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# The Construction of 4-Regular Polyhedra Containing Triangles, Quadrilaterals and Pentagons *

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**Abstract**

In this paper, several series of 4-regular polyhedra including triangular, quadrilateral and pentagonal faces have been constructed by pasting patches of belts and hats. The sufficient and necessary condition for their existences are also given by describing the construction. Our finding is an effective complement to earlier researches most focused on 3-regular polyhedra for carbon molecular models.

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# 1 Introduction

It is known that polyhedra are widespread as structural models in chemistry. Using the underlying geometrical and symmetrical principles to envisage and classify polyhedral molecules and clusters, presents an enormous challenge at an interface between mathematics and chemistry [4]. Since the famous fullerene $C_{60}$ was discovered in 1985 [27], there have been numerous theoretical progresses in this line of research [14, 19]. A problem that has been a source of fascination to scientists is building a rich treasure house for hypothetical candidates of carbon molecules.

First, we introduce some definations. Let $P$ denotes a 3-dimensional (convex) polytope [20] or a polyhedral graph, i.e., a graph consists with the vertices and the edges of a 3-polytope. The famous Steinitz's result [20, 31] shows that a graph is the polyhedral graph of a 3-polytope if and only if it is planar and 3-connected. A polyhedron is $k$-regular if all its vertices have the same degree $k$. By the planarity and connectivity, we can know that for a $k$-regular polyhedral graph, $k = 3, 4$ or 5. Moreover, the $p$-vector $p(P)$ of a polyhedron $P$ is a sequence $(p_3, ..., p_i, ...)$, where $p_i$ denote the number the $i$-gons of $P$. Then

$$f = \sum_{i\geq 3} p_i, 2e = \sum_{i\geq 3} ip_i = kv,$$

and the Euler formula becomes [16, 20]

$$\sum_{i\geq 3}(2k + 2i - ki)p_i = 4k.$$

If $k = 3$ then

$$3p_3 + 2p_4 + p_5 = 12 + \sum_{i\geq 7}(i - 6)p_i. \tag{1.1}$$

If $k = 4$ then

$$p_3 = 8 + \sum_{i\geq 5}(i - 4)p_i. \tag{1.2}$$

If $k = 5$ then

$$p_3 = 20 + \sum_{i\geq 4}(3i - 10)p_i. \tag{1.3}$$

The Euler formula is related to the Gauss-Bonnet formula in differential geometry [8, 29]. Hence $c_k(i) = \frac{2k+2i-ki}{2k}$ can be considered as the curvature of a face of size $i$ in $k$-regular polyhedra. Note that $c_3(i) = \frac{6-i}{6}, c_4(i) = \frac{4-i}{4}, c_5(i) = \frac{10-3i}{10}$. Most works are focused on positive curvature $c_k(i) > 0$, and nonnegative curvature $c_k(i) \geq 0$. For example, a 3-regular polyhedron of nonnegative curvature only consists of 3-, 4-, 5- and 6-gons, and $3p_3 + 2p_4 + p_5 + 0p_6 = 12$.

A sequence of nonegative integer $p = (p_3, \cdots, p_i, \cdots)$ is called a $p$-vector if it satifies the Euler formula of plane graph, where $p_i$ is considered as the number the $i$-gons of the plane graph. For shorter, we write out only the beginning part of a $p$-vector which interests us and leaving out the infinite sequence of zeros following it. We say a $p$-vector $p = (p_3, \cdots, p_i, \cdots)$ is realizable if there exists a polyhedron $P$ such that $p = p(P)$. In general, $p$ is 3-, 4- or 5-realizable if the polyhedral graph is 3-, 4- or 5-regular, respectively. There some questions about $p$-vector are arised frequently:

(1) What $p$-vectors are realizable?

(2) What values of $p_6$ are 3-realizable?

(3) What values of $p_4$ are 4-realizable?

