multiple enumerations of vertices in the center. More exactly, (N – 1) pairs of vertices are redundant. In addition, to eliminate repetition, it is necessary to subtract once all the remaining (n_i – 2) vertices of each of the N adjacent faces.

$$V = \sum v - 2(N-1) - \sum (n_i - 2) = \sum v - \sum n_i - 2N + 2 + 2N = \sum v - \sum n_i + 2 \tag{6}$$

Similar relations are not difficult to obtain for the number of edges and faces.

$$E = \sum e - (N-1) - \sum (n_i - 1) = \sum e - \sum n_i - N + N + 1 = \sum e - \sum n_i + 1 \tag{7}$$

$$F = \sum f - N \tag{8}$$

Combining these expressions, we obtain the following general formula for edge-sharing polyhedra

$$V - E + F = N + 1 \tag{9}$$

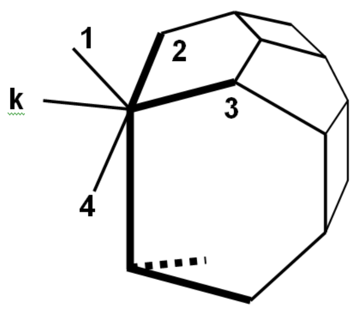

Fig. 3 (a) Edge-sharing polyhedron

3.3 Vertex sharing

3.3.1 Examples

Let us first analyze the simplest examples of structures formed by polyhedra with one common vertex (Fig. 4). We consider the case when their adjacent polyhedral angles add up to 4π. For a tetrahedron divided into four smaller tetrahedra, $V = 5$, $E = 10$, and $F = 10$. Therefore, $V - E + F = 5$ and we again arrive at formula (9), since in this case $N = 4$.

Let us now consider the entire class of n-gonal bipyramids. It is obvious that in this case $V = n + 3$. For the edges we have two sets of inclined edges of n edges each and a double set in the horizontal plane. Taking into account the two central vertical edges, we obtain $E = 4n + 2$. For the faces, there are two sets of inclined faces, two sets of vertical faces and one set of horizontal faces, i.e. $F = 5n$. We obtain that $V - E + F = 2n + 1$. Considering that in this case the total number of polyhedra $N = 2n$, we again arrive at formula (9).

A similar calculation is not difficult to perform for “biprisms” with a common base (Fig. 4c). Note that most often biprisms are called prisms with a common lateral side (Fresnel biprism, [6]). In this case, $V = 3n + 3$, $E = 8n + 2$, $F = 7n$. Again we obtain $V - E + F = 2n + 1$. Consequently, formula (9) is also valid in this case. It can be verified that formula (9) is valid for cuboctahedron (Fig. 4d) and cuboid 2×2×2 (Fig. 4e). The first of them is obtained by truncating eight vertex regions, one of which is shown in Fig. 4e.

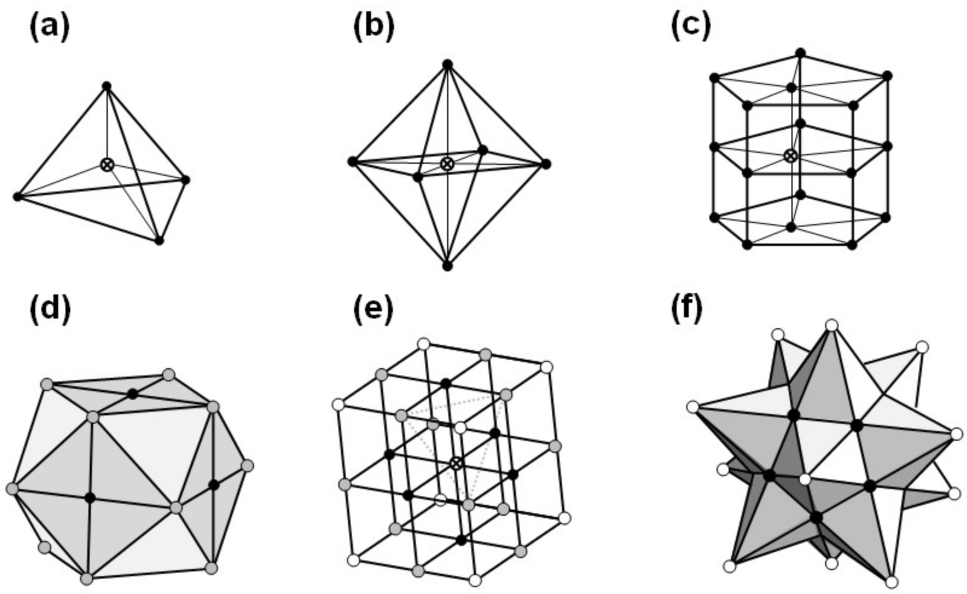

Fig. 4 (a) tetrahedron, (b) bipyramid, (c) biprism, (d) cubooctahedron, (e) cuboid 2×2×2, (f) small stellated dodecahedron

