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Tables of the Topological Characteristics of Polyhexes (Condensed Aromatic Hydrocarbons). II.* Sextet Polynomial

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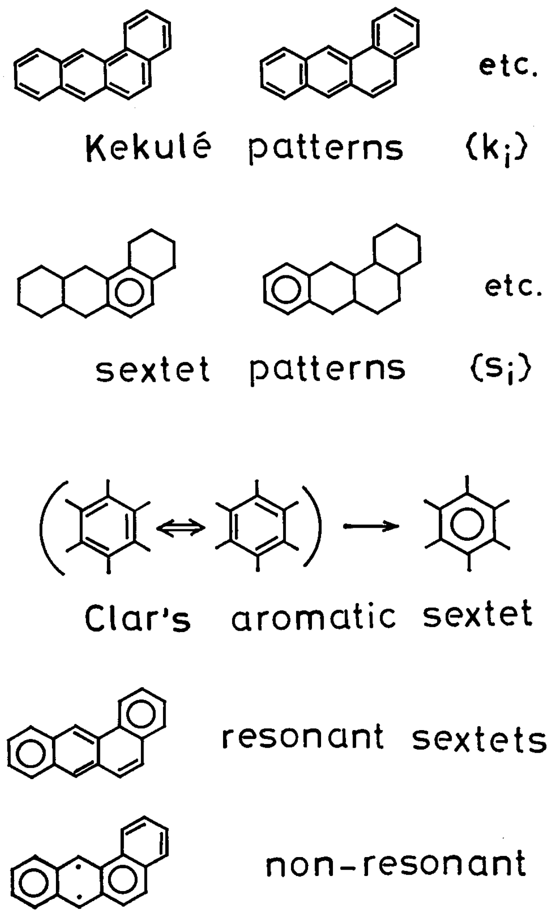
We will be concerned with such polyhex graphs (G's), or hexagonal animals, that have non-zero perfect matching number, or Kekulé number ($K(G)$), or are 1-factorable.[1-3] Let us call such polyhex as Kekulé polyhex. There have been known a group of polyhexes with an even number of points but with zero $K(G)$.[4-6] Those graphs will not be treated here, although interesting mathematical problems are being discussed.[6,7]

The present authors have proposed to define the sextet pattern s_i and sextet polynomial $B_G(x)$ for characterizing both the topological and chemical properties of the Kekulé polyhex representing the carbon atom skeleton of a condensed polycyclic aromatic hydrocarbon molecule.[8-10] A number of variant resonance-theoretical quantities were shown to be mathematically related with each other through the sextet polynomial. A novel one-to-one correspondence between the sextet patterns $\{s_i\}$ and the Kekulé patterns $\{k_i\}$, or perfect matching pattern, was found and analyzed by the use of the sextet polynomial. Analysis of the topological dependency of the above-mentioned properties is of potential importance not only in chemistry but also in graph theory. It is thus worth preparing an extensive list of the sextet polynomials of typical series of polyhex graphs and an exposition of their recursion relations hitherto known.

According to Clar, if a set of three conjugated double bonds are drawn in a hexagon for one of the Kekulé patterns of a polyhex graph, an aromatic sextet can be assigned to that hexagon and is designated by a circle in it.[5] Two or more aromatic sextets can mutually be resonant if the remainder of the graph has at least one Kekulé pattern (See Figure).[8-10] Define the resonant sextet number, $r(G, k)$, as the number of ways in which k resonant sextets can be chosen from G. Define $r(G, 0)=1$ for any G including a vacant graph ϕ. With the set of such $r(G, k)$'s the sextet polynomial is defined as

* Part I of this series is: T. Yamaguchi, M. Suzuki, and H. Hosoya, Natural Sci. Rept. Ochanomizu Univ., **26** (1975), 39.



Figure

$$B_G(x)=\sum_{k=0}^{m} r(G, k)x^k , \tag{1}$$

where x is simply a parameter to hold k.