In fact, the 3-realizable of bifaced polyhedra is of major importance in chemical application [1]. A bifaced polyhedron is a polyhedron only has faces of two kinds of sizes, $p_a$ $a$-gons and $p_b$ $b$-gons ($3 \leq a < b$), so its $p$-vector $p = (\cdots, p_a, \cdots, p_b)$, where $p_i = 0$, if $i \neq a, b$. Fullerenes [27] and Pentaheptites [10] are two particular cases of this kind, which have $p = (0, 0, p_5, p_6)$ and $p = (0, 0, p_5, 0, p_7)$, respectively. For $p = (0, 0, p_5, ..., p_b), b \geq 7$ defined as fulleroids [5, 15], Jendrol' et al. [23] and Kardǒ [25] found necessary and sufficient conditions for some of their existence. More generally, Deza and coworkers have considered a number of polyhedra with different vertex degrees and various $p$-vectors. Their early work [11] has solved the classification of some bifaced regular polyhedra, whose $p$-vectors $p = (0, p_4, 0, p_6)$, $p = (0, 0, p_5, p_6)$, $p = (p_3, p_4)$. Then in 2004 [17], they recalled the well-known method of Goldberg-Coxeter construction to build a large collection of 3- and 4-valent plane graphs, while some related structural properties, such as zigzags and central circuits, are described in [7, 9]. Attention has turned to symmetry as another important research object, and more recently to some 3-regular polyhedra with face size

$i \leq 6$[8] and some 4-regular self-dual polyhedra with faces of size 2,3, and 4 [16].

Herein, restricting our effort to some 4-regular polyhedral graphs with 5-gons (see ref.[22] for our previous work on this topic), which are worth of studying in chemical and biological contexts for at least two reasons. First, 4-valent polyhedra are expected to appear in some supermolecules and clusters, such as space fullerenes [28] and crystal structures [6]. Second, polyhedral structures having all pentagal capsomeres are observed in virus capsids, such as polyoma virus for example[30].

We begin, in the next section, by recalling some preliminaries and listing our main result, while the proof is given in the third section. Conclusions and references will close this article.

## 2 Preliminaries and the main theorem

The progresses of 3- and 4- realizable of polyhedra are summarized in following theorems, which provide some necessary knowledge for the present paper.

**Theorem 2.1** *(1) [20, Grünbaum] or [18, Eberhard] For every sequence* $(p_k|3 \leq k \neq 6)$ *of nonnegative integers satisfying (1.1), there exist values of* $p_6$ *such that the sequence* $(p_k|k \geq 3)$ *is 3-realizable;*

*(2) [20, Grünbaum] and [24, Jucovic] For every solution* $(p_k|3 \leq k \neq 4)$ *of nonnegative integers satisfying (1.2), a values* $p_4$ *exists such that the sequence* $(p_k|k \geq 3)$ *is 4-realizable.*

In the case of 3-realizable of polyhedra of nonnegative curvature, we have $p_i = 0$, if $i \geq 7$ and the $p$-vector is shortened by $(p_3, p_4, p_5, p_6)$. Let $\mathbb{N}_0$ be the set of all natural numbers and 0, i.e. $\mathbb{N}_0 = \{0, 1, 2, \cdots\}$.

**Theorem 2.2** *[21, Grünbaum and Motzkin] and [29, Plastria] or [20]*

*(1) The p-vector* $(0, 6, 0, p_6)$ *and* $(0, 0, 12, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{1\}$*;*

*(2) The p-vector* $(4, 0, 0, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0^e \setminus \{2\}$*;*

*(3) The p-vector* $(3, 1, 1, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0^o \setminus \{1\}$,

*where* $\mathbb{N}_0^e$ *and* $\mathbb{N}_0^o$ *denote the sets of even and odd number of* $\mathbb{N}_0$*, respectively.*

In particular, the following theorem relates to the isolated pentagon rule in fullerenes.

