

# On the Polyhedral Graphs with Positive Combinatorial Curvature

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*Abstract: The purpose of this article is to introduce a refinement of DeVos-Mohar conjecture in which the number of vertices of polyhedral graphs with positive combinatorial curvature, which are neither prisms, nor antiprisms, (PCC graphs) plays a significant role. According to the conjecture proposed by DeVos and Mohar, for the maximal vertex number  $V_{\max}$  of a PCC graph, the inequality  $VLB=120 \leq V_{\max} \leq VUB=3444$  is fulfilled. In this paper we show that the lower bound  $VLB$  can be improved. The improved lower bound is  $VLB = 138$ . It is also verified that there are no regular, vertex-homogenous PCC graphs with vertex number greater than 120. We conjecture that for PCC graphs the minimum value of combinatorial curvatures is not less than  $1/380$ . If the conjecture is true this implies that the upper bound  $VUB$  is not greater than 760. Moreover, it is also conjectured that there are no PCC graphs having faces with side-number greater than 19, except two trivalent polyhedral graphs containing 20- and 22-sided faces, respectively.*

*Keywords: combinatorial curvature, planar graph, polyhedra, vertex corona*

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## 1 Introduction

If all of the vertices of a polyhedral graph  $G_P$  have positive combinatorial curvatures only, then  $G_P$  is said to be a graph with positive combinatorial curvature [1,2,3]. Let  $\mathfrak{R}$  be the set of polyhedral graphs with positive combinatorial curvature, which does not contain the graphs of prisms and antiprisms. A graph included in  $\mathfrak{R}$  is called a PCC graph. DeVos and Mohar proposed the following conjecture, which is still open: For the maximal vertex number  $V_{\max}$  of PCC graphs in  $\mathfrak{R}$ , the inequality  $120 \leq V_{\max} \leq 3444$  is fulfilled [1]. In this paper we show that the conjectured lower bound ( $V_{LB}=120$ ) can be improved. It will be verified that for any PCC graph, the maximum number of vertices is not less than 138.

## 2 Background: Definitions and Notation

Consider a polyhedral graph with vertex number  $V$ . The combinatorial curvature  $\Phi(X_j)$  of an  $r$ -valent vertex  $X_j$  ( $j=1,2,\dots,V$ ) is defined as

$$\Phi(X_j) = 1 - \frac{r}{2} + \frac{1}{n_{j,1}} + \frac{1}{n_{j,2}} + \dots + \frac{1}{n_{j,r(j)}} \quad (1)$$

where  $n_{j,1}, n_{j,2}, \dots, n_{j,r(j)}$  are the side-numbers of  $r$  polygons incident with vertex  $X_j$ . It is known that for an arbitrary polyhedral graph the sum of combinatorial curvatures satisfies the relation [1,2,3]

$$\sum_{j=1}^V \Phi(X_j) = \chi \quad (2)$$

In Eq.(2)  $\chi$  is the Euler-characteristic, which equals 2 for polyhedral graphs. The fundamental properties of PCC graphs can be summarized as follows:

- i The set of PCC graphs ( $\mathfrak{R}$ ) is finite [1]. All prisms and antiprisms are represented by polyhedral graphs with positive combinatorial curvature, but their number is infinite.
- ii The number of vertices is not greater than 3444 [1].
- iii The maximal number of edges incident to a vertex is less than 6. This implies that if a PCC graph has a vertex of valency 5, it contains at least four triangles, if it has a vertex of valency 4, then it contains at least one triangle.
- iv The graph of the snub icosidodecahedron with 60 vertices is the largest PCC graph which has vertices of valency 5, only.

From Eq.(2) it follows that the number of vertices  $V$  of a PCC graph can be easily estimated if we know the minimum value  $\Phi_{\min}$  of the possible combinatorial curvatures. In this case we have  $V \leq 2/\Phi_{\min}$ . It is obvious that the maximum value of  $\Phi(X_j)$  is  $1/2$ , this value is valid for the tetrahedron. A polyhedral graph is called a vertex homogenous graph (VH-graph), if its combinatorial curvatures are equal in each vertex (i.e.  $\Phi(X_j) = 2/V$  is fulfilled for  $j=1,2,\dots,V$ ). For example, Platonic and Archimedean polyhedra, prisms and antiprisms are represented by VH graphs. It is obvious that every VH-graph which is neither a prism nor an antiprism is a PCC graph.

A polyhedral graph  $G_p$  is called a regular ( $\rho$ -regular) graph if all vertices of  $G_p$  have the same valency  $\rho$ , where  $\rho = 3, 4$  or  $5$ . It is worth noting that among PCC graphs there can exist vertices with identical (equal) positive combinatorial curvatures, but with different numbers of valency. It is conjectured that every vertex homogenous graph is regular.

Consider a subset  $\mathfrak{R}_S = \mathfrak{R}_S(n_1, n_2, \dots, n_k, \dots, n_K)$  of  $\mathfrak{R}$  where  $n_k$  stands for the side number of faces, for which  $3 \leq n_1 < n_2 < \dots < n_k, \dots < n_K, k=1, 2, \dots, K$ , and  $K \geq 1$  is a positive integer. This means that the number of possible face types is equal to  $K$  for any graphs in subset  $\mathfrak{R}_S$ . (In other words, all polyhedral graphs in  $\mathfrak{R}_S$  have faces with  $K$  different side-numbers, exactly). In certain cases,  $\mathfrak{R}_S$  is identical to the empty set, i.e.  $\mathfrak{R}_S = \emptyset$ . In case  $K=1$ , we have  $\mathfrak{R}_S(n_1) = \emptyset$  if  $n_1=4$  or  $n_1 \geq 6$ . The graph of dodecahedron is the unique PCC graph which is composed of pentagons only. For example, it is easy to see that  $\mathfrak{R}_S(5,10) = \emptyset$ , because there are no PCC graphs composed of 5- and 10-gons.

For set  $\mathfrak{R}_S(n_1, n_2, \dots, n_k, \dots, n_K)$  we define the upper bound  $V_{US}$  on the maximum vertex number as follows

$$V_{US} = \left\{ \max V(G_S) \mid G_S \in \mathfrak{R}_S \right\} \quad (3)$$

In Eq.(3)  $V(G_S)$  denotes the number of vertices of an arbitrary graph  $G_S \in \mathfrak{R}_S$ . If  $\mathfrak{R}_S$  is identical to the empty set, then  $V_{US} = 0$ , by definition. It is obvious that inequality  $V_{US} \leq 3444$  holds for any subset  $\mathfrak{R}_S$ . In other words, for an arbitrary PCC graph in  $\mathfrak{R}_S$ , the corresponding vertex number is not greater than 3444 [1].