The number of the sextet patterns is then equal to $B_G(1)$. The one-to-one correspondence between $\{s_i\}$ and $\{k_i\}$ is written down as

$$B_G(1)=K(G) . \tag{2}$$

In order to hold this relation in all the polyhex graphs the "super sextet" should be introduced. The detailed discussion on the super sextet is given elsewhere.[9,10)]

In Table I are given the $B_G(x)$ and $B'_G(x)$ for small polyhexes, where $B_G'(x)$ is the first derivative of $B_G(x)$ with respect to x. The value $B'_G(1)$ gives the total number of aromatic sextets for the set of $\{s_i\}$ of G.[8-10)] The code numbers for small polyhexes are taken from Ref. 2. In Table II are given the list of the known recursion relations for various series of polyhexes with the necessary sets of initial entities.[10)] Tentative symbols such as D_n or $P_{1,n}$ are taken from Ref. 10 but with minor alteration where necessary. In Table III are given the general expressions for the sextet polynomials of several series of polyhex graphs.[10]

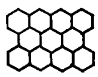
If one introduces the operator expression, relations among complicated recursion relations of the sextet polynomials can be understood systematically.[11,12] Define the step-up operator $\hat{\boldsymbol{O}}$ for a given sextet polynomial, $X_n(x)$, as $X_n(x)=\hat{\boldsymbol{O}}X_{n-1}(x)$. The recursion relation $P_{1,n}(x)=2P_{1,n-1}(x)-P_{1,n-2}(x)$ for the first entry in Table II can be expressed as

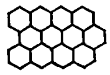
$$(\hat{\boldsymbol{O}}^2-2\hat{\boldsymbol{O}}+1)P_{1,n}(x)=(\hat{\boldsymbol{O}}-1)^2P_{1,n}(x)=0 .$$

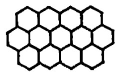
Then the operator expression for the recursion relation of $P_{1,n}$ is simply given by

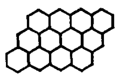
$$(\hat{\boldsymbol{O}}-1)^2=0 .$$

It is worthy of notice that the operator expressions for the following series of graphs form an interesting hierarchical structure:

$(\hat{\boldsymbol{O}}-1)^3=0$ for $R_{2,n}$ 

$(\hat{\boldsymbol{O}}-1)^4=0$ for $B_{3,n}$ 

$(\hat{\boldsymbol{O}}-1)^5=0$ for $C_{3,n}$ 

$(\hat{\boldsymbol{O}}-1)^6=0$ for $P_{3,n}$. 

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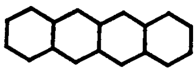
[12] H. Hosoya and A. Motoyama, J. Math. Phys., in prss

Table I—1

G	$r(G, k)$				$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3		
1C0001	1	1			2	1
2C0001	1	2			3	2
3C0001	1	3			4	3
3C0002	1	3	1		5	5
4C0001	1	4			5	4
4C0002	1	4	2		7	8
4C0003, 4	1	4	3		8	10
4C0005	1	4	3	1	9	13
4P2001	1	4	1		6	6


1C0001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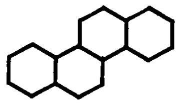
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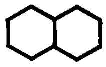
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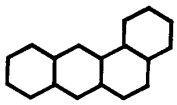
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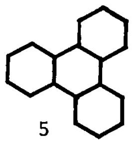
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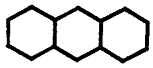
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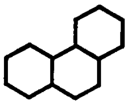
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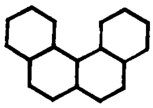
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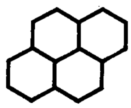

4P2001

Table I—2

G	$r(G, k)$				$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3		
5C0001	1	5			6	5
5C0002	1	5	3		9	11
5C0003	1	5	4		10	13
5C0004, 5	1	5	5		11	15
5C0006, 7	1	5	5	1	12	18
5C0008-10*	1	5	6	1	13	20
5C0011*	1	5	5	2	13	21
5C0012	1	5	6	2	14	23
5P2001	1	5	3		9	11
5P2002	1	4	4		9	12
5P2003	1	5	4	1	11	16

* Numbering has been interchanged between 5C0010 and 11, which were originally assigned in Ref. 2.