**Theorem 2.3** *[26, Klein and Liu] For every positive integers* $n (n = 20$ *or* $n \geq 25)$ *there exist a polyhedra with* $p_5 = 12$ *and* $p_6 = n$ *such that any two pentagons are disjoint.*

**Theorem 2.4** *[29, Plastria]*

*(1) The p-vectors* $(2, 2, 2, p_6), (1, 3, 3, p_6), (0, 4, 4, p_6), (0, 3, 6, p_6)$ *and* $(0, 2, 8, p_6)$ *is 3-realizable for any* $p_6 \in \mathbb{N}_0$*;*

*(2) The p-vectors* $(2, 1, 4, p_6)$ *and* $(1, 2, 5, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{0\}$*;*

*(3) The p-vectors* $(2, 0, 6, p_6)$ *and* $(0, 5, 2, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{1\}$*;*

*(4) The p-vectors* $(1, 4, 1, p_6), (1, 1, 7, p_6)$ *and* $(0, 1, 10, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{0, 1\}$*;*

*(5) The p-vector* $(3, 0, 3, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{0, 2, 4\}$*;*

*(6) The p-vector* $(2, 3, 0, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{1, 3, 7\}$*;*

*(7) The p-vector* $(1, 0, 9, p_6)$ *is 3-realizable if and only if* $p_6 \in \mathbb{N}_0 \setminus \{0, 1, 2, 4\}$.

These results have solved completely the 3-realizable of $p$-vectors of nonnegative curvature on the plane or the sphere. Plastria [29] also obtained similar results on the torus, the projective plane and the Klein bottle almost.

In the case of 4-realizable of polyhedra of nonnegative curvature, the similarly question becomes easier: $p_i = 0, i \geq 5$, and the shorter $p$-vector is $(p_3, p_4)$.

**Theorem 2.5** *[20, Grünbaum] The p-vector* $(8, p_4)$ *is 4-realizable if and only if* $p_4 \in \mathbb{N}_0 \setminus \{1\}$.

The polyhedra $(0,6,0,p_6)$, $(0,0,12,p_6)$,$(4,0,0,p_6)$ in Theorem 2.2 (1), (2) and $(8,p_4,0,0)$ Theorem 2.5 relate to bifaced polyhedra with only a- and b-gonal faces and $3 \le a < b$. If both $p_a$ and $p_b$ are fixed, then the polyhedron is fixed and trival. If $p_b$ is variational and $p_a$ is fixed in a bifaced polyhedron, then the curvature of $b$-gon must be zero. This means $2k+2b-kb=0$, i.e., $\frac{1}{b}+\frac{1}{k}=\frac{1}{2}$. Considering the planarity of the polyhedral graph, this equation has only two solutions $(k,b)=(3,6)$ and $(4,4)$. For $k=3$, i.e., 3-regular bifaced polyhedra, there are three sub-solutions ($b=6$): $(a,p_a)=(5,12)$ (the famous family of fullerenes), $(4,6)$ (BN-fullerenes) and $(3,4)$. For $k=4$, there only one sub-solution ($b=4$): $(a,p_a)=(3,8)$ (octahedrites [12, 13]). If both $p_a$ and $p_b$ are variational, the $a$-gons must be the positive curvature faces and $b$-gons must be the negative curvature faces. No matter what $k=3,4$ or 5, there are infinity sub-solutions:

$$\begin{aligned}
k=3: &\quad (6-a)p_a &= 12+(b-6)p_b, &\quad a=3,4,5,\ b=7,8,\cdots;\\
k=4: &\quad p_3 &= 8+(b-4)p_b, &\quad b=5,6,\cdots;\\
k=5: &\quad p_3 &= 20+(3b-10)p_b, &\quad b=4,5,\cdots.
\end{aligned}$$

In this paper, we derive a sufficient and necessary condition on the $p$-vector of the family of polyhedra with $k=4, b=5$ and also some zero-curvature 4-gons. Now the $p$-vector is $(p_3,p_4,p_5)$ and Euler formula is

$$p_3 = 8 + p_5.$$

Using similarly methods with Grünbaum and Motzkin's work, we prove the following main result:

**Theorem 2.6** *The p-vector $p=(p_5+8,p_4,p_5)$ is 4-realizable if and only if $p \notin \{(9,0,1),$ $(11,0,3),(13,0,5),(8,1,0),(9,1,1),(9,2,1)\}$.*

# 3 Proof of the main theorem

For certain polyhedra with small number of pentagons, the existence, especially the inexistence can be proved by the performing computer program–*Plantri* [2, 3]. Using the program, we exhaustively enumerate all polyhedra (i.e. all 4-regular and 3-connected planar graph) for certain small value $p_5$. And obtain the existence and inexistence from these results.

The method of proving existence of certain polyhedra with large number of pentagons is similar to the proof Theorem 2.1 and 2.2.

Our proofs begin with the definition of two families of certain configurations, belts $B$ and hats $H$, and the proofs are done by the manipulation of pasting them. The belts and hats are some patches containing 3-gons, 4-gons and 5-gons, see Fig. 1 and Fig. 2. In these patches, all 3-valent vertices (which are called boundary vertices) lie on one or two 4-gonal faces (the boundary cycle of which are called boundary of the patch), and all other vertices are 4-valent. Thus, a belt is a patch with two boundaries, whereas a hat is one with a single boundary. In general, belts and hats are labeled $B_n^m$ and $H_n^m$, where the superscript $m$ and the subscript $n$ denotes the number of $p_4$ except boundary 4-cycles and $p_5$, respectively. When doing the manipulation of belts and hats, we paste their corresponding bounderies together, i.e., the coresponding 4-cycles overlap each other. Accordingly, all 3-valent (boundary) vertices transform to 4-valent with the disappearance of 4-gonal boundaries, and therefore a 4-regular polyhedron is constructed. For example, as shown in Fig. 1, if pasting the boundary of $H_0^0$ to the boundary of $H_6^0$, then a polyhedron $H_6^0+H_0^0$ is obtained, and if pasting two boundaries of $B_8^0$, respectively, to the boundary of $H_0^0$ and the boundary of $H_6^0$, then a polyhedra $H_6^0+B_8^0+H_0^0$ is also obtained. The manipulation of pasting many of belts $B_0^4$ are also called Infaltion [29] and $m$-elongation [7, 9] along a central circuit with length 4.

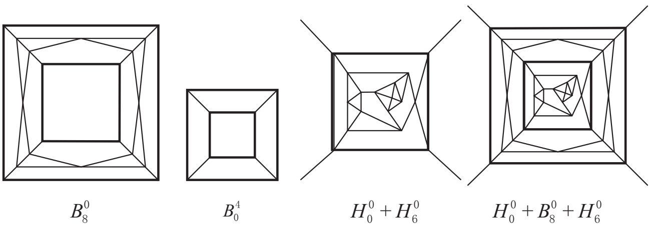


Fig. 1. Belt $B_8^0$, $B_0^4$ and Schlegel projections of polyhedrons $H_6^0+H_0^0$ and $H_6^0+B_8^0+H_0^0$.

**Lemma 3.1** *The p-vector* $p=(p_5+8,0,p_5)$ *is 4-realizable if and only if* $p_5\in\mathbb{N}_0\backslash\{1,3,5\}$.

**Proof:** We construct the polyhedron $P$ by belt $B_8^0$ and hats shown in Fig. 2.

Case 1: $6 \leq p_5 \leq 13$. Let $P = H_0^0 + H_{p_5}^0$, if $6 \leq p_5 \leq 11$ and $P = H_6^0 + H_{p_5-6}^0$ otherwise.

Case 2: $p_5 \geq 14$. Then there exist nonnegative integer $k, r$ such that $p_5 - 6 = 8k + r, 0 \leq r \leq 7$. Now $6 \leq r + 6 \leq 13$. Hence, by Case 1, we may set $P = H_0^0 + kB_8^0 + H_{r+6}^0$, if $0 \leq r \leq 5$ and $P = H_6^0 + kB_8^0 + H_r^0$ otherwise.