Graphs  $G_{S,1}, G_{S,2}, \dots, G_{S,z}, \dots, G_{S,Z} \in \mathfrak{R}_S(n_1, n_2, \dots, n_k, \dots, n_K)$  are called maximal (more exactly maximal with respect to  $\mathfrak{R}_S$ ) if equality  $V_{US} = V(G_{S,1}) = V(G_{S,2}), \dots = V(G_{S,Z})$  is fulfilled for  $z=1, 2, \dots, Z$ , where  $Z$  is a positive integer. Considering the polyhedral graphs consisting of triangles, there are only three vertex homogenous graphs in  $\mathfrak{R}_S(3)$ . Among these polyhedra only the tetrahedron and the icosahedron are represented by PCC graphs, the octahedron is a triangular antiprism. The graph of icosahedron with vertex number of 12 is the unique maximal PCC graph in  $\mathfrak{R}_S(3)$ . It is worth noting that in  $\mathfrak{R}_S(3,4)$  there exist four distinct polyhedra represented by VH-graphs with vertex number of 24. All of them are characterized by maximal PCC graphs (the snub cube which has two different chiralities, the rhombicuboctahedron and the Miller polyhedron (called pseudo-rhombicuboctahedron) which is not Archimedean). In  $\mathfrak{R}_S(5,6)$  there is only one VH-graph, this maximal PCC graph corresponds to the truncated icosahedron (the so-called Buckminster fullerene).

In **Fig. 1** the great rhombicosidodecahedron (truncated icosidodecahedron) is shown. It has 120 vertices, 180 edges and 62 faces of regular polygons: 30 squares, 20 hexagons and 12 decagons. The graph of the great rhombicosidodecahedron is a VH-graph, since values of combinatorial curvatures are equal for all vertices,  $(1-3/2 + (1/4+1/6+1/10)) = 1/60$ .

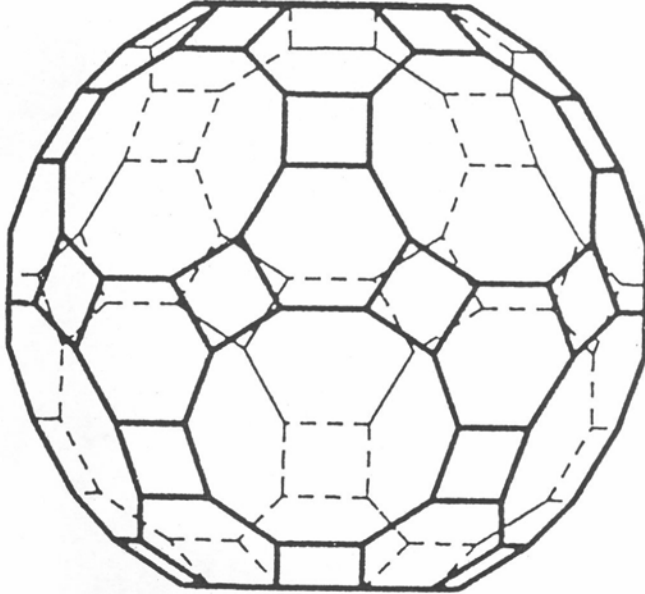


Figure 1

The great rhombicosidodecahedron

As far as the lower bound of maximum vertex number is concerned, the conjectured number of vertices for PCC graphs is equal to 120 [1]. This is identical to the vertex number of the great rhombicosidodecahedron [1]. The theoretical upper bound of maximum vertex number ( $V_{UB} = 3444$ ) found by DeVos and Mohar corresponds to a vertex number of a “hypothetic” trivalent VH-graph composed only of 3-, 7- and 41-gons. We will show that there exist no trivalent PCC graphs composed of 3-, 7- and 41-gons for which the vertex numbers are equal to 3444. Moreover, it will be verified that there exist PCC graphs with vertex numbers greater than 120.

### 3 Results

The main results are represented by the following six theorems.

**Theorem 1** There is no trivalent PCC graph in  $\mathfrak{R}_S(3,7,b)$  if  $b > 11$  positive integer.

**Proof.** The proof is based on computational results obtained by checking the fulfillment of necessary conditions given in the form of various equations and inequalities. We used the following three lemmas:

**Lemma 1** Consider a trivalent polyhedral graph composed of  $\alpha$ -,  $\beta$ - and  $\gamma$ -sided polygons. Let us denote by  $N_\alpha$ ,  $N_\beta$  and  $N_\gamma$  the corresponding number of faces. The

following well-known necessary conditions for the existence of such a graph (polyhedron) are easily derivable from Euler's formula:

$$\frac{1}{N_P}(\alpha N_\alpha + \beta N_\beta + \gamma N_\gamma) < 6 \quad (4)$$

$$(6 - \alpha)N_\alpha + (6 - \beta)N_\beta + (6 - \gamma)N_\gamma = 12 \quad (5)$$

where  $N_\alpha + N_\beta + N_\gamma = N_P$

**Lemma 2** There are no edge-neighbor triangles in a trivalent polyhedral graph with vertex number greater than 4. (The exceptional case of  $V=4$  corresponds to the graph representing a tetrahedron).

To prove this, let us suppose that there are two edge-neighbor triangles (i.e. two triangles with a common edge) in a trivalent polyhedral graph  $G_T$ . By deleting vertices  $X_A$  and  $X_C$  of the neighbor triangles we have separated graph components. (See Fig. 2)

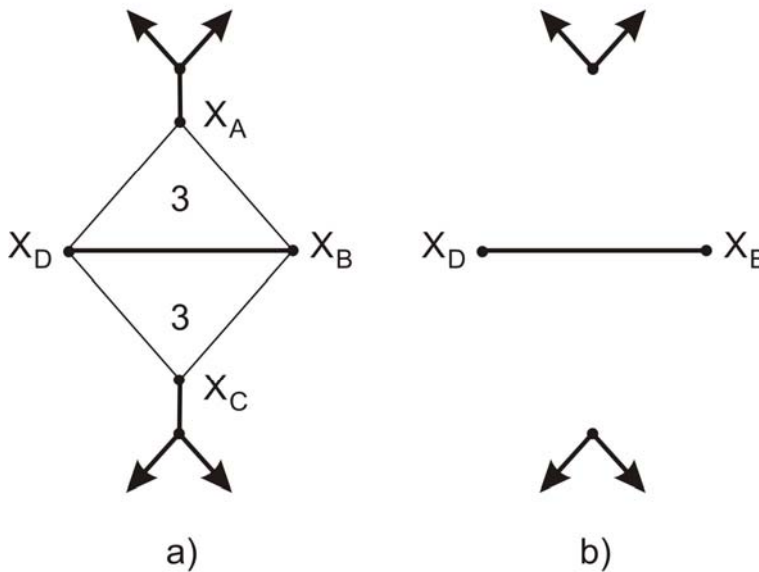


Figure 2

A 2-connected, trivalent, planar graph including edge-neighbor triangles  
 (a) The original graph. (b) The graph obtained by deleting vertices  $X_A$  and  $X_C$ .

It follows that  $G_T$  must be only 2-connected; consequently it is a non-polyhedral graph. This implies that all triangles are isolated in a trivalent polyhedral graph. As an example, the smallest 2-connected, planar, non-polyhedral, trivalent graph

is illustrated in **Fig. 3a**. It is worth noting that this graph can be represented by a non-convex polyhedron. (See. **Fig. 3b**.) (From the previous considerations it follows that there are no trivalent PCC graphs composed of 3- and 7-gons only.)

