Polygonal Systems Including the Corannulene and Coronene Homologs: Novel Applications of Pólya's Theorem

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A system of Class Q_q is a polygonal system consisting of one central q-gon circumscribed by q other polygons, which may possess different sizes. As chemical graphs, these systems represent polycyclic conjugated hydrocarbons, which include homologous series of $C_{20}H_{10}$ corannulene and $C_{24}H_{12}$ coronene along with many other molecules of interest in organic chemistry. The problem of isomer enumeration for the Q_q systems is solved completely in terms of generating functions by means of Pólya's theorem.

Introduction

A polycyclic conjugated hydrocarbon is represented as a chemical graph [1] by a system P of simply connected polygons, a polygonal system. By definition, any two polygons in P should either share exactly one edge or be disjoint. In consequence, only vertices of degree two and three will be present, corresponding to secondary and tertiary carbon atoms, respectively. Certain classes of P systems have recently been enumerated [2–5]. Specifically, twenty-three classes of polygonal systems (**I–XXIII**) were defined, and we shall refer to some of these classes below by the Roman numerals; for a full definition of the different forms, the article [3] may be consulted.

In general, the enumeration of isomers is a well-established branch of chemistry. In this connection, the famous Pólya theorem [6, 7] has found very many applications; only a small extract of the relevant literature can be cited here [6–16]. Also several of the classes of polygonal systems referred to above can be enumerated by simple applications of the Pólya theorem. In the following, the applications to the classes **VI** and **XIV** are demonstrated. The main part of the present work represents additional novel applications of Pólya's theorem: the enumerations for classes **V** and **XI** along with extensions of these cases. The results are supposed to be of considerable interest in organic chemistry since several important molecules are represented by the pertinent chemical graphs; $C_{20}H_{10}$ corannulene and $C_{24}H_{12}$ coronene are among them.

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Pólya's Theorem

In the formulation of Harary et al. [11]: The generating function $C(x)$ which enumerates equivalence classes of functions determined by the permutation group A is obtained by substituting the figure counting series $c(x)$ in the cycle index $Z(A)$ as follows. Each variable s_r in $Z(A)$ is replaced by $c(x^r)$. Symbolically we write: $C(x) = Z(A, c(x))$.

Here is not the place to expand fully the contents of Pólya's theorem. It seems more appropriate to describe the special applications with a few necessary explanations.

In all cases of the present work, the figure counting series reflects the variable polygon sizes. Specifically, the powers of x, say i, indicate the number of vertices of degree two in a particular polygon, corresponding to the number of hydrogen atoms at the pertinent ring. Hence $i = 0, 1, 2, 3, \dots$, and

$$c(x) = \frac{1}{1-x} = 1 + x + x^2 + x^3 + \dots . \quad (1)$$

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Preliminary Examples

Consider the polygonal systems of class **VI** [3, 4], viz. the tetracyclic (pyrene-like) systems with two internal vertices each. In this case the permutation group (A) isomorphic with the symmetry group D_2 is appropriate, and the cycle index reads

$$Z(D_2)=\frac{1}{4}(s_1^4+s_2^2+2s_1^2 s_2)\,. \qquad (2)$$

Here one has to insert

$$s_1=c(x)=\frac{1}{1-x}\,,\quad s_2=c(x^2)=\frac{1}{1-x^2}\,, \qquad (3)$$

which yields

$$Z(D_2,c(x))=\frac{1}{4}\left[\frac{1}{(1-x)^4}+\frac{1}{(1-x^2)^2}+\frac{2}{(1-x)^2(1-x^2)}\right]$$
$$=\frac{1}{(1-x)^2(1-x^2)^2}=1+2x+5x^2+8x^3 \quad (4)$$
$$+14x^4+20x^5+30x^6+40x^7+55x^8+\dots\,.$$

This means, for instance, that there are 14 distinct systems of class **VI** with $h=4$, 20 with $h=5$, etc. The result is consistent with the generating functions derived previously [3, 4] in a different and more complicated way.

