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Closed–Form Formulas for Zhang–Zhang Polynomials of Hexagonal Graphene Flakes $O(k, m, n)$ with $k, m = 1$–7 and Arbitrary n

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Abstract

We report a closed-form formula for the ZZ polynomials of hexagonal graphene flakes $O(k, m, n)$ with $k, m = 1, 2, 3, \ldots, 7$ and an arbitrary value of n. The discovered formula,

$$\mathrm{ZZ}\left(O\left(k,\, m\,, n\right), x\right) = \sum_{i=0}^{k\cdot m} \sum_{j=0}^{\left\lfloor \frac{k\cdot m}{2} \right\rfloor - 1} \sum_{l=0}^{(k-2)(m-2)} \sum_{h=0}^{l} c_{lj} \binom{l}{h} \binom{k\cdot m-2j-l}{i-2j-l} \binom{n+j+h}{i} \left(1+x\right)^{i},$$

where c_{lj} denotes structural parameters dependent on k and m but independent of n, is obtained by a combinatorial analysis of large families of isostructural hexagonal flakes. The presented results extend the available body of information on the ZZ polynomials of hexagonal graphene flakes $O(k, m, n)$ by a factor of 10. The main reason for presenting these numerical results is to provide the chemical and mathematical communities with reference data necessary for deriving, understanding, and testing general ZZ polynomial formulas valid for a hexagonal flake $O(k, m, n)$ with arbitrary values of the structural parameters k, m, and n.

1 Introduction

In 1996, Heping Zhang and Fuji Zhang introduced to chemical graph theory a combinatorial polynomial

$$\mathrm{ZZ}\left(\boldsymbol{B}, x\right) = \sum_{k=0}^{Cl} c_k x^k, \tag{1}$$

usually referred to in the recent literature as the Clar covering polynomial, Zhang-Zhang polynomial, or ZZ polynomial, which provides a generating function for the sequence $[c_0, c_1, \ldots, c_{Cl}]$, where c_k represents the number of Clar covers of order k for a given benzenoid $\boldsymbol{B}$ and the number Cl, usually referred to as the Clar number of $\boldsymbol{B}$, denotes the maximal number of aromatic sextets that can be accommodated in $\boldsymbol{B}$. (To keep this communication to a reasonable length, we refrain here from repeating all the formal definitions and refer the novice reader to the original papers of Zhang and Zhang [1–5] together with their two more recent reviews of the field [6, 7], an excellent pedagogical introduction to the topic of ZZ polynomials written by Gutman, Furtula, and Balaban [8], and our earlier papers on this topic [9–12].) Somewhat surprisingly, it soon turned out that the computation of the full sequence $[c_0, c_1, \ldots, c_{Cl}]$ of Clar cover numbers for a given benzenoid $\boldsymbol{B}$—given naturally by the coefficients of the ZZ polynomial of $\boldsymbol{B}$—is performed much more conveniently and robustly than the determination of a single of these numbers, owing to the inviting recursive properties of ZZ polynomials demonstrated in the original papers of Zhang and Zhang [1, 3, 4] and restated in slightly different verse by other authors [8, 9]. The theoretical development was soon augmented with practical considerations allowing to formulate fast and robust algorithms for computing ZZ polynomials [1, 8–10, 13] and resulting in freely available computer programs (initially ZZCalculator [9] and finally ZZDecomposer [11, 12, 14, 15]). With these automatized programs, a characterization and enumeration of Clar covers of an arbitrary pericondensed benzenoid [16] containing up to about 500 carbon atoms became a routine task. Even more importantly, ZZDecomposer allowed for determination and derivation of closed-form formulas for ZZ polynomials of whole isostructural families of benzenoids, allowing to extend the analogous heroic effort of determination of the number of Kekulé structures reported in the literature by Cyvin, Cyvin, Gutman, and their collaborators some three decades earlier. (For a detailed account, see [16] and numerous references therein including [17–28].) ZZDecomposer has been used in many applications [9–11, 29–39] to find closed-form formulas of

ZZ polynomials for various families of basic catacondensed and pericondensed benzenoids, substantially extending the total body of previously available results [1–5, 8, 40–45]. The rapid development of Clar theory stimulated by these discoveries in recent years lead to many new interesting applications and connections to other branches of chemistry, graph theory, and combinatorics [13, 34, 35, 43–67].

Despite of many successful applications of ZZDecomposer to finding closed-form formulas of ZZ polynomials for basic benzenoid families, two important groups of benzenoid structures, hexagonal graphene flakes $O(k, m, n)$ and oblate rectangles $Or(m, n)$, persistently defy revealing their closed-form ZZ polynomial formulas. In a recent article [68], we have presented a compilation of all the known facts pertaining to the ZZ polynomials of these two families of structures, augmenting the existing body of information with a compact, determinantal formula for the ZZ polynomial of $O(2, m, n)$ suggested by an extension of the John-Sachs theory of Kekulé structures. Here, we only briefly summarize the available facts for hexagonal graphene flakes $O(k, m, n)$ again, before we present our new results, which double or triple the amount of so-far accumulated information on Clar cover enumeration of hexagonal graphene flakes. We would like to stress, sharply and clearly, that the ultimate goal of our research is discovering the Holy Grail of the Clar theory: a ZZ polynomial formula of a general hexagonal flake $O(k, m, n)$ applicable for arbitrary values of the structural parameters k, m, and n. While, unfortunately, the presented here results do not attain this goal, they constitute an important step toward it. We hope that the presented here equations give additional insight into how such a general formula for $\mathrm{ZZ}(O(k, m, n), x)$ might look like and may suggest a path leading to its discovery. In addition, once such a formula is discovered, the presented here results give a set of testing examples against which the newly formulated theory should be critically evaluated.