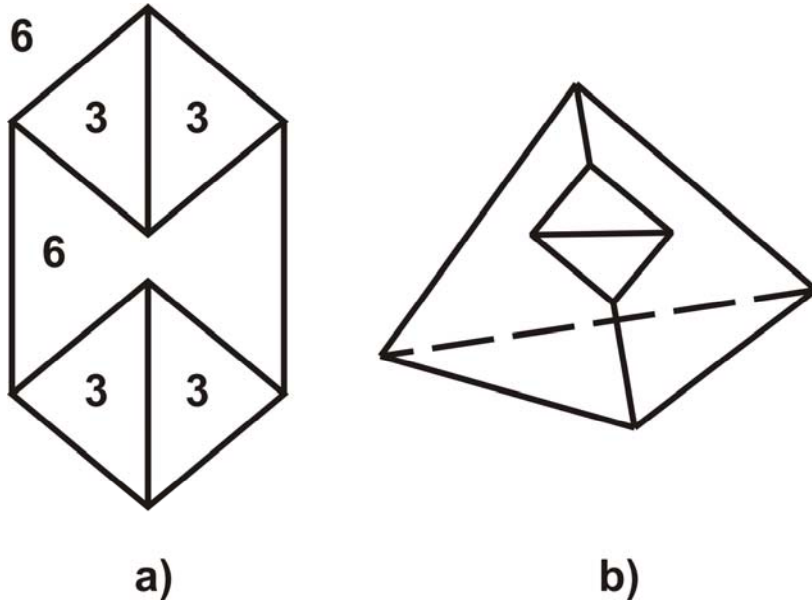


Figure 3

The smallest 2-connected, trivalent planar graph (a) and its 3-dimensional representation (b)

**Lemma 3** Consider a trivalent polyhedral graph composed of  $\alpha$ -,  $\beta$ - and  $\gamma$ -sided polygons. As it is illustrated in **Fig. 4**, by taking into consideration the types of vertex coronas, each vertex can be classified into 10 distinct classes denoted by  $C_{\alpha,\alpha,\alpha}$ ,  $C_{\alpha,\alpha,\beta}$ , ...,  $C_{\gamma,\gamma,\gamma}$ , respectively. Let  $V_1, V_2, \dots, V_{10}$  be the corresponding numbers of vertices belonging to different vertex configurations. It can be proved that [4]

$$\frac{1}{V} \sum_{i=1}^{10} V_i M_i = \frac{\langle n^2 \rangle}{\langle n \rangle} \quad (6)$$

In Eq.(4)  $V=V_1 + V_2 + \dots + V_{10}$ , quantities  $M_1, M_2, \dots, M_{10}$  are the corresponding vertex coordination numbers shown in **Fig. 4**, and

$$\langle n^k \rangle = \frac{1}{N_p} (\alpha^k N_\alpha + \beta^k N_\beta + \gamma^k N_\gamma) \quad (7)$$

is the  $k$ th moment of the side numbers of polygons [4]. It should be noted that an extended version of Eq.(6) is valid for 4- and 5-regular polyhedral graphs [4].

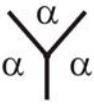


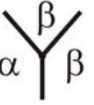

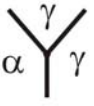




 $C_{\alpha,\alpha,\alpha}$ $M_1 = \frac{\alpha+\alpha+\alpha}{3}$	 $C_{\alpha,\alpha,\beta}$ $M_2 = \frac{\alpha+\alpha+\beta}{3}$	 $C_{\alpha,\alpha,\gamma}$ $M_3 = \frac{\alpha+\alpha+\gamma}{3}$	 $C_{\alpha,\beta,\beta}$ $M_4 = \frac{\alpha+\beta+\beta}{3}$	 $C_{\alpha,\beta,\gamma}$ $M_5 = \frac{\alpha+\beta+\gamma}{3}$
 $C_{\alpha,\gamma,\gamma}$ $M_6 = \frac{\alpha+\gamma+\gamma}{3}$	 $C_{\beta,\beta,\beta}$ $M_7 = \frac{\beta+\beta+\beta}{3}$	 $C_{\beta,\beta,\gamma}$ $M_8 = \frac{\beta+\beta+\gamma}{3}$	 $C_{\beta,\gamma,\gamma}$ $M_9 = \frac{\beta+\gamma+\gamma}{3}$	 $C_{\gamma,\gamma,\gamma}$ $M_{10} = \frac{\gamma+\gamma+\gamma}{3}$

Figure 4

The ten possible vertex arrangements (vertex coronas) in a trivalent polyhedral graph

By using the three lemmas outlined above, the main steps of the proof are as follows:

- 1 Consider a subset  $\mathfrak{R}_{SG}(3,a,b)$  of  $\mathfrak{R}_S(3,a,b)$ . We assume that  $\mathfrak{R}_{SG}(3,a,b)$  contains trivalent PCC graphs consisting of 3-gons, a-gons and b-gons only, and for any graph of  $\mathfrak{R}_{SG}(3,a,b)$  the following inequalities are fulfilled:

$$6 \leq a < b \quad (8a)$$

$$\Phi(3, a, b) = 1 - \frac{3}{2} + \frac{1}{3} + \frac{1}{a} + \frac{1}{b} > 0 \quad (8b)$$

$$\Phi(3, b, b) = 1 - \frac{3}{2} + \frac{1}{3} + \frac{1}{b} + \frac{1}{b} \leq 0 \quad (8c)$$

$$\Phi(a, a, a) = 1 - \frac{3}{2} + \frac{1}{a} + \frac{1}{a} + \frac{1}{a} \leq 0 \quad (8d)$$

In the equations above,  $\Phi(3,a,a)$ ,  $\Phi(3,a,b)$ ,  $\Phi(3,b,b)$  and  $\Phi(a,a,a)$  denote the corresponding combinatorial curvatures. Every graph included in  $\mathfrak{R}_{SG}$  has a positive combinatorial curvature in vertices of type of  $V(3,a,a)$  and  $V(3,a,b)$ , for which  $\Phi(3,a,a) > \Phi(3,a,b) > 0$  is fulfilled.

It is easily seen that only the following PCC graphs satisfy the conditions formulated by Eqs.(8a-8d): all trivalent polyhedral graphs in  $\mathfrak{R}_S(3,6,b)$  if  $b \geq 12$ , in  $\mathfrak{R}_S(3,7,b)$  if  $12 \leq b \leq 41$ , in  $\mathfrak{R}_S(3,8,b)$  if  $12 \leq b \leq 23$ , in  $\mathfrak{R}_S(3,9,b)$  if  $12 \leq b \leq 17$ , in  $\mathfrak{R}_S(3,10,b)$  if  $12 \leq b \leq 14$  and  $\mathfrak{R}_S(3,11,12)$ .

- 2 Let  $N_3$ ,  $N_a$  and  $N_b$  be the number of 3-,  $a$ - and  $b$ -sided faces, respectively. Since  $\mathfrak{R}_{SG}$  is a subset of trivalent polyhedral graphs, according to Lemma 1 we have

$$(3N_3 + aN_a + bN_b) < 6N \quad (9)$$

$$3N_3 + (6 - a)N_a + (6 - b)N_b = 12 \quad (10)$$

where  $N = N_3 + N_a + N_b$ .