Consider now the pentacyclic systems **XIV** [3, 4] with three internal vertices each. With respect to $A=C_2$ one finds

$$Z(C_2)=\frac{1}{2}(s_1^5+s_1 s_2^2) \qquad (5)$$

and, after inserting from (3),

$$Z(C_2,c(x))=\frac{1+x^2}{(1-x)^3(1-x^2)^2} \qquad (6)$$
$$=1+3x+9x^2+19x^3+38x^4$$
$$+66x^5+110x^6+170x^7+255x^8+\dots\,,$$

in consistency with the previous result [4].

Classes of Circulenes

Definitions

Consider a system P which consists of a central q-gon circumscribed by q polygons of arbitrary sizes. Denote the class of such systems by Q_q. Here $q=3$, 4, 5, ..., corresponding to triangle, tetragon, pentagon, etc. A member of Q_q corresponds to a polycyclic conjugated hydrocarbon with the formula $C_{2q+h}H_h$, where h is the hydrogen content. Both the closed-shell molecules and unstable (open-shell) radicals are included; in particular, all odd-carbon compounds of the considered category are radicals. The numbers of nonisomorphic systems in Q_q are counted by the generating function $C_q(x)=Z(D_q, c(x))$. In the expansion of $C_q(x)$ into its counting series, the powers of x indicate the hydrogen content, h, in each of the members of Q_q. For every q, the expansion of $C_q(x)$ starts obviously with $1+x$ for $h=0$, 1. The appropriate figure counting series is given in (1).

Central Triangle or Tetragon

The classes Q_3 and Q_4 are identical with **V** and **XI**, respectively. The corresponding generating functions have been derived previously [4, 5] according to somewhat complicated combinatorial analyses. Pólya's theorem gives the same results straightforwardly in the following way:

$$C_3(x)=\frac{1}{6}\left[\frac{1}{(1-x)^3}+\frac{3}{(1-x)(1-x^2)}+\frac{2}{1-x^3}\right]$$
$$=\frac{1}{(1-x)(1-x^2)(1-x^3)}$$
$$=1+x+2x^2+3x^3+4x^4+5x^5$$
$$+7x^6+8x^7+10x^8+\dots\,, \qquad (7)$$

$$C_4(x)=\frac{1}{8}$$
$$\cdot\left[\frac{1}{(1-x)^4}+\frac{2}{(1-x)^2(1-x^2)}+\frac{3}{(1-x^2)^2}+\frac{2}{1-x^4}\right]$$
$$=\frac{1-x+x^2}{(1-x)^2(1-x^2)(1-x^4)}$$
$$=1+x+3x^2+4x^3+8x^4+10x^5$$
$$+16x^6+20x^7+29x^8+\dots\,. \qquad (8)$$

Central Pentagon

The smallest system of the class Q_5 is depicted in Fig. 1; it corresponds to a cluster with ten carbon atoms. The five sites of the polygons, which are to be subjected to variations in sizes, are indicated by inscribed numerals. Herefrom the cycle index $Z(D_5)$ is derived as shown in Table 1. In this table, the symmetry operations of D_5 are correlated with the permuta-

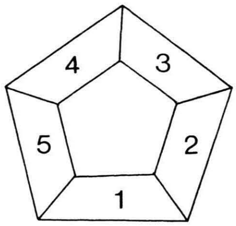

Fig. 1. The smallest system of the class Q_5 ($h=0$).

Table 1. Cycle index for the class Q_5 under the permutation group isomorphic with D_5.

D_5	Permutations	Contribution to cycle index
E	(1) (2) (3) (4) (5)	s_1^5
$2C_5$	(12345), (54321)	$2s_5$
$2C_5^2$	(13524), (42531)	$2s_5$
$5C_2$	(1) (25) (34), (2) (13) (45), (3) (24) (15), (4) (35) (12), (5) (14) (23)	$5s_1 s_2^2$

tions of the sites and expressed in terms of cycles. In the contributions to the cycle index, a subscript to s indicates the length of a cycle, while the superscript gives the number of the cycles in question for a given permutation. The contributions should be added and divided by the group order, which here is ten. In conclusion,

$$Z(D_5)=\frac{1}{10}(s_1^5+5s_1 s_2^2+4s_5). \quad (9)$$

On inserting $s_r=(1-x^r)^{-1}$ according to the prescription in Pólya's theorem, one obtains

$$C_5(x)=\frac{1}{10}\left[\frac{1}{(1-x)^5}+\frac{5}{(1-x)(1-x^2)^2}+\frac{4}{1-x^5}\right] \quad (10)$$

$$=\frac{1-x+2x^3-x^5+x^6}{(1-x)^2(1-x^2)^2(1-x^5)}=1+x+3x^2+5x^3+10x^4+16x^5+26x^6+38x^7+57x^8+\dots .$$