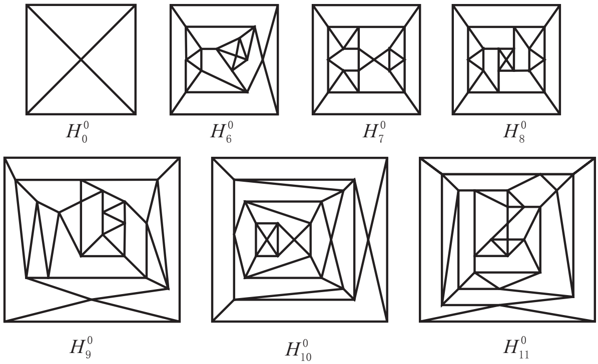


Fig. 2. Some hats with $p_4 = 0$.

Case 3: $p_5 \leq 5$. If $p_5 = 0$ then let $P = H_0^0 + H_0^0$ be the octahedron. The polyhedra with $p_5 = 2, 4$ are listed in Fig. 3. There exists no polyhedron with $p_5 = 1, 3, 5$ and $p_4 = 0$.

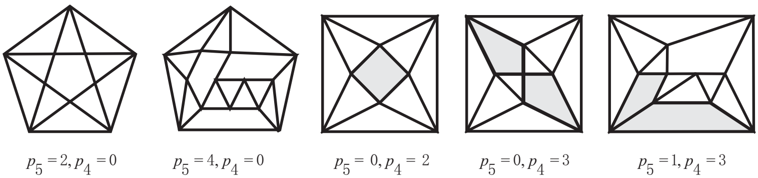


Fig. 3. Some polyhedra with little $p_5$ and $p_4$.

**Lemma 3.2** *The p-vector* $(p_5 + 8, 1, p_5)$ *is 4-realizable if and only if* $p_5 \in \mathbb{N}_0 \setminus \{0, 1\}$.

**Proof:** In the same way, we construct the polyhedron $P$ by belt $B_8^0$ and some hats shown in Fig. 2 and Fig. 4.

Case 1: $2 \leq p_5 \leq 9$. Let $P = H_0^0 + H_{p_5}^1$, if $2 \leq p_5 \leq 7$ and $P = H_6^0 + H_{p_5-6}^1$ otherwise.

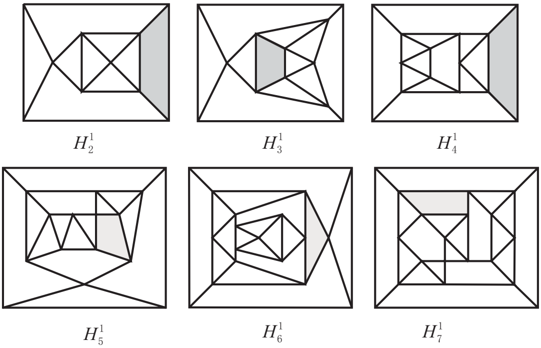


Fig. 4. Some hats with $p_4 = 1$.

Case 2: $p_5 \geq 10$. Then there exist nonnegative integer $k, r$ such that $p_5 - 2 = 8k + r, 0 \leq r \leq 7$. Now $2 \leq r + 2 \leq 9$. Hence, by Case 1, we may set $P = H_0^0 + kB_8^0 + H_{r+2}^1$, if $0 \leq r \leq 5$ and $P = H_6^0 + kB_8^0 + H_{r-4}^1$ otherwise.

Case 3: There exists no polyhedron with $p_5 = 0, 1$ and $p_4 = 1$.

**Lemma 3.3** *The p-vector* $(p_5 + 8, 2, p_5)$ *is 4-realizable if and only if* $p_5 \in \mathbb{N}_0 \setminus \{1\}$.