- 3 From Eqs.(8a-8d) it follows that not only the triangles are isolated but all  $b$ -sided faces as well. (See **Fig. 5**)

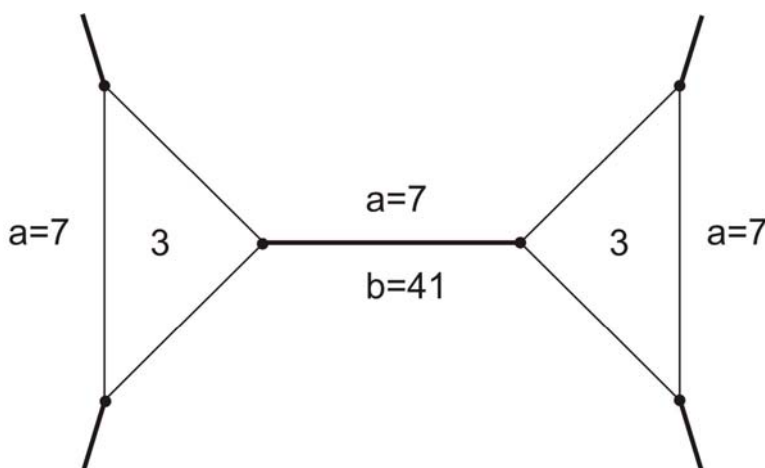


Figure 5

Isolated triangles in a trivalent PCC graph of  $\mathfrak{R}_{SG}$  composed only of 3-, $a$ - and  $b$ -sided polygons

Moreover, we can conclude that each vertex is incident with a vertex of an isolated triangle. Hence, for any graph of  $\mathfrak{R}_{SG}$  we obtain

$$3N_3 = V \quad (11)$$

Since each vertex is incident with a vertex of an  $a$ -sided polygon as well, inequality

$$V \leq aN_a \quad (12)$$

yields. (See **Fig. 5**).

- 4 From Eqs.(11-12) we have

$$aN_a - V = aN_a - 3N_3 \geq 0 \quad (13)$$



Consequently,

$$\frac{aN_a}{3} \geq N_3 \quad (14)$$

- 5 Since all triangles and all b-sided polygons are isolated, this implies that there is no polyhedral graph in  $\mathfrak{R}_{SG}$  for which b is an odd integer. This can be easily verified on the basis of **Fig. 6**.

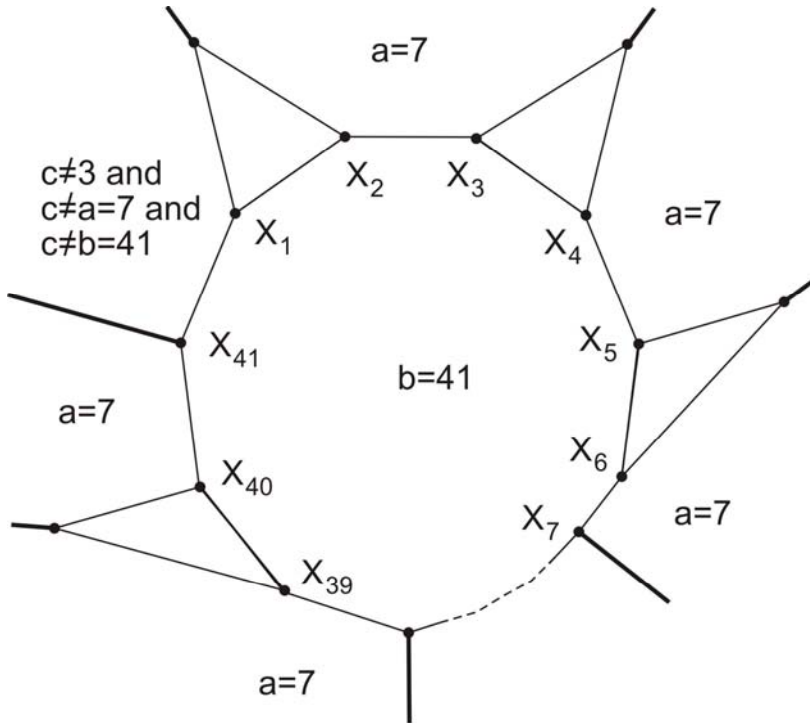


Figure 6

The neighborhood of b-sided faces in a PCC graph of  $\mathfrak{R}_{SG}$  composed only of 3-, a- and b-sided polygons (for case: a=7 and b=41)

As we can conclude, the edge neighbors of b-sided polygons are or triangles either a-sided polygons, only. The sum of triangles and a-sided polygons should be equal to b, but two a-sided polygons having common edges with a b-sided one, cannot be edge-neighbors. Moreover, as it is demonstrated in **Fig. 6**, if b is an even number, then inequality

$$N_3 \geq \frac{b}{2} N_b \quad (15)$$

should be fulfilled. From Eqs.(11-15) we obtain

$$aN_a \geq 3N_3 = V \geq \frac{3b}{2}N_b \quad (16)$$

Inequality (16) gives a necessary condition for the existence of a graph in  $\mathfrak{R}_{SG}$ .

- 6 Because all triangles and b-sided polygons are isolated, and inequalities (12-16) are valid, this implies that there exist only two types of vertices (vertex coronas) which should be taken into account for graphs in  $\mathfrak{R}_{SG}$ . These are denoted by  $C_{3,a,a}$  and  $C_{3,a,b}$ . In this case,  $\alpha=3$ ,  $\beta=a$  and  $\gamma=b$  are the corresponding side-numbers of polygons incident with a common vertex. (See Fig. 4.)
- 7 According to Lemmas 2 and 3, as a particular case, from Eq.(6) it follows:

$$\frac{V(3,a,a)M(3,a,a) + V(3,a,b)M(3,a,b)}{V(3,a,a) + V(3,a,b)} = \frac{\langle n^2 \rangle}{\langle n \rangle} \quad (17)$$

where  $V(3,a,a)$  and  $V(3,b,b)$  are the numbers of vertices belonging to the vertex coronas  $C_{3,a,a}$  and  $C_{3,a,b}$  and  $M(3,a,a)=(3+a+a)/3$  and  $M(3,a,b)=(3+a+b)/3$  are the corresponding vertex coordination numbers. It is obvious that Eq.(17) represents a useful necessary condition for checking the existence of PCC graphs.

- 8 Equations (4-17) can be efficiently used to predict whether a particular subset of trivalent PCC graphs exists or not. More exactly, if there is no solution to Eqs. (4-17) for positive integers  $a$ ,  $b$ ,  $N_3$ ,  $N_a$  and  $N_b$  we can conclude that this subset of PCC graphs is empty. Based on the concept outlined above, we checked by computer all possible cases concerning the existence of trivalent PCC graphs in  $\mathfrak{R}_{SG}$ . By performing computations, we verified, that there do not exist trivalent PCC graphs in  $\mathfrak{R}_S(3,7,b)$  if  $b > 11$ . Consequently, there are no trivalent PCC graphs composed of 3-, 7- and 41-gons, only.

**Theorem 2** There is no trivalent PCC graph in  $\mathfrak{R}_S(3,8,b)$  if  $b > 22$  positive integer. Moreover, if  $b=22$  there exists a trivalent PCC graph  $G_x$  in  $\mathfrak{R}_S(3,8,22)$  composed of 3-, 8- and 22-gons, for which  $V(G_x) = 66$ .

**Proof.** In this case, there are two types of vertex corona with positive combinatorial curvature (denoted by  $C_{3,8,8}$  and  $C_{3,8,b}$ ) which should be taken into account. The proof performed by computer was based on the same concept that was used in Theorem 1. We found that in a particular case when  $b=22$ , there exists a trivalent PCC graph composed of 3-, 8- and 22-gons for which  $N_3=22$ ,  $N_8=11$  and  $N_{22}=2$ . This graph denoted by  $G_{22}$  corresponds to a truncated 11-gonal prism. In Fig. 7 the corresponding Schlegel diagram is shown.