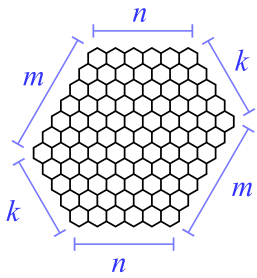

Figure 1. Graphical definition of hexagonal graphene flakes $O\,(k, m, n)$.

2 Review of available results on ZZ polynomials of $O(k, m, n)$

Hexagonal graphene flakes $O\,(k, m, n)$ are defined graphically in Fig. 1. The structural parameters k, m, and n can take on any positive integer value starting from 1. Since the ZZ polynomial of $O\,(k, m, n)$ is invariant under the group S_3 of permutations of the structural parameters (it should be obvious for the reader how to establish the bijection between the sets of Clar covers of these six structures using geometrical rotations and reflections), we consider in this section explicitly only the hexagonal graphene flakes $O\,(k, m, n)$ for which $k \leq m \leq n$. In the case when $k = 1$, the hexagonal graphene flake $O\,(1, m, n)$ reduces to a parallelogram $M\,(m, n)$, for which the ZZ polynomial is long known [9, 30, 42]. Very limited amount of information is available for the ZZ polynomials of the remaining hexagonal graphene flakes $O\,(k, m, n)$ with $k \geq 2$. For $(k = 2, m = 2)$ and $(k = 3, m = 3)$, the closed-form ZZ polynomial formulas were given originally by Eqs. (35) and (37) of [10], respectively. Formal demonstration of the validity of these formulas was presented in [11] (Eqs. (47)–(51) for $(k = 2, m = 2)$ and Eqs. (66)–(71) for $(k = 3, m = 3)$), together with a derivation of a closed-form formula for the ZZ polynomial of $O\,(k = 2, m = 3, n)$ (Eqs. (52)–(65)) [10, 11]. A slightly more organized way of displaying these results was employed in [36] (Eqs. (12a–c) for $(k = 2, m = 2)$ and Eqs. (25a–c) for $(k = 2, m = 3)$) and in [37] (Eq. (13) for $(k = 3, m = 3)$). Finally, the ZZ polynomial of $O\,(k = 2, m = 4, n)$ has been reported as Eq. (54) of [37]. All the known formulas obtained in this way can be summarized concisely as

$$\mathrm{ZZ}\left(O\left(1,m,n\right),x\right) = \sum_{i=0}^{\min(m,n)} \left[\binom{m}{i}\binom{n}{i}\right](1+x)^{i} \tag{2}$$

$$\mathrm{ZZ}\left(O\left(2,\,2\,,n\right),x\right) = \sum_{i=0}^{4} \left[\binom{4}{i}\binom{n}{i}+\binom{4-2}{i-2}\binom{n+1}{i}\right](1+x)^{i} \tag{3}$$

$$\mathrm{ZZ}\left(O\left(2,\,3\,,n\right),x\right) = \sum_{i=0}^{6} \left[\binom{6}{i}\binom{n}{i}+3\binom{6-2}{i-2}\binom{n+1}{i}+\binom{6-4}{i-4}\binom{n+2}{i}\right](1+x)^{i} \tag{4}$$

$$\begin{aligned}\mathrm{ZZ}\left(O\left(2,\,4\,,n\right),x\right) = \sum_{i=0}^{8} & \left[\binom{8}{i}\binom{n}{i}+6\binom{8-2}{i-2}\binom{n+1}{i}\right. \\ & \left.+6\binom{8-4}{i-4}\binom{n+2}{i}+\binom{8-6}{i-6}\binom{n+3}{i}\right](1+x)^{i}\end{aligned} \tag{5}$$

$$\begin{aligned}\mathrm{ZZ}\left(O\left(3,\,3\,,n\right),x\right) = \sum_{i=0}^{9} & \left[\binom{9}{i}\binom{n}{i}+\left(10\binom{9-2}{i-2}-\binom{9-3}{i-2}\right)\binom{n+1}{i}\right. \\ & +\left(20\binom{9-4}{i-4}+\binom{9-6}{i-3}-\binom{9-6}{i-5}\right)\binom{n+2}{i} \\ & \left.+\left(10\binom{9-6}{i-6}+\binom{9-7}{i-5}+\binom{9-6}{i-5}\right)\binom{n+3}{i}+\binom{9-7}{i-7}\binom{n+4}{i}\right](1+x)^{i}\end{aligned} \tag{6}$$

Recently, motivated by the great successes of the John-Sachs theory [69–75] in finding determinantal formulas for the number of Kekulé structures of benzenoid hydrocarbons, [17, 21, 73, 76, 77] we performed [78] an *ad hoc* extension of this theory to the world of Clar covers, which resulted [68] in discovering a determinantal ZZ polynomial formula applicable to hexagonal graphene flakes $O\left(2,m,n\right)$ with arbitrary values of the