The distribution into symmetry groups for the Q_5 systems was also worked out. Let the pentagonal (D_{5h}), mirror-symmetrical (C_{2v}) and unsymmetrical (C_s) system be counted by the generating functions $P(x)$, $M(x)$ and $A(x)$, respectively. Here the symmetries refer to planar chemical graphs. The crucial results are given in the following, but the details of their derivation are omitted for the sake of brevity. Firstly, $P(x)=(1-x^5)^{-1}$ and

$$M(x)=\frac{x(1+3x+x^2)}{(1-x^2)^2(1-x^5)} \quad (11)$$
$$=x+3x^2+3x^3+6x^4+5x^5+10x^6+\dots .$$

Secondly, $A(x)$ may be determined by means of $J(x)$, the generating function for crude totals with respect to four degrees of freedom [5];

$$J(x)=P(x)+5M(x)+10A(x)=\frac{1}{(1-x)^5}. \quad (12)$$

From (11) and (12), all the numbers of Table 2 are accessible. The total numbers of nonisomorphic systems in class Q_5 are given by $P(x)+M(x)+A(x)$, a generating function equal to $C_5(x)$ of (10). These totals are found in Table 3 under the column $q=5$ along

Table 2. Numbers of isomers of polycyclic conjugated hydrocarbons with six rings and five internal carbons in one ring (class Q_5).

h	Formula	D_{5h}	C_{2v}	C_s
0	C_{10}	1	0	0
1	$C_{11}H$	0	1	0
2	$C_{12}H_2$	0	3	0
3	$C_{13}H_3$	0	3	2
4	$C_{14}H_4$	0	6	4
5	$C_{15}H_5$	1	5	10
6	$C_{16}H_6$	0	10	16
7	$C_{17}H_7$	0	10	28
8	$C_{18}H_8$	0	15	42
9	$C_{19}H_9$	0	15	64
10	$C_{20}H_{10}$	1	20	90
11	$C_{21}H_{11}$	0	21	126
12	$C_{22}H_{12}$	0	28	168

Table 3. Total numbers of isomers of polycyclic conjugated hydrocarbons with $q+1$ rings and q internal carbons in one ring (class Q_q).

	q					
h	3	4	5	6	7	8
0	1	1	1	1	1	1
1	1	1	1	1	1	1
2	2	3	3	4	4	5
3	3	4	5	7	8	10
4	4	8	10	16	20	29
5	5	10	16	26	38	57
6	7	16	26	50	76	126
7	8	20	38	76	133	232
8	10	29	57	126	232	440
9	12	35	79	185	375	750
10	14	47	111	280	600	1282
11	16	56	147	392	912	2052
12	19	72	196	561	1368	3260