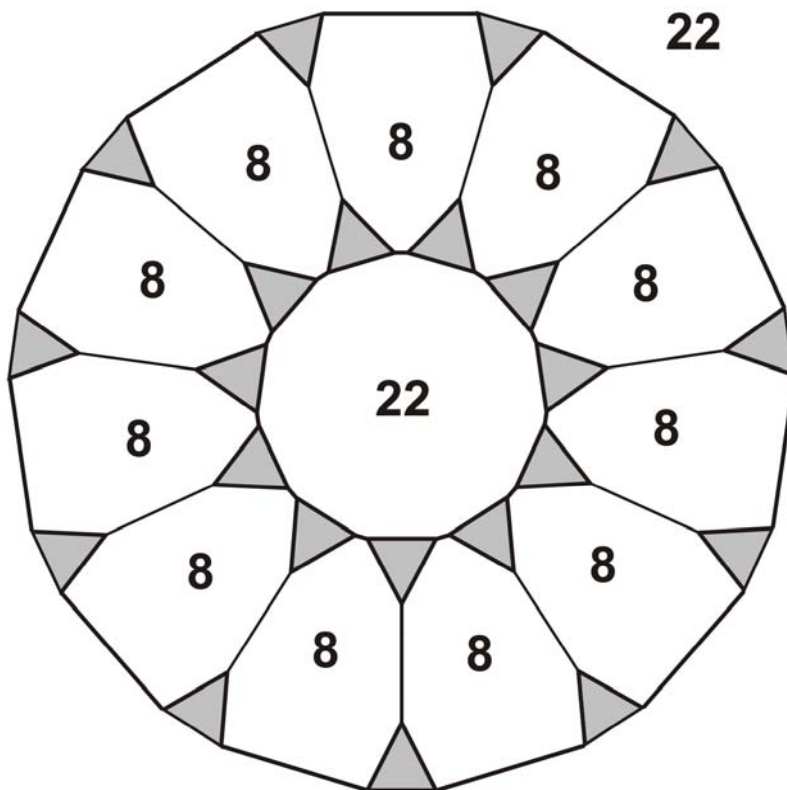


Figure 7

The Schlegel diagram of the PCC graph  $G_{22}$  (truncated 11-gonal prism)

We conjecture that the trivalent graph  $G_{22}$  is maximal with respect to set  $\mathfrak{R}_S(3,8,22)$  where  $V_{US} = 66$ . It is supposed that  $G_{22}$  is the unique PCC graph containing 22-sided faces. Moreover, we assume that there exists only one PCC graph with 20-sided faces. This graph denoted by  $G_{20}$  which is composed of 20 triangles, 10 octagons and two 20-sided polygons, corresponds to a truncated 10-gonal prism. Based on previous considerations, the following conjecture can be formulated: There are no PCC graphs having faces with side-number greater than 19, except the two trivalent polyhedral graphs  $G_{20}$  and  $G_{22}$  containing 20- and 22-sided faces, respectively.

**Theorem 3** There exists a trivalent PCC graph  $G_y$  in  $\mathfrak{R}_S(4,6,11)$  for which  $V(G_y) = 132$ .

**Proof.** For trivalent graphs included in  $\mathfrak{R}_S(4,6,11)$ , we have from Euler's formula that  $2N_4 - 5N_{11} = 12$ . Additionally, there are 5 types of vertex coronas with positive combinatorial curvature (denoted by  $C_{4,4,4}$ ,  $C_{4,4,6}$ ,  $C_{4,4,11}$ ,  $C_{4,6,6}$  and  $C_{4,6,11}$ ) which should be taken into consideration when using Eq.(6) for computational purposes.

In this case,  $\alpha=4$ ,  $\beta=6$  and  $\gamma=11$  are the side-numbers of polygons which are incident with a common vertex. (See **Fig. 4** ) For graphs in  $\mathfrak{R}_S(4,6,11)$ , the minimal value of combinatorial curvature is  $\Phi_{\min} = 1 - 3/2 + (1/4 + 1/6 + 1/11) = 1/132$ . Theoretically, this implies that the possible maximum vertex number is not greater than 264. A computer search gave that the maximum vertex number of PCC graphs in  $\mathfrak{R}_S(4,6,11)$  is less than 198.

In order to find the largest PCC graphs included in  $\mathfrak{R}_S(4,6,11)$ , we preselected seven “possible” subclasses of polyhedral graphs (candidates) whose existence could be expected. For the 7 subclasses denoted by  $\mathbf{G}_A$ ,  $\mathbf{G}_B$ , ..., and  $\mathbf{G}_G$ , the computed topological parameters ( $N_4$ ,  $N_6$ ,  $N_{11}$ ,  $V(4,4,11)$ ,  $V(4,6,6)$ ,  $V(4,6,11)$  and  $V$ ) are summarized in Table 1. Quantities  $V(4,4,11)$ ,  $V(4,6,6)$  and  $V(4,6,11)$  are the numbers of vertices belonging to the three vertex coronas denoted by  $C_{4,4,11}$ ,  $C_{4,6,6}$  and  $C_{4,6,11}$ , respectively. (A common feature of graphs included in the seven subclasses is that they do not contain vertex coronas of type  $C_{4,4,4}$ , and  $C_{4,4,6}$ , which implies that  $V(4,4,4) = V(4,4,6) = 0$ .)

Subset of graphs	Topological parameters						
	$N_4$	$N_6$	$N_{11}$	$V(4,4,11)$	$V(4,6,6)$	$V(4,6,11)$	$V$
<b>GA</b>	36	20	12	12	0	120	132
<b>GB</b>	36	26	12	0	12	132	144
<b>GC</b>	41	24	14	10	0	144	154
<b>GD</b>	41	29	14	0	10	154	164
<b>GE</b>	46	28	16	8	0	168	176
<b>GF</b>	46	32	16	0	8	176	184
<b>GG</b>	51	32	18	6	0	192	198

Table 1

Computed topological quantities for 7 subclasses of possible PCC graphs

From the computed results given in Table 1, it is clear that there do not exist trivalent PCC graphs in  $\mathfrak{R}_S(4,6,11)$  with vertex number greater than 198. By analyzing the local structure of vertex coronas of graphs in Table 1, two cases should be taken into consideration.

CASE 1 concerns the subsets  $\mathbf{G}_B$ ,  $\mathbf{G}_D$  and  $\mathbf{G}_F$  in Table 1. Graphs in  $\mathbf{G}_B$ ,  $\mathbf{G}_D$  and  $\mathbf{G}_F$  have vertex coronas of type  $C_{4,6,6}$  and  $C_{4,6,11}$  with positive vertex numbers. It is easy to show that subsets  $\mathbf{G}_B$ ,  $\mathbf{G}_D$  and  $\mathbf{G}_F$  do not contain PCC graphs. The proof is based on the following observations. Each 11-gon is isolated, and each of them is surrounded by six 4-gons and five 6-gons, exactly. (There are no edge-neighbor hexagons since  $V(6,6,11)=0$ .) Consequently, among 6+5 neighbors of an arbitrary 11-gon there must exist two edge-neighbor squares. But, this is impossible because  $V(4,4,4) = V(4,4,6) = V(4,4,11) = 0$  is fulfilled.