**Proof:** We construct the polyhedron $P$ by belt $B_8^0$ and hats shown in Fig. 2, Fig. 4 and Fig. 5.

Case 1: $2 \leq p_5 \leq 9$. Let $P = H_0^0 + H_{p_5}^2$, if $2 \leq p_5 \leq 5$ and $P = H_2^1 + H_{p_5-2}^1$ otherwise.

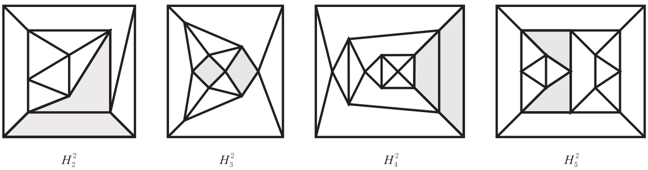


Fig. 5. Some hats with $p_4 = 2$.

Case 2: $p_5 \geq 10$. Then there exist nonnegative integer $k, r$ such that $p_5 - 2 = 8k + r, 0 \leq r \leq 7$. Now $2 \leq r + 2 \leq 9$. Hence, by Case 1, we may set $P = H_0^0 + kB_8^0 + H_{r+2}^2$, if $0 \leq r \leq 3$ and $P = H_2^1 + kB_8^0 + H_r^1$ otherwise.

Case 3: $p_5 \le 1$. The polyhedron with $p_5 = 0$ is listed in Fig. 3. There exists no polyhedron with $p_5 = 1$ and $p_4 = 2$.

**Lemma 3.4** *The p-vector* $(p_5 + 8, 3, p_5)$ *is 4-realizable for all nonnegative integer* $p_5$*.*

**Proof:** We construct the polyhedron $P$ by belt $B_8^0$ and hats shown in Fig. 2, Fig. 4, Fig. 5 and Fig. 6.

Case 1: $2 \le p_5 \le 9$. Let $P = H_0^0 + H_{p_5}^3$, if $2 \le p_5 \le 5$ and $P = H_{p_5-2}^1 + H_2^2$ otherwise.

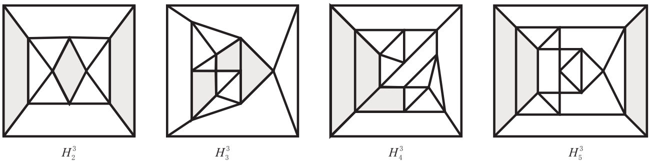


Fig. 6. Some hats with $p_4 = 3$.

Case 2: $p_5 \ge 10$. Then there exist nonnegative integer $k, r$ such that $p_5 - 2 = 8k + r, 0 \le r \le 7$. Now $2 \le r + 2 \le 9$. Hence, by Case 1, we may set $P = H_0^0 + kB_8^0 + H_{r+2}^3$, if $0 \le r \le 3$ and $P = H_r^1 + kB_8^0 + H_2^2$ otherwise.

Case 3: $p_5 \le 2$. The polyhedra with $p_5 = 0, 1$ are listed in Fig. 3.

**Lemma 3.5** *The p-vector* $(p_5 + 8, 4, p_5)$ *is 4-realizable for all nonnegative integer* $p_5$*.*

**Proof:** We construct the polyhedron $P$ by belts $B_8^0, B_0^4$ and hats shown in Fig. 2, Fig. 7 and Fig. 8.

Case 1: $1 \le p_5 \le 5$. Let $P = H_0^0 + H_{p_5}^4$.

Case 2: $p_5 = 0$ or $p_5 \ge 6$. By Lemma 3.1, there exist a polyhedron $P'$ with $p_5$ pentagons and 0 quadrilaterals such that $P' = H_a^0 + kB_8^0 + H_b^0$, where $k, a, b \in \mathbb{N}_0$ and $8k + a + b = p_5$. Then $P = H_a^0 + kB_8^0 + B_0^4 + H_b^0$ is the expected polyhedron.