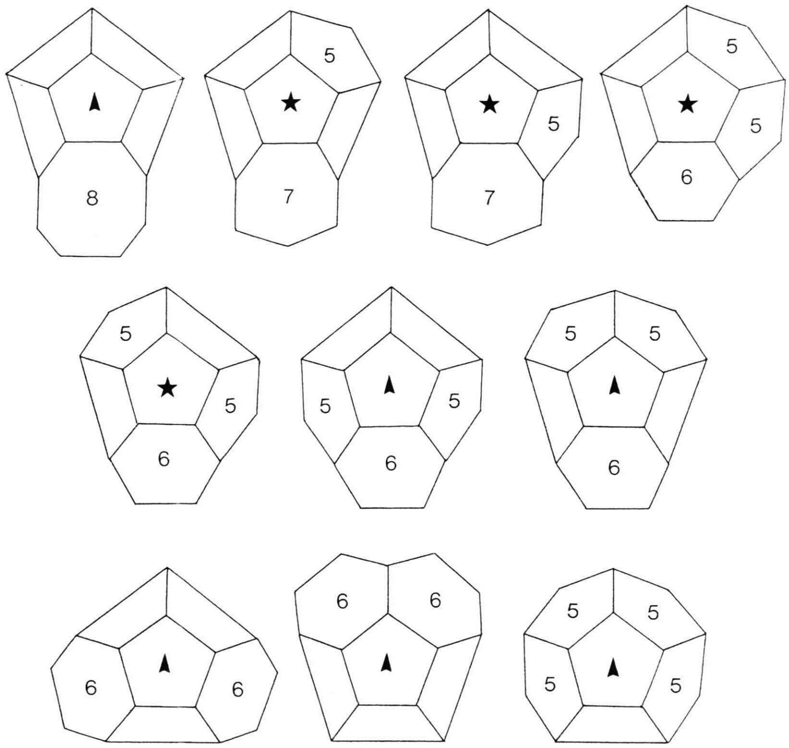

Fig. 2. The $C_{14}H_4$ systems of class Q_5. The central pentagon is marked with an arrowhead in the C_{2v} systems, and with an asterisk in the C_s systems. The sizes of the other polygons, when larger than four, are indicated by inscribed numerals.

with the numerical results for other Q_q classes. For the sake of illustration, the ten nonisomorphic Q_5 systems with $h=4$ are depicted in Fig. 2; they are distributed according to $6C_{2v}+4C_s$. Notice the agreement between $6C_{2v}$ and the term $6x^4$ in (11).

Central Hexagon, Heptagon or Octagon

Pólya's theorem was also applied to the classes Q_6, Q_7 and Q_8. The cycle indices are

$$Z(D_6)=\frac{1}{12}(s_1^6+3s_1^2 s_2^2+4s_2^3+2s_3^2+2s_6), \quad (13)$$

$$Z(D_7)=\frac{1}{14}(s_1^7+7s_1 s_2^3+6s_7), \quad (14)$$

$$Z(D_8)=\frac{1}{16}(s_1^8+4s_1^2 s_2^3+5s_2^4+2s_4^2+4s_8). \quad (15)$$

After inserting the figure counting series (1) according to the prescribed rules, one obtains

$$C_6(x)=\frac{1-x+x^2+x^3+2x^4-x^5+2x^6+x^8}{(1-x)^2(1-x^2)^2(1-x^3)(1-x^6)}, \quad (16)$$

$$C_7(x)=\frac{1-2x+x^2+4x^3-2x^4-2x^5+4x^6}{(1-x)^3(1-x^2)^3(1-x^7)}, \quad (17)$$

$$C_8(x)=\frac{1-3x+5x^2-2x^3+2x^4-2x^5+7x^6-6x^7+7x^8-3x^9+2x^{10}}{(1-x)^4(1-x^2)^2(1-x^4)(1-x^8)}. \quad (18)$$

Expressions for the expanded forms of the functions occurring on the right-hand sides of (16)–(18) are readily obtained from the data given in Table 3.

Chemical Relevance

The Q_q systems for $h=0$ correspond to carbon clusters void of hydrogens (formula C_{2q}). Although the polygonal systems usually are drawn as geometrically planar, these clusters may be associated with cage structures, specifically q-gonal prisms. In particular, the C_8 cluster for $q=4$ corresponds to a cube. Several of the polygonal prism structures of elemental carbon have been considered [17] in connection with the fullerene studies, where C_{60} buckminsterfullerene [18, 19] is the outstanding representative, but not belonging to the class Q_q itself.