CASE 2 concerns the subsets  $\mathbf{G}_A$ ,  $\mathbf{G}_C$ ,  $\mathbf{G}_E$  and  $\mathbf{G}_G$  in Table 1. Graphs in  $\mathbf{G}_A$ ,  $\mathbf{G}_C$ ,  $\mathbf{G}_E$  and  $\mathbf{G}_G$  have vertex coronas of type  $C_{4,4,11}$  and  $C_{4,6,11}$  with positive vertex

numbers. In this case, the following conclusions can be drawn: It is easily seen that every 11-gon and every hexagon are isolated. Additionally, each vertex is incident with a vertex of an 11-gon, this implies that  $11N_{11}=V$ .

In the following we suppose that all neighborhoods of every 11-gon are identical, that is, each 11-gon is surrounded by  $H$  hexagons and  $(11-H)$  squares exactly, where  $H$  is a positive integer not greater than five.

Figure 8 shows the four possible neighborhoods of an isolated hexagon in a hypothetical PCC graph. From this figure, we can conclude that among the edge-neighbors of a 6-sided polygon there exist always three squares and three 11-sided polygons, exactly (See Fig. 8a.)

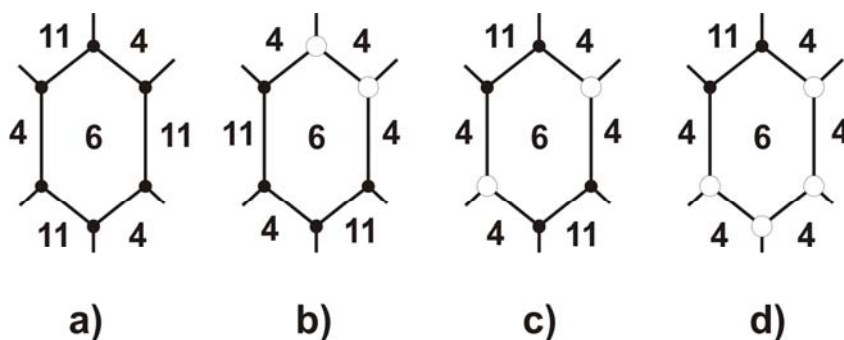


Figure 8

The possible edge-neighbor arrangements of a 6-sided polygon

The previous considerations imply that for the number of common edges, the following equalities should be fulfilled:  $3N_6=HN_{11}$  and  $2N_{11} = (11-H)N_4$ . Since  $N_4 = (12-5N_{11})/2$ , we obtain that  $H = 11 - 2N_4/N_{11} = 6 - 12/N_{11}$ . From this latter equation we can determine the possible solutions for  $H$ . It can be stated that the proper solutions are:  $H=3$  if  $N_{11}=4$ ,  $H=4$  if  $N_{11}=6$  and  $H=5$  if  $N_{11}=12$ .

From this it follows that in subset  $\mathbf{G}_C$ ,  $\mathbf{G}_E$  and  $\mathbf{G}_G$  there do not exist PCC graphs having identical neighborhoods for any 11-gons. It should be emphasized that the results obtained above are only valid, when it is supposed that each isolated 11-gon has identical neighborhood, that is, each 11-sided polygon is surrounded by  $H$  hexagons and  $(11-H)$  squares, exactly.

After analyzing the topological structure of vertex coronas, it was conjectured that only the existence of PCC graphs belonging to  $\mathbf{G}_A$  could be expected (case  $H=5$ ,  $N_{11}=12$ ). It is easy to show that there exists a simple polyhedron which corresponds to a trivalent graph  $\mathbf{G}_{AR}$  in subclass  $\mathbf{G}_A$ . By transforming the great rhombicosidodecahedron we can generate a new polyhedron, which has the same topological parameters as graphs in  $\mathbf{G}_A$ . This simple topological transformation of the great rhombicosidodecahedron can be performed by dividing six squares into two parts. As a result of this operation, we obtain  $6 \cdot 2 + 24 = 36$  squares, 20

hexagons and 12 eleven-sided polygons. (See **Fig. 1**.) Consequently, the number of new vertices, faces and edges will be 132, 68 and 198, respectively. (As can be stated, each 11-gon is surrounded by  $H=5$  hexagons and  $(11-H)=6$  squares.)

The trivalent polyhedron contains two different types of vertices. The corresponding combinatorial curvatures are as follows:  $1-3/2+(1/4+1/4+1/11) = 1/11$  and  $1-3/2+(1/4+1/6+1/11)=1/132$ . It is conjectured that graph  $G_{AR}$  of this new polyhedron is maximal, that is  $G_{AR}$  with vertex number of 132 is the “largest trivalent PCC graph” in  $\mathfrak{R}_S(4,6,11)$ .

**Theorem 4** There exists a non-cubic (non-trivalent) PCC graph which contains 138 vertices.

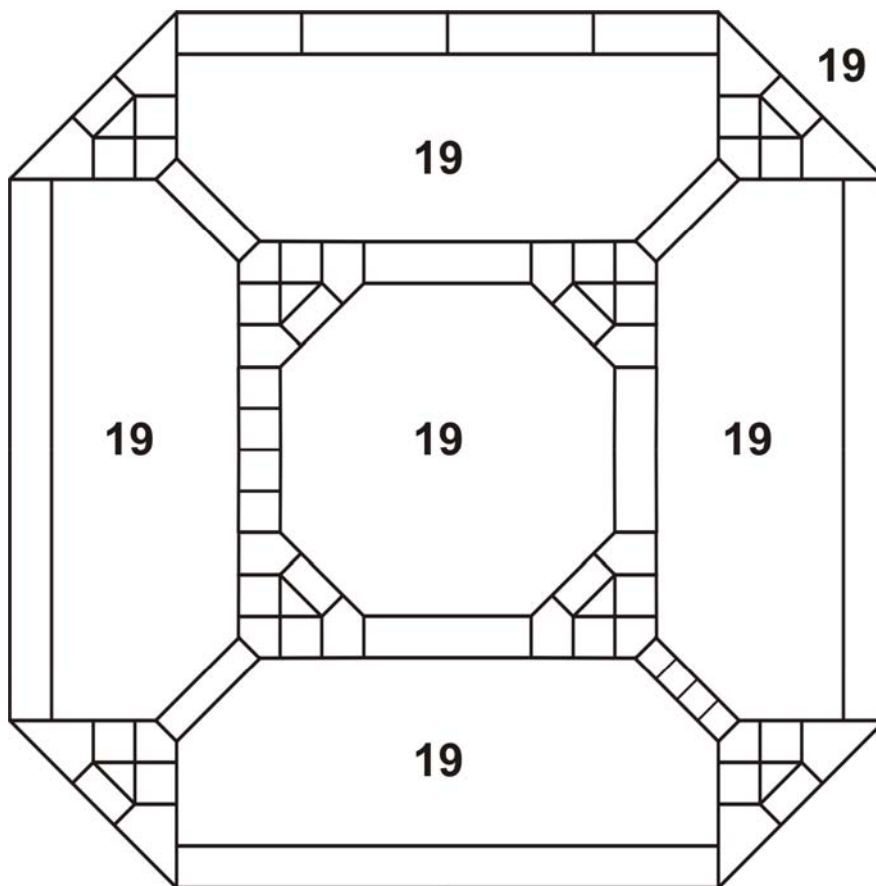


Figure 9

A non-cubic PCC graph with vertex number of 138

**Proof.** In **Fig. 9** the Schlegel diagram of this polyhedron is shown. It has 138 vertices, 219 edges and 83 faces (8 triangles, 45 squares, 24 pentagons and six 19-

gons). As can be seen, there are 114 trivalent and 24 four-valent vertices. The minimum value of combinatorial curvatures is  $1-3/2+(1/4+1/5+1/19) = 1/380$ . Based on this observation, it is conjectured that for PCC graphs, the minimum value of combinatorial curvatures is not less than  $1/380$ . If the conjecture is true, a simple consequence is that the upper bound  $V_{UB}$  of vertices is 760.