**Lemma 3.6** *The p-vector* $(9, p_4, 1)$ *is 4-realizable for all integer* $p_4 \ge 3$*.*

**Proof:** We construct the polyhedron $P$ by belt $B_0^4$ and hats shown in Fig. 8.

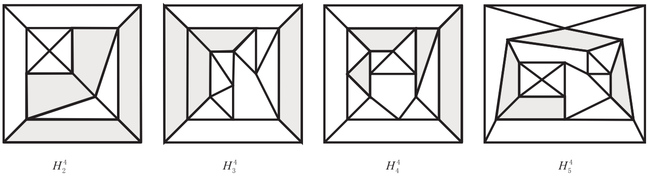


Fig. 7. Some hats with $p_4 = 4$.

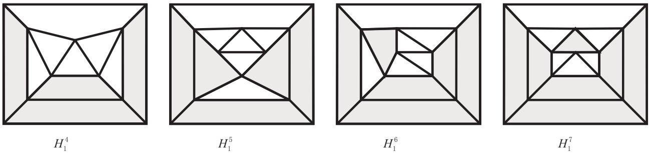


Fig. 8. Some polyhedra with $p_5 = 1$.

Case 1: $4 \leq p_4 \leq 7$. Let $P = H_0^0 + H_1^{p_4}$.

Case 2: $p_4 \geq 8$. Then there exist nonnegative integer $l, s$ such that $p_4 - 4 = 4l + s, 0 \leq s \leq 3$. Now $4 \leq s + 4 \leq 7$. Hence, by Case 1, we may set $P = H_0^0 + lB_0^4 + H_1^{s+4}$.

Case 3: $p_4 \leq 3$. The polyhedra with $p_4 = 3$ are listed in Fig. 3. There exists no polyhedron with $p_5 = 1$ and $p_4 = 0, 1, 2$.

Now it is the time to prove our main result.

**Proof of Theorem 2.6:** Case 1: $p_5 = 0$. This is just the result of Theorem 2.5.

Case 2: $p_5 = 1$. This has been solved in Lemma 3.6.

Case 3: $0 \leq p_4 \leq 4$. They are the results of Lemmas 3.1 to 3.5.

Case 4: $p_4 \geq 5$ and $p_5 \geq 2$. Then there exist nonnegative integer $l, s$ such that $p_4 - 1 = 4l + s$, $0 \leq s \leq 3$. Now $1 \leq s + 1 \leq 4$. Hence, by Lemmas 3.2 to 3.5, there exists a polyhedron $P'$ with $p$-vector $(p_5 + 8, s + 1, p_5)$ and $P' = H_a^{m_a} + kB_8^0 + H_b^{m_b}$, where $a, b, k, m_a, m_b \in \mathbb{N}_0$ and $m_a + m_b = s + 1, a + b + 8k = p_5$. Now let $P = H_a^{m_a} + kB_8^0 + lB_0^4 + H_b^{m_b}$, where $m_a + m_b + 4l = s + 1 + 4l = p_4, a + b + 8k = p_5$. It easy to see that $P$ is the required polyhedron.

# 4 Conclusions

Using belts and hats as building patches, two new classes of 4-regular polyhedra containing pentagons have been constructed. One has only faces of 3-gons and 5-gons, the other has faces of 3-gons, 4-gons and 5-gons. Furthermore, the sufficient and necessary condition for their existence is given.

It has also been shown that 3-regular polyhedra are feasible candidates for carbon molecular models. So the justification of chemical polyhedra is just limit to 3-regular. Likewise, the study of 4-regular polyhedra may be of another interest in forming blueprint for supermolecules and clusters. This systematic research therefore is an effective complement to earlier works.

The symmetry principle derived from nature plays an important role in determining the structure of molecules. Applying symmetry constraints to these polyhedra provide potential models for virus capsids. For patches of belts and hats, they all have positive curvaturtes and main building blocks are pentagons. The construction provides a novel insight into the structural puzzles that especial viruses whose capsomers are all pentamers. The further consideration of such polyhedra with high symmetry shall be discussed in detail elsewise.

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