Also for $h>0$ many Q_q systems correspond to interesting molecules in organic chemistry. First of all, one has the celebrated set of circulenes: [5]circulene or $C_{20}H_{10}$ corannulene; [6]circulene or $C_{24}H_{12}$ coronene; [7]circulene, $C_{28}H_{14}$. In this set of homologs, a [q]circulene as a member of Q_q consists of a q-gon circumscribed exclusively by hexagons. Corannulene ($q=5$) was synthesized for the first time by Barth and Lawton [20]. More recently, the same molecule has attracted new interest and two new syntheses of it have been reported [21, 22]. Additional references to corannulene are found elsewhere [23, 24]. Coronene ($q=6$) is well known [25]. Also [7]circulene has been synthesized [26], while a synthesis of [8]circulene has been attempted [27], but has remained unsuccessful. On the other hand, another member belonging to the Q_8 class (formula $C_{28}H_{12}$) has been prepared under the name tetrametheno-tetraphenylene [28, 29]. In this connection, Hellwinkel [29] has proposed the corannulene concept to structures which nicely fit into our definition of Q_q. He has depicted not less than thirty-two hypothetic molecules of this category with good prospects for possible syntheses; they span from $q=3$ to $q=16$. A representative of the Q_4 class ($C_{20}H_{12}$) is known chemically [30]. From the present work it is inferred that there are, for instance, 111 Q_q-type isomers of $C_{20}H_{10}$ (including corannulene), 561 $C_{24}H_{12}$ (including coronene) and 3260 $C_{28}H_{12}$; cf. Table 3. Notice that both h and q are determined uniquely when the chemical formula is given. The numbers of isomers increase rapidly with q for [q]circulenes. For $q=7$ and $q=8$ they are 2828 ($C_{28}H_{14}$) and 15581 ($C_{32}H_{16}$), respectively (outside the range of Table 3). Agranat et al. [31] depicted seven systems of the class Q_q, ranging from $q=5$ to $q=10$ and called them corannulenes like Hellwinkel [29]. However, the authors [31] extended the corannulene concept to systems which include primitive coronoids [23] and do not belong to Q_q; those systems are represented by $C_{48}H_{24}$ kekulene [32, 33] and other cycloarenes [33–35]. For the sake of clarity one should mention that most of the chemical compounds representing Q_q are structurally nonplanar. However, this does not imply any controversy inasmuch as they are represented by planar graphs.

Generalization

The solution for the numbers of nonisomorphic systems in Q_q was generalized to arbitrary q. It is sufficient here to specify the cycle index in the general case, viz.:

$$Z(D_q)=\frac{1}{2q}\left[\sum_{j\mid q}\varphi(q/j)\, s_{q/j}^{j}+z(s_1,s_2)\right] \quad (j=1,2,\ldots,q),$$

$$z(s_1,s_2)=\begin{cases} q\, s_1\, s_2^{(q-1)/2} & (q \text{ odd}). \\ \tfrac{1}{2}q\,[s_1^2\, s_2^{(q/2)-1}+s_2^{q/2}] & (q \text{ even}). \end{cases} \tag{19}$$

Here the Euler φ function has been employed: For t being a positive integer, $\varphi(t)$ is the number of positive integers smaller than t, no divisor of which (greater than unity) is a divisor of t; $\varphi(t)=1, 1, 2, 2, 4, 2, 6, 4, \ldots$ for $t=1, 2, \ldots, 8, \ldots$. The summation is taken over the integers j whenever q is divisible by j.

Let C_{hq} be the numbers of isomers in Q_q with h hydrogens; in other words,

$$C_q(x)=\sum_{h=0}^{\infty} C_{hq}\, x^h=\frac{1}{2q}\sum_{j\mid q}\left[\varphi(q/j)\,(1-x^{q/j})^{-j}+c_q(x)\right], \tag{20}$$

$$c_q(x)=\begin{cases} q(1-x)^{-1}(1-x^2)^{-(q-1)/2} & (q \text{ odd}). \\ \tfrac{1}{2}q\,[(1-x)^{-2}(1-x^2)^{-(q/2)+1}+(1-x^2)^{-q/2}] & (q \text{ even}). \end{cases} \tag{21}$$

Now the general relations (19) can be applied to the degenerate systems with $q=2$. One obtains

$$C_{h2}=\lfloor h/2 \rfloor+1, \tag{22}$$

where the floor function is employed: $\lfloor h/2 \rfloor=h/2$ (h even); $\lfloor h/2 \rfloor=(h-1)/2$ (h odd). But we have also

$$C_{2q}=\lfloor q/2 \rfloor+1, \tag{23}$$

at least for $q\geq 3$ (cf. Table 3), as is obtained from a simple combinatorial analysis. It is natural to define $C_{21}=1$, $C_{22}=2$. Hence $C_{h2}=C_{2q}$ for $h=q$ ($h, q\geq 1$). Similarly, when (19) is applied to $q=1$, one obtains

$C_{h1}=1$ (for all h). Also $C_{1q}=1$ ($q \geq 3$), and we define $C_{11}=C_{12}=1$; hence $C_{h1}=C_{1q}$ for $h=q$ ($h, q \geq 1$). In conclusion, the C_{hq} ($h, q \geq 1$) numbers define an infinite matrix, **C**, of which the first elements are listed below (compare with Table 3):

1	1	1	1	1	...
1	2	2	3	3	...
1	2	3	4	5	...
1	3	4	8	10	...
1	3	5	10	16	... .
.	.	.			