**Theorem 5** There is no 3-regular, vertex homogenous PCC graph with vertex number greater than 120.

**Proof.** It is important to note that a number  $0 < \Phi_C \leq 1/4$  cannot be the constant positive combinatorial curvature of a VH graph, if  $2/\Phi_C$  is not a positive integer. A consequence of this observation is that there are no 3-regular, vertex homogenous PCC graphs composed of 5- and 7-gons only, because  $\Phi_C = \Phi(5,5,7) = 1-3/2+(1/5+1/5+1/7) = 3/70$ , consequently  $2/\Phi_C = 140/3 = 46,667$ .

Starting with the concept outlined in Ref.[1], consider a list of positive integers with  $a_1 \leq \dots \leq a_L$ . We say that a vertex  $X$  has a vertex pattern  $V(a_1, \dots, a_i, \dots, a_L)$  if the faces incident with  $X$  may be ordered  $f_1, \dots, f_i, \dots, f_L$  so that  $f_i$  has size  $a_i$  for  $1 \leq i \leq L$ . The complete list of the possible vertex patterns (V-patterns) is given in Ref.[1]. We define a vertex pattern  $V(a_1, \dots, a_i, \dots, a_L)$  to be “bed” if there is no regular VH graphs which contain  $V(a_1, \dots, a_i, \dots, a_L)$ . By definition, a V-pattern which is not bed, is called “good”. For example, considering 5-regular PCC graphs,  $V(3,3,3,3,5)$  is a good V-pattern. This belongs to the graph of the snub icosidodecahedron with 60 vertices which is the “largest” graph among 5-regular PCC graphs.

The candidates of 3-regular vertex-homogenous graphs can be classified into 5 groups which are denoted by  $\Pi_0$ ,  $\Pi_1$ ,  $\Pi_2$ ,  $\Pi_3$  and  $\Pi_4$ , respectively.  $\Pi_0$  contains the monofaced,  $\Pi_1$ ,  $\Pi_2$ ,  $\Pi_3$  contains the bifaced, and  $\Pi_4$  includes the possible trifaced graphs, respectively.

Group  $\Pi_0$  includes only the tetrahedron and the dodecahedron, since the cube is a 4-sided prism. The graph of the dodecahedron is the largest PCC graph in Group  $\Pi_0$ .

Group  $\Pi_1$  contains the following V-patterns:  $V(3,5,5)$ ,  $V(3,6,6)$ ,  $V(3,7,7)$ ,  $(3,8,8)$ ,  $V(3,9,9)$ ,  $V(3,10,10)$  and  $V(3,11,11)$ . It is easy to show that  $V(3,11,11)$  is a bed V-pattern. It follows that the graph belonging to  $V(3,10,10)$  is considered as the largest 3-regular, vertex-homogenous graph in Group  $\Pi_1$ . This graph represents the truncated dodecahedron with 60 vertices.

Group  $\Pi_2$  includes only three V-patterns:  $V(4,5,5)$ ,  $V(4,6,6)$  and  $V(4,7,7)$ . It can be verified that  $V(4,5,5)$  and  $V(4,7,7)$  are bed V-patterns. The only good V-pattern is  $V(4,6,6)$  which corresponds to the truncated octahedron with 24 vertices.

Group  $\Pi_3$  contains five V-patterns:  $V(5,5,6)$ ,  $V(5,5,7)$ ,  $V(5,5,8)$ ,  $(5,5,9)$  and  $V(5,6,6)$ . It is easy to see that the graph belonging to  $V(5,6,6)$  is considered as the

largest 3-regular, vertex-homogenous PCC graph in Group  $\Pi_3$ . This is equivalent to the Buckminster fullerene with 60 vertices.

Group  $\Pi_4$  includes V-patterns represented by  $V(c_1, c_2, c_3)$  where inequality  $3 \leq c_1 < c_2 < c_3$  holds. It is clear that  $V(c_1, c_2, c_3)$  are good V-patterns only if  $c_1, c_2, c_3$  are even integers. This condition is satisfied only for two particular cases:  $V(4, 6, 8)$  and  $V(4, 6, 10)$ . The first one corresponds to the truncated cuboctahedron (rhombicuboctahedron) with 48 vertices, while the second one belongs to the great rhombicosidodecahedron with 120 vertices. We can conclude that the largest 3-regular, vertex homogenous PCC graph is represented by the great rhombicosidodecahedron.

**Theorem 6** There is no 4-regular, vertex homogenous PCC graph with vertex number greater than 60.

**Proof.** For 4-regular PCC graphs the possible V-patterns are as follows:  $V(3, 3, 3, c)$  if  $3 \leq c$ ,  $V(3, 3, 4, c)$  if  $4 \leq c \leq 11$ ,  $V(3, 3, 5, c)$  if  $5 \leq c \leq 7$  and  $V(3, 4, 4, c)$  if  $4 \leq c \leq 5$ . The graph of the small rhombicosidodecahedron composed of 20 triangles, 30 squares and 12 pentagons is a 4-regular VH graph with 60 vertices. This means that  $V(3, 3, 4, 5)$  is a good V-pattern. For 4-regular, vertex homogenous PCC graphs the following relationships are valid:

$$V\Phi_p = 2 \tag{18a}$$

$$2E = 4V = \sum_k kN_k \tag{18b}$$

$$\sum_{k \geq 3} (4 - k)N_k = 8 \tag{18c}$$

where  $\Phi_p$  is the positive combinatorial curvature,  $E$  is the number of edges, and  $N_k$  is the number of  $k$ -sided faces for  $k \geq 3$ .

Among the possible vertex patterns there are only 4 types for which the vertex numbers of the corresponding 4-regular, VH graphs are greater than 60. These are:  $V(3, 3, 4, 11)$ ,  $V(3, 3, 4, 10)$ ,  $V(3, 3, 4, 9)$  and  $V(3, 3, 5, 7)$ . We will verify that all of them are bad V-patterns. The proof is based on the following considerations. By definition, a  $k$ -sided face  $f_k$  is called an isolated face, if  $f_k$  has no  $k$ -sided edge-neighbor faces. It is easy to see that 4-regular, VH graphs characterized by vertex-patterns  $V(3, 3, 4, 11)$ ,  $V(3, 3, 4, 10)$ ,  $V(3, 3, 4, 9)$  and  $V(3, 3, 5, 7)$  cannot exist if all faces are isolated. We only need to prove that for graphs belonging to patterns  $V(3, 3, 4, 11)$ ,  $V(3, 3, 4, 10)$ ,  $V(3, 3, 4, 9)$ ,  $V(3, 3, 5, 7)$  the equality  $E=3N_3$  holds. This implies that all faces are isolated. We suppose (for a contradiction) that  $V(3, 3, 4, 11)$ ,  $V(3, 3, 4, 10)$ ,  $V(3, 3, 4, 9)$  and  $V(3, 3, 5, 7)$  are good V-patterns. Using an extended version of Eq.(6) given in Ref.[4], we can conclude that the corresponding numbers of vertices are: 264, 120, 72 and 210, while the corresponding face numbers are:  $(N_3=176, N_4=66, N_{11}=24)$ ;  $(N_3=80, N_4=30,$