It can be assumed that formula (9) is valid for any set of polyhedra with a common vertex. To prove this statement, we introduce a number of auxiliary definitions and notations.

3.3.2 Vertex classification

1) Central vertex

2) Black vertices are directly connected to the center (Fig. 4).

3) Gray vertices belong to adjacent polyhedra, without being black.

4) White vertices belong to only one polyhedron.

The numbers of such vertices will be designated as V^b, V^g and V^w. In Fig. 4, the first two figures (a, b, c) have only black vertices in addition to the central vertex. Figure (d) also has gray vertices, and figures (e, f) also have white vertices, although the latter has no gray vertices. The structure in Fig. 2b also has all the types of vertices.

3.3.3 Black polyhedron

The black vertices are the vertices of a certain polyhedron, which we will also call black. The black vertices belonging to one of polyhedra can be considered as the vertices of the outer face of the black polyhedron. For topological analysis, it does not matter that such "faces" may not be flat. It is enough that the black polyhedron is topologically equivalent to a sphere. Therefore, we can consider that the black polyhedron is formed by a set of pyramids with a common vertex. Fig. 5a shows a set of black vertices of a certain structure. A square face of the black polyhedron is highlighted.

The main characteristics of the compound black polyhedron, including both its external and internal elements, will be marked with an asterisk. In parallel, we will

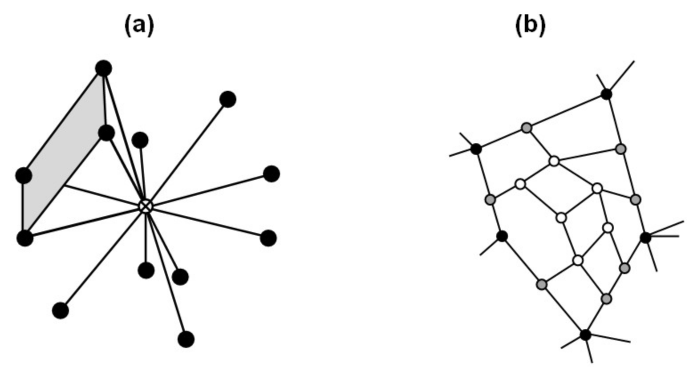

Fig. 5 (a) black vertexes of a polydedron, (b) vertices located on the outer surface of a polyhedron at vertex-sharing connection. Black vertexes are connected with center. Grey

vertices lie on adjacent faces of two polyhedrons. White vertices belong to only one polyhedron.

consider the surface polyhedron, the characteristics of which we will designate with the symbol "S". There are following simple relationships between them

$$V^{¿}=V^{s}+1$$

$$E^{¿}=E^{S}+V^{S} \qquad (10)$$

$$F=F^{S}+E^{S}$$

Here we have taken into account that the number of internal edges of the black polyhedron is equal to the number of vertices on the surface, and the number of internal faces between adjacent pyramids is equal to the number of surface edges. For the black polyhedron as a whole, we obtain the following relation.

$$V^{¿}-E^{¿}+F^{¿}=V^{s}+1-E^{S}-V^{S}+F^{S}+E^{S}=1+F^{S} \qquad (11)$$

And since F^S is equal to the number of composite figures N (pyramids), we obtain the same relationship for the elements of the black polyhedron.

$$V^{¿}-E^{¿}+F^{¿}=N+1 \qquad (12)$$

Note that for the surface polyhedron considered here, the usual Euler equation is naturally satisfied

$$V^{S}-E^{S}+F^{S}=2, \qquad (13)$$

which can be rewritten as follows

$$E^{S}=V^{S}+N-2 \qquad (14)$$

3.3.4 Designations of external elements

A part of the external surface of the general structure, limited by the planes of the faces of one of the internal pyramids, will be called a cap. Each cap in turn can be composed of a certain number of faces that are external to the structure as a whole. Some of the vertices of such caps are in planes that are continuations of the internal faces of the black polyhedron. Topologically, we can assume that they are located on the boundaries of the faces of the black polyhedron. The remaining vertices are internal to one of the caps (Fig. 5b). Vertices located on the boundaries between the faces of the black polyhedron are gray, and internal vertices are white. Recall that we designated the number of such vertices as V^g and V^w, respectively.