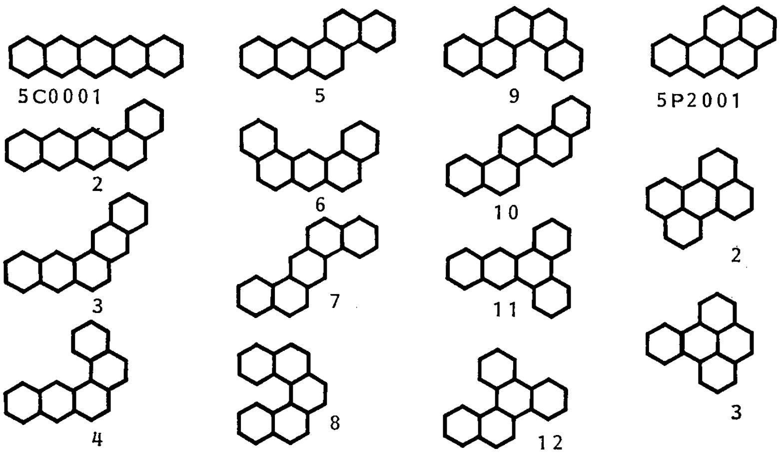


Table I—3

G	$r(G, k)$				$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3		
6C0001	1	6			7	6
6C0002	1	6	4		11	14
6C0003	1	6	6		13	18
6C0004, 5	1	6	7		14	20
6C0006, 7	1	6	8		15	22
6C0008, 9	1	6	7	2	16	26
6C0010, 11	1	6	8	2	17	28
6C0012-15	1	6	9	2	18	30

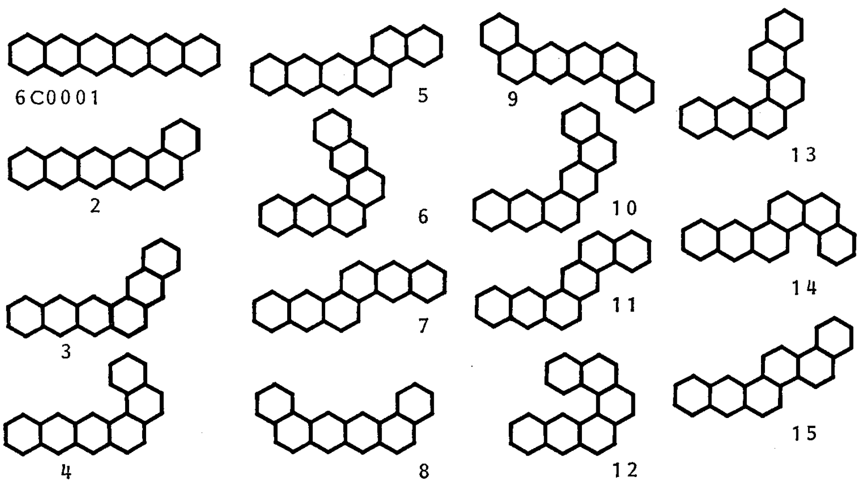


Table I—4

G	$r(G,k)$				$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3		
6C0016-19	1	6	9	3	19	33
6C0020-25	1	6	10	4	21	38
6C0026	1	6	7	3	17	29
6C0027	1	6	8	4	19	34
6C0028	1	6	9	3	19	33
6C0029, 30	1	6	9	4	20	36

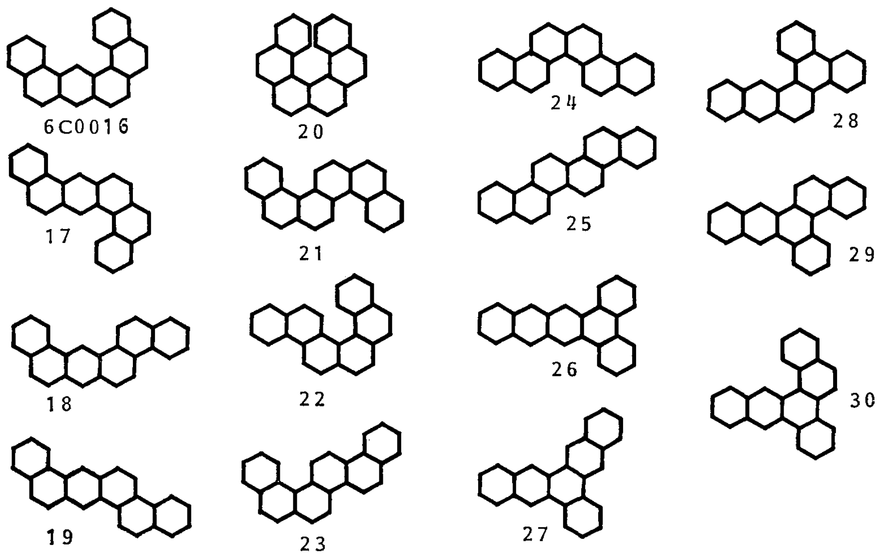
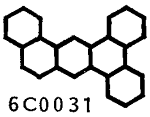