$N_{10}=12$ ); ( $N_3=48$ ,  $N_4=18$ ,  $N_9=8$ ) and ( $N_3=140$ ,  $N_5=42$ ,  $N_7=30$ ), respectively. Consequently, we obtain  $3N_3=528=E$ ,  $4N_4=11N_{11}=264=V$  for case  $V(3,3,4,11)$ ;  $3N_3=240=E$ ,  $4N_4=10N_{10}=120=V$  for case  $V(3,3,4,10)$ ;  $3N_3=144=E$ ,  $4N_4=9N_9=72=V$  for case  $V(3,3,4,9)$  and  $3N_3=420=E$ ,  $5N_5=7N_7=210=V$  for case  $V(3,3,5,7)$ . For all cases we have that  $E=3N_3$  is fulfilled. We obtain a contradiction to the assumption that  $V(3,3,4,11)$ ,  $V(3,3,4,10)$ ,  $V(3,3,4,9)$  and  $V(3,3,5,7)$  are good V-patterns.

## 4 Final Remarks

The classification of polyhedral PCC graphs cannot be regarded complete as yet. In fact, work is in progress in this direction, and we hope that in subsequent publications an account on that will be given. To characterize quantitatively the geometric structure of PCC graphs, we introduced two topological shape factors  $\Lambda$  and  $\Omega$  defined as

$$\Lambda(G) = \Phi_{\max}(G) / \Phi_{\min}(G) \quad (19)$$

$$\text{and } \Omega(G) = \frac{380}{39} V(G) \Phi_{\min}(G) \quad (20)$$

In Eqs.(19-20), for an arbitrary graph  $G \in \mathfrak{R}$ ,  $V(G)$ ,  $\Phi_{\max}(G)$  and  $\Phi_{\min}(G)$  stand for the corresponding vertex number, the maximal and minimal combinatorial curvatures, respectively.

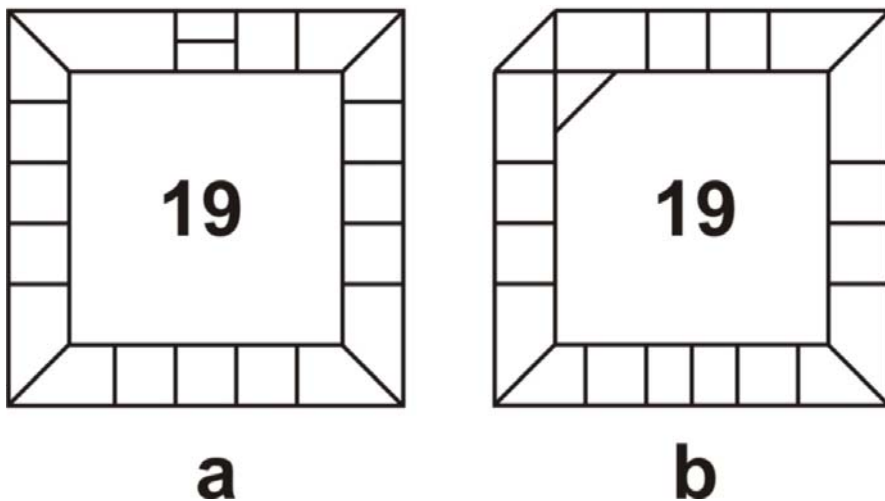


Figure 10

Non vertex-homogenous PCC graphs: a cubic graph with vertex number of 40 (a) and a non-cubic graph with vertex number of 39 (b)

Shape factors  $\Lambda(G)$  and  $\Omega(G)$  are finite positive numbers, for which relationships  $\Lambda \geq 1$  and  $\Omega \leq 2 \cdot 380/39 = 19.487$  are fulfilled. Since  $V(G)\Phi_{\max}(G) \geq 2 \geq V(G)\Phi_{\min}(G)$  we have

$$\Lambda(G)\Omega(G) \geq \frac{760}{39} \geq \frac{\Omega(G)}{\Lambda(G)} \quad (21)$$

It follows that  $\Lambda=1$  and  $\Omega=760/39=19.487$  if the graph  $G$  is vertex-homogenous. We conjecture that for any non vertex-homogeneous PCC graph, the following inequalities are valid:

$$1 < \Lambda(G) \leq 380/5 = 76 \quad (22)$$

and

$$1 \leq \Omega(G) \leq \frac{380 \cdot 7}{39 \cdot 4} = 17.0513 \quad (23)$$

If the conjecture represented by Eq.(22) is true, then the upper bound of  $\Lambda$  is sharp. It is reasonable to suppose that the upper bound (i.e.  $\Lambda=76$ ) is valid only for the trivalent PCC graph shown in **Fig. 10a**. Moreover, it is conjectured that the lower and upper bounds of  $\Omega$  are sharp. We suppose that equality  $\Omega=1$  is fulfilled only for the non-cubic PCC graph depicted in **Fig. 10b**. For example, equality  $\Omega = 17.0513$  holds for a 7-sided polyhedron where the minimum value of combinatorial curvatures is equal to  $1-4/2+(1/3+1/3+1/3+1/4)=1/4$ . This heptahedron has 7 vertices, 12 edges, its faces consist of 4 triangles and 3 quadrilaterals [5]. A common feature of PCC graphs shown in **Fig. 9** and **Fig. 10** is that the minimum values of combinatorial curvatures are identical:  $1-3/2+1/4+1/5+1/19=1/380$ .

## Conclusions

According to the conjecture proposed by DeVos and Mohar, for the maximal vertex number  $V_{\max}$  of a PCC graph (a polyhedral graph with positive combinatorial curvature, which is neither a prism, nor an antiprism), the inequality  $120 \leq V_{\max} \leq 3444$  is fulfilled. In this paper we verified that the lower bound (120) is not sharp, consequently, it can be improved. Based on theoretical investigations and numerical computations we obtained the following results:

- i For any PCC graph the maximum number of vertices is not less than 138.
- ii There is no trivalent PCC graph in  $\mathfrak{R}_S(3,7,b)$  if  $b > 11$  positive integer.
- iii There is no trivalent PCC graph in  $\mathfrak{R}_S(3,8,b)$  if  $b > 22$  positive integer. Moreover, if  $b=22$  there exists a trivalent PCC graph  $G_x$  in  $\mathfrak{R}_S(3,8,22)$  composed of 3-, 8- and 22-gons, for which  $V(G_x)=66$ .
- iv There exists a trivalent PCC graph  $G_y$  in  $\mathfrak{R}_S(4,6,11)$  for which  $V(G_y)=132$ .

- v There exists a non-cubic PCC graph which contains 138 vertices.
- vi There are no regular, vertex homogenous PCC graphs with vertex number greater than 120. The graph of the great rhombicosidodecahedron with 120 vertices is the largest regular, vertex homogenous PCC graph.
- vii It is conjectured that there are no PCC graphs having faces with side-number greater than 19, except the two trivalent polyhedral graphs  $G_{20}$  and  $G_{22}$  containing 20- and 22-sided faces, respectively.
- viii Moreover it is also conjectured that for PCC graphs the minimum value of positive combinatorial curvatures is not less than  $1/380$ .

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