Both black and gray vertices are located on the boundaries between faces of the black polyhedron. The total number of boundary edges between the nearest boundary vertices will be designated as E^{b}. We will also introduce notations for the number of edges between gray and white vertices E^{gw} and for the number of edges between white vertices E^{w}. Finally, the number of faces near the boundary and internal faces for each cap is denoted as F^{b} and F^{w}, respectively.

3.3.5 Formula derivation

To derive the main formula, we need two auxiliary relations. First, note that the number of boundary edges of a single cap is equal to the sum of the black and gray vertices located on this boundary, i.e. $E^{b}_{i} = V^{S}_{i} + V^{g}_{i}$. Let us sum this relation over all N caps, taking into account the doubling of edges and of the number of gray vertices.

$$2E^{b} = \sum deg\left(V_{k}^{S}\right) + 2V^{g} = 2E^{S} + 2V^{g} \tag{15}$$

Here we took into account that when summing over all polyhedra, each black vertex is repeated as many times as its degree, i.e. the number of converging black edges. In the total sum over all black vertices, such edges are also repeated twice, i.e.

$$\sum V_{i}^{S} = 2E^{S} \tag{16}$$

Therefore,

$$E^{b} = E^{S} + V^{g} \tag{17}$$

Based on formula (2) for a separate cap we have

$$\left(V_{i}^{S} + V_{i}^{g} + V_{i}^{w}\right) - \left(E_{i}^{b} + E_{i}^{gw} + E_{i}^{w}\right) + \left(F_{i}^{b} + F_{i}^{w}\right) = 1 \tag{18}$$

Summing this expression over all caps, taking into account (16), we obtain

$$\left(2E^{S} + 2V^{g} + V^{w}\right) - \left(2E^{b} + E^{gw} + E^{w}\right) + \left(F^{b} + F^{w}\right) = N \tag{19}$$

Now we transform the combination of the main parameters of the general structure using the characteristics of the black polyhedron, and then rearrange the terms of this expression so as to use formula (19).

$$V - E + F = \left(V^{¿} + V^{g} + V^{w}\right) - \left(E^{¿} + E^{b} + E^{gw} + E^{w} - E^{S}\right) + \left(F^{¿} + F^{b} + F^{w} - F^{S}\right)$$

$$¿\left(V^{¿} - E^{¿} + F^{¿}\right) + V^{g} + V^{w} - \left(E^{b} + E^{gw} + E^{w}\right) + E^{S} + \left(F^{b} + F^{w} - N\right)$$

$$¿\left(V^{¿} - E^{¿} + F^{¿}\right) + 2E^{S} + 2V^{g} + V^{w} - \left(2E^{b} + E^{gw} + E^{w}\right) + \left(F¿¿b + F^{w}\right) - N¿$$

$$¿V^{¿}-E^{¿}+F^{¿} \quad (20)$$

Here we have added the right side of equation (17) and subtracted its left side.

Thus, taking into account (12), it can be stated that for any system of adjacent convex polyhedra with one common vertex, the following expression is indeed valid.

$$V-E+F=N+1 \quad (21)$$

3.4. Multiple connections

3.4.1 Examples

We have considered the cases of adjacency of polyhedra with one common element. But, as the examples show, expression (21) remains valid for case of multiple connections of polyhedra. Various examples are shown in Fig. 6. The simplest case of multiple face-sharing of polyhedra is N-section prismatic tubes (Fig. 5a) with k-gonal rings. In this case, the following relations are valid: $V = k + kN$, $E = k + 2kN$, $F = 1 + (k + 1)N$. Therefore, in this case we also obtain the previous relation

$$V-E+F=k+kN-k-2kN+1+kN+N=N+1 \quad (22)$$

An example of double edge-sharing is shown in Fig. 6b. It is easy to check that in this case $V = 12$, $E = 12 + 12 = 24$, $F = 4 + 8 + 5 = 17$. That is, $V - E + F = 12 - 24 + 17 = 5$. This means that formula (21) is satisfied in this case as well.