Table I—5

G	$r(G,k)$					$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3	4		
6C0031	1	6	9	5	1	22	43
6C0032-34	1	6	10	5		22	41
6C0035, 36	1	6	10	5	1	23	45
6C0037	1	6	10	6	1	24	48
6P2002	1	4	4			9	12
6P2003	1	6	5			12	16
6P2004	1	5	6			12	17
6P2005	1	6	6			13	18
6P2006	1	6	6	1		14	21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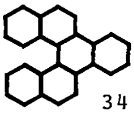
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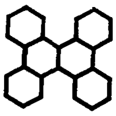
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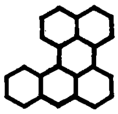
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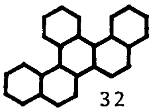
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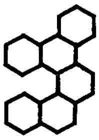
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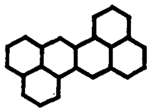
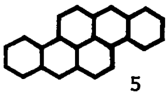

6P2002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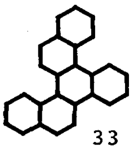
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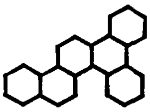
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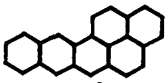
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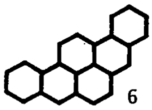
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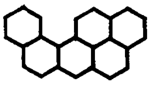
Table I—6

G	$r(G,k)$					$B_G(1)$	$B_G'(1)$
	$k=0$	1	2	3	4		
6P2007, 8	1	6	7	1		15	23
6P2009	1	5	7	2		15	25
6P2010, 11	1	6	7	2		16	26
6P2012	1	6	8	2		17	28
6P2013	1	6	7	3		17	29
6P2014	1	6	8	4	1	20	38
6P4002	1	6	3			10	12
6P4003	1	6	6	1		14	21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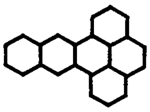
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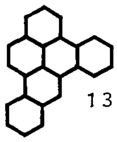
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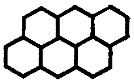
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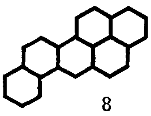
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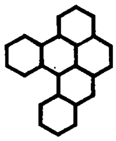
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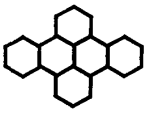
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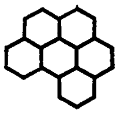
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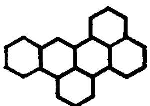
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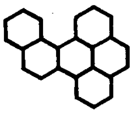
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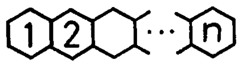
Table II—1

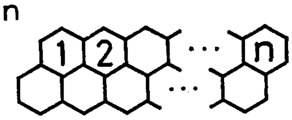
$P_{1,n}$



$P_{1,0}(x)=1$
$P_{1,1}(x)=1+x$

$$P_{1,n}(x)=2P_{1,n-1}(x)-P_{1,n-2}(x)$$

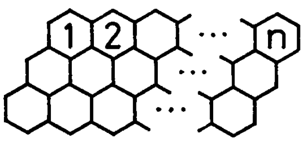
$P_{2,n}$



$P_{2,0}(x)=1$
$P_{2,1}(x)=1+2x$
$P_{2,2}(x)=1+4x+x^2$
$P_{2,3}(x)=1+6x+3x^2$

$$P_{2,n}(x)=4P_{2,n-1}(x)-6P_{2,n-2}(x)+4P_{2,n-3}(x)-P_{2,n-4}(x)$$

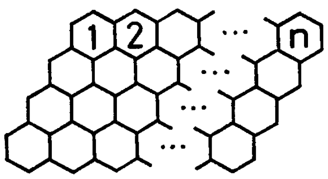
$P_{3,n}$



$P_{3,0}(x)=1$
$P_{3,1}(x)=1+3x$
$P_{3,2}(x)=1+6x+3x^2$
$P_{3,3}(x)=1+9x+9x^2+x^3$
$P_{3,4}(x)=1+12x+18x^2+4x^3$
$P_{3,5}(x)=1+15x+30x^2+10x^3$

$$P_{3,n}(x)=6P_{3,n-1}(x)-15P_{3,n-3}(x)+20P_{3,n-3}(x)-15P_{3,n-4}(x)$$
$$+6P_{3,n-5}(x)-P_{3,n-6}(x)$$