Theorem

$C_{hq}=C_{qh}$; the matrix **C** is symmetrical.

After the above analysis and definitions it is sufficient to prove the theorem for $h, q \geq 3$ when the numbers count nondegenerate systems. Consider the systems counted by C_{hq}, where h hydrogens are distributed among the q edges of the central q-gon. Produce the corresponding systems counted by C_{qh} (central h-gon and q hydrogens) in the following way: Take the same distribution of the radial edges from the central h-gon among the spaces in-between the q hydrogens. In this way a one-to-one correspondence is established between the two sets of systems, and it is also clear that the distributions into symmetry groups for these two sets are the same.

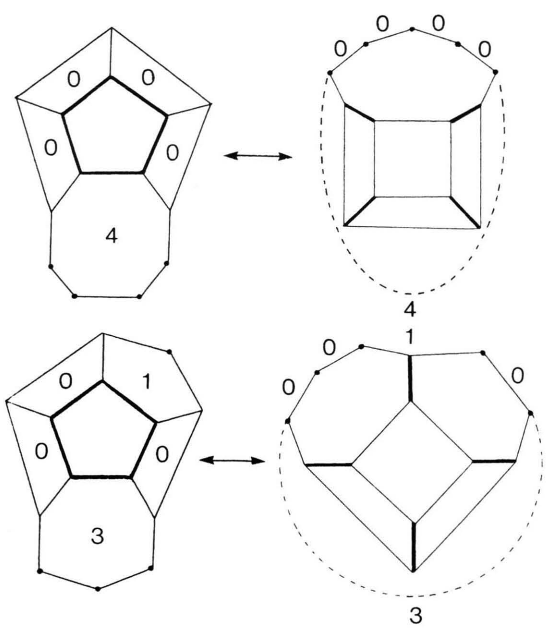

Fig. 3. Two pairs of corresponding systems. *Left* column: class Q_5; the numerals indicate numbers of vertices of degree two (symbolized by black dots) as distributed between consecutive vertices of degree three. *Right* column: class Q_4; the numerals indicate numbers of vertices of degree three as distributed between consecutive vertices of degree two (black dots).

As an example, consider the ten ($6\,C_{2v}+4\,C_s$) systems with a central pentagon and four hydrogens each. According to the theorem, there should exist exactly ten nonisomorphic systems with a central tetragon and five hydrogens each, and they should be distributed according to $6\,C_{2v}+4\,C_s$. In Fig. 3 the correlations between two pairs of systems from Q_5 and Q_4 are explained, where the Q_5 systems are taken as the two first ones in Figure 2. A formal proof of the present theorem is presented in the Appendix.

Supplementary Remarks

The results presented here can be related to an earlier publication of Fujita [36] on cage-shaped molecules. This author considered the number of isomers of certain classes by substitution of methylene units into the edges of a parent skeleton. For example, he derived all adamantane isomers using the edges of the tetrahedrane skeleton for the appropriate insertion of methylene units. Consequently, on invoking Mark tables [37] and coset representation theory Fujita derived all the 32 adamantane isomers in agreement with previous results of Balaban [38]. Fujita's approach is applicable to the present problem. For instance, if we consider the outer edges of the graph shown in Fig. 1, then by appropriate insertions of methylene units all the isomers of Fig. 2 are derived.

Appendix: Formal Proof of the Theorem

Let G be the graph of a system in Q_q with h hydrogens and C its boundary. G is completely determined by the arrangement of the vertices of degree two (say black vertices) and vertices of degree three (say white) on C. In fact G is obtained from C by inserting a q-gon in the internal area of C and connecting the white vertices on C with the corresponding vertices of the q-gon. If we now change the colours of the vertices on C in G, we obtain a new cycle C′, from which a graph G′ is constructed as described above. Clearly, the graph G′ represents a Q_h system with q hydrogens. Thus a one-to-one correspondence is established between the Q_q systems with h hydrogens and Q_h systems with q hydrogens. Hence $C_{hq}=C_{qh}$.

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