Formula (21) is also valid for more complex vertex-sharing structures. Figures 6c–e shows various multi-cage fragments of the two most common gas hydrate frameworks sI and sII. Each of these tetrahedrally coordinated frameworks is formed by two types of

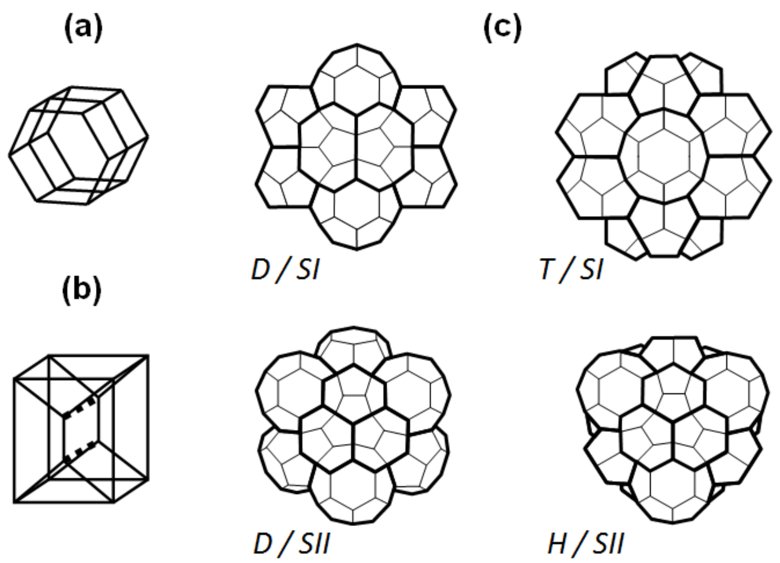

Fig. 6 (a) hexagonal tube with multiple face-sharing of prisms, (b) double edge-sharing connection of prisms, (c) multi-cage fragments of gas hydrate frameworks.

Table Topological characteristics of multiple vertex-sharing fragments

Cage	D/sI	T/sI	D/sII	H/sII
n_1	20	24	20	28
V	172	184	172	198
E	296	320	296	346
F	138	152	138	166
$V - E + F$	14	16	14	18
$f = n_1/2 + 2$	12	14	12	16

polyhedra. The polyhedra of the first framework are D (20) and T(24), and those of the second are again D and H (28). The number of vertices n_1 is given in brackets. The fragments in Figure 6c–e represent different dense single-layer sheaths of polyhedra around the central polyhedron. The total numbers of vertices (molecules), edges (hydrogen bonds), and faces (H-bonded cycles) were previously calculated for these fragments [7]. This statistics is convenient for checking relation (21). For each fragment, the number of vertex-sharing connections is equal to the number of vertices of the internal polyhedron.

Table 1 shows the main characteristics of these fragments that were calculated earlier. The total number of polyhedra on the surface of each fragment is equal to the number of faces of the internal polyhedron. With tetrahedral coordination of bonds, three edges converge at each vertex of individual polyhedra (cubic graphs). Therefore, for each polyhedron, the number of edges is one and a half times greater than the number of vertices. According to Euler's formula (1), the number of faces of the internal polyhedron, equal to the number of polyhedra on the surface, is determined by the ratio $f = n_1/2 + 2$ (last line in Table). Taking into account the internal polyhedron, it is easy to verify the validity of formula (21) for the considered multi-cage fragments.

3.4.2 Proof of the basic formula for multiple connections

The method of proving the validity of formula (21) for any multiple connections consists of analyzing the changes in the system parameters when one polyhedron is disconnected from the original multi-polyhedral structure. In this case, the validity of this formula for one connection has already been proven. This is the method of backward induction. The validity of Euler's formula (1) itself is proven in a similar way when one vertex is successively removed.

First, let us consider the case of a face-sharing compound, where the face is an n-gon. Let us also denote the parameters of the removed polyhedron as v, e, f. In this case, the change in the parameters of the general structure is $\Delta V = v - n$, $\Delta E = e - n$, $\Delta F = f - 1$, i.e. $\Delta(V - E + F) = (v - e + f) - 1 = 2 - 1 = 1$. We have established that with successive removal of one polyhedron, the expression $V - E + F$ decreases by one. But for two polyhedra, equation (3) is valid. Therefore, in the general case, this expression is indeed equal to $N + 1$.