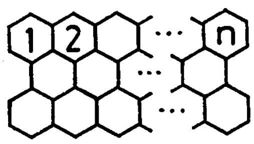
$P_{4,n}$



$P_{4,0}(x)=1$
$P_{4,1}(x)=1+4x$
$P_{4,2}(x)=1+8x+6x^2$
$P_{4,3}(x)=1+12x+18x^2+4x^3$
$P_{4,4}(x)=1+16x+36x^2+16x^3+x^4$
$P_{4,5}(x)=1+20x+60x^2+40x^3+5x^4$
$P_{4,6}(x)=1+24x+90x^2+80x^3+15x^4$
$P_{4,7}(x)=1+28x+126x^2+140x^3+35x^4$

$$P_{4,n}(x)=8P_{4,n-1}(x)-28P_{4,n-2}(x)+56P_{4,n-3}(x)-70P_{4,n-4}(x)$$
$$+56P_{4,n-5}(x)-28P_{4,n-6}(x)+8P_{4,n-7}(x)-P_{4,n-8}(x)$$

$R_{2,n}$

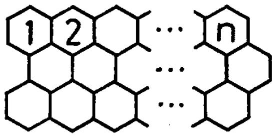


$R_{2,0}(x)=1$
$R_{2,1}(x)=1+2x+x^2$
$R_{2,2}(x)=1+4x+4x^2$

$$R_{2,n}(x)=3R_{2,n-1}(x)-3R_{2,n-2}(x)+R_{2,n-3}(x)$$

Table II—2

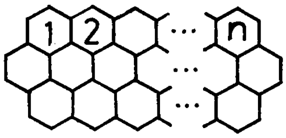
$B_{3,n}$



$B_{3,0}(x)=1$
$B_{3,1}(x)=1+3x+x^2$
$B_{3,2}(x)=1+6x+6x^2+x^3$
$B_{3,3}(x)=1+9x+15x^2+5x^3$

$$B_{3,n}(x)=4B_{3,n-1}(x)-6B_{3,n-2}(x)+4B_{3,n-3}(x)-B_{3,n-4}(x)$$

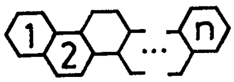
$C_{3,n}$



$C_{3,0}(x)=1$
$C_{3,1}(x)=1+4x+x^2$
$C_{3,2}(x)=1+8x+9x^2+2x^3$
$C_{3,3}(x)=1+12x+24x^2+12x^3+x^4$
$C_{3,4}(x)=1+16x+46x^2+36x^3+6x^4$

$$C_{3,n}(x)=5C_{3,n-1}(x)-10C_{3,n-2}(x)+10C_{3,n-3}(x)-5C_{3,n-4}(x)+C_{3,n-5}(x)$$

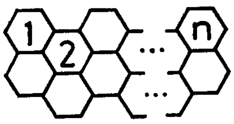
$W_{1,n}$



$W_{1,0}(x)=1$
$W_{1,1}(x)=1+x$

$$W_{1,n}(x)=W_{1,n-1}(x)+W_{1,n-2}(x)$$

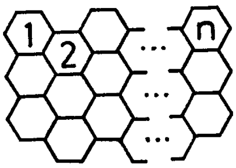
$W_{2,n}$



$W_{2,0}(x)=1$
$W_{2,1}(x)=1+2x$
$W_{2,2}(x)=1+4x+x^2$

$$W_{2,n}(x)=(1+x)\,W_{2,n-1}(x)+x\cdot W_{2,n-2}(x)-x^2\cdot W_{2,n-3}(x)$$

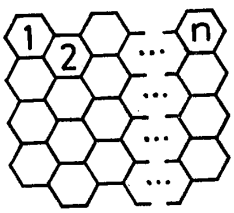
$W_{3,n}$



$W_{3,0}(x)=1$
$W_{3,1}(x)=1+3x$
$W_{3,2}(x)=1+6x+3x^2$
$W_{3,3}(x)=1+9x+15x^2+5x^3$

$$W_{3,n}(x)=(1+x)\,W_{3,n-1}(x)+(2x+x^2)\,W_{3,n-2}(x)-x^2\cdot W_{3,n-3}(x)-x^3\cdot W_{3,n-4}(x)$$

$W_{4,n}$

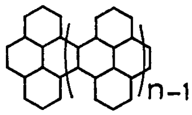


$W_{4,0}(x)=1$
$W_{4,1}(x)=1+4x$
$W_{4,2}(x)=1+8x+6x^2$
$W_{4,3}(x)=1+12x+28x^2+14x^3$
$W_{4,4}(x)=1+16x+66x^2+76x^3+31x^4$

$$W_{4,n}(x)=(1+2x)\,W_{4,n-1}(x)+(2x+x^2)\,W_{4,n-2}(x)-(3x^2+x^3)\,W_{4,n-3}(x)-x^3\cdot W_{4,n-4}(x)+x^4\cdot W_{4,n-5}(x)$$

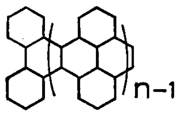
Table II—3

N_n



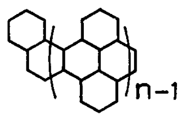
$N_0(x)=1$
$N_1(x)=1+4x+x^2$

Q_n



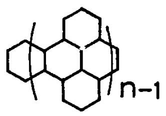
$Q_0(x)=1$
$Q_1(x)=1+3x+x^2$

S_n



$S_0(x)=1$
$S_1(x)=1+2x$

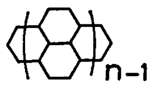
T_n



$T_0(x)=1$
$T_1(x)=1+x$

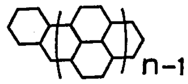
$$X_n(x)=(1+4x+x^2)X_{n-1}(x)-x^2\cdot X_{n-2}(x) \quad (X=N, Q, S, T)$$

U_n



$U_0(x)=1$
$U_1(x)=1+x$

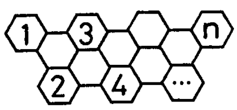
V_n



$V_0(x)=1$
$V_1(x)=1+2x$

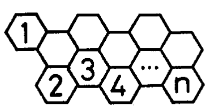
$$X_n(x)=(1+2x)X_{n-1}(x)+x(1-x)X_{n-2}(x) \quad (X=U, V)$$

D_n



$D_0(x)=1$
$D_1(x)=1+x$
$D_2(x)=1+2x+x^2$

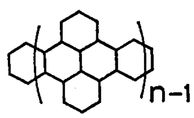
E_n



$E_0(x)=1$
$E_1(x)=1+x$
$E_2(x)=1+3x+x^2$

$$X_n(x)=(1+x)X_{n-1}(x)+x\cdot X_{n-2}(x)-x^2\cdot X_{n-3}(x) \quad (X=D, E)$$

F_n



$F_0(x)=0$*
$F_1(x)=1+x$

$$F_n(x)=(1+5x+3x^2+x^3)F_{n-1}(x)-x^2\cdot F_{n-2}(x)$$

---

* Note that only for this series of graphs the initial condition $F_0(x)=0$ is different from unity.

Table III

$$W_{1,n}(x)=\sum_{i=0}^{[n+1/2]}\binom{n-i+1}{i}x^i$$

$$P_{m,n}(x)=\sum_{i=0}^{m}\binom{m}{i}\binom{n}{i}x^i \qquad (m\leqq n)$$

$$R_{m,n}(x)=(1+nx)^m$$

$$B_{3,n}(x)=1+3nx+n(2n-1)x^2+\frac{n(n-1)(2n-1)}{6}x^3$$

$$C_{3,n}(x)=1+4nx+\frac{n(7n-5)}{2}x^2+n(n-1)^2x^3+\frac{n(n-1)^2(n-2)}{12}x^4$$