A similar situation occurs in the case of edge sharing (Fig. 3) when removing one polyhedron, which has two adjacent faces in the form of polygons with the number of sides n_1 and n_2. Here, $\Delta V = v - n_1 - n_2 + 2$, $\Delta E = e - n_1 - n_2 + 1$, $\Delta F = f - 2$, i.e. $\Delta(V - E + F) = (v - e + f) - 1 = 1$.

In the vertex-sharing case, when deleting one polyhedron, it is necessary to consider k faces with a common vertex (Fig. 3, upper part). Let these faces be polygons with n_i angles, where i varies from 1 to k. In this case, $\Delta V = v - (n_1 + n_2 + \ldots.+ n_k) + k + k - 1$. Here the sum $(n_1 + n_2 + \ldots n_k)$ compensates for the deletion of vertices belonging to the faces adjacent to the central vertex (black and gray vertices). The first term k eliminates double counting of black vertices. The second k eliminates k-fold counting repetition of the central vertex in the sum $(n_1 + n_2 + \ldots+ n_k)$. It remains to subtract one, since the central vertex still needs to be excluded from the total number of vertices of the polyhedron being deleted. Similarly, $\Delta E = e - (n_1 + n_2 + \ldots.+ n_k) + k$, $\Delta F = f - k$. Therefore, $\Delta(V - E + F) = (v - e + f) - 1 = 1$. Thus, for any removal of one adjacent polyhedron, $\Delta(V - E + F) = 1$. -

Now consider the general case of a structure without holes. Let an arbitrary number of faces become external when a polyhedron is removed (Fig. 1b). These faces form a simply connected set. One can always perform such a deletion. Otherwise the connectivity of the structure as a whole changes (the number of holes changes or the general structure is divided into two parts). The set of components of the polyhedron to be deleted (vertices, edges, and faces, the numbers of which are denoted as v, e, f) can be divided into two subsets: the external components to be deleted and the internal components shared with the remaining part (v_{in}, e_{in}, f_{in}). In this case, we get:

$$\Delta(V - E + F) = (v - e + f) - (v_{¿} - e_{¿} + f_{¿}) = 2 - 1 = 1 \quad (23)$$

Here, for the polyhedron to be removed, we used formulas (1) and (2). This is also true when two parts of the inner surface of the polyhedron being removed (Fig. 1b) are connected by a single vertex (articulation point of the graph). To prove formula (2) in this case, you only need to add one edge, forming a triangle at the junction. In this case, ΔV = 0, ΔE = 1, ΔF = 1, i.e. the value of V – E + F does not change. Thus, for any removal of one adjacent polyhedron Δ(V – E + F) = 1, which means that the general formula is valid for any system of adjacent polyhedra.

3.5 Weak compounds

Stable structures are of primary interest. But the general formula obtained is easily generalized to the case of "light touches". For cases when two polyhedra have only one common vertex or one common edge, the validity of formula (21) is proved by following simple transformations.

$$(V_1+V_2-1)-(E_1+E_2)+(F_1+F_2)=2+2-1=N+1 \tag{24}$$

$$(V_1+V_2-2)-(E_1+E_2-1)+(F_1+F_2)=2+2-1=N+1 \tag{25}$$

4 Conclusions

The right side of expression (5) for face sharing of polyhedra can also be written as N + 1, since in this case two polyhedra are adjacent. That is, the range of applicability of formula (21) turns out to be very wide.

The formulas for adjacent polyhedra are based on the Euler formula for a single polyhedron and are a consequence of this formula. At the same time, formula (21) is a generalization of the Euler formula and passes into it when the number of adjacent polyhedra is two. This allows us to take a new look at the Euler formula itself, in which 2 is 1 + *N*, as well as at the concept of topological simple-connectedness and multi-connectedness.

Physicochemical applications of the obtained formula can be related to computer modeling and structural analysis algorithms based on the adjacency matrix, since in this case the characteristics *V*, *E* and *F* are quite easily calculated.

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Author contributions All the results were obtained by me (MVK) personally.

Data availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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