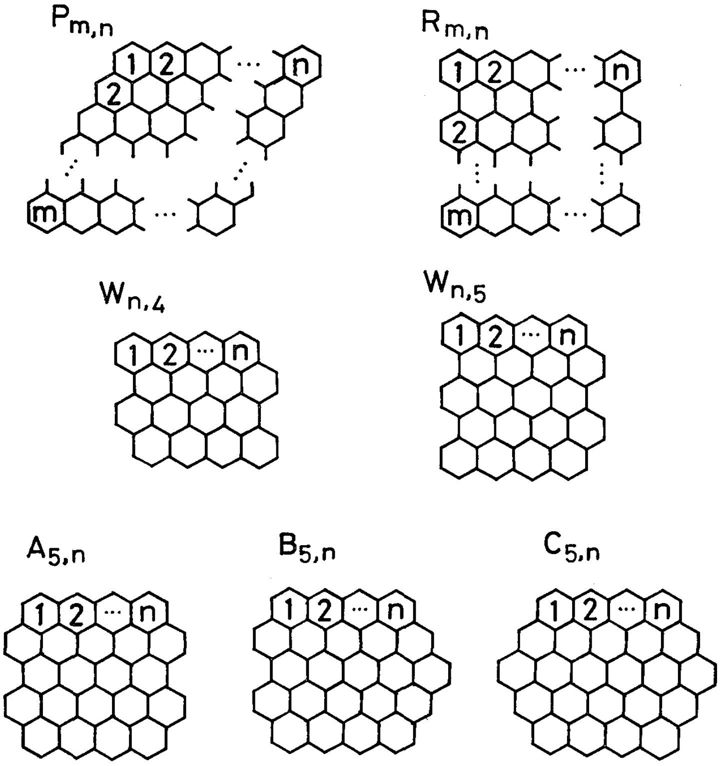
$$W_{n,4}(x)=1+4nx+\frac{3n(3n-1)}{2}x^2+\frac{n(n-1)(5n-1)}{3}x^3+\frac{n(n-1)(5n^2-5n+2)}{24}x^4$$

$$W_{n,5}(x)=1+5nx+2n(4n-1)x^2+\frac{n(10n^2-9n+1)}{2}x^3$$
$$+\frac{n(n-1)(2n-1)(4n-1)}{6}x^4+\frac{n(n-1)(2n-1)(2n^2-2n+1)}{30}x^5$$

$$A_{5,n}(x)=1+7nx+3n(5n-2)x^2+\frac{n(41n^2-51n+13)}{3}x^3$$
$$+\frac{n(n-1)(75n^2-103n+32)}{12}x^4+\frac{n(n-1)(89n^3-251n^2+214n-76)}{60}x^5$$
$$+\frac{n(n-1)(n-2)(21n^3-52n^2+47n-20)}{120}x^6+\frac{n(n-1)^3(n-2)(n^2-2n+2)}{120}x^7$$

$$B_{5,n}(x)=1+8nx+\frac{n(37n-19)}{2}x^2+\frac{n(112n^2-165n+59)}{6}x^3$$
$$+\frac{n(n-1)(29n^2-53n+23)}{3}x^4+\frac{n(n-1)(82n^3-293n^2+337n-128)}{30}x^5$$
$$+\frac{n(n-1)(n-2)(152n^3-564n^2+679n-285)}{360}x^6$$
$$+\frac{n(n-1)(n-2)(12n^4-74n^3+168n^2-163n+63)}{360}x^7$$
$$+\frac{n(n-1)^2(n-2)^2(n-3)(3n^2-9n+8)}{2880}x^8$$

$$C_{5,n}(x)=1+9nx+\frac{9n(5n-3)}{2}x^2+\frac{n(149n^2-249n+106)}{6}x^3$$
$$+\frac{n(n-1)^2(86n-103)}{6}x^4+\frac{n(n-1)^2(28n^2-89n+72)}{6}x^5$$
$$+\frac{n(n-1)(n-2)(316n^3-1464n^2+2201n-1059)}{360}x^6$$
$$+\frac{n(n-1)(n-2)(236n^4-1784n^3+4921n^2-5749n+2430)}{2520}x^7$$
$$+\frac{n(n-1)(n-2)(n-3)(105n^4-838n^3+2427n^2-2918n+1272)}{20160}x^8$$
$$+\frac{n(n-1)^2(n-2)^3(n-3)^2(n-4)}{8640}x^9$$


$P_{m,n}$
$R_{m,n}$
$W_{n,4}$
$W_{n,5}$
$A_{5,n}$
$B_{5,n}$
$C_{5,n}$

Errata to Ref. 2 (T. Yamaguchi, M. Suzuki, and H. Hosoya: Natl. Sci. Rept. Ochanomizu Univ., **26** (1975), 39)

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Diagram for Table I-2

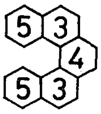
5C0008 

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Table I-3

	B
5P2001	11

Diagram

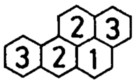
5P2001 

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Table I-9

	B
6P2013	29

Diagram

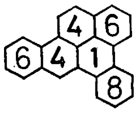
6P2013 

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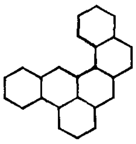
Diagram for Table I-8

6P1017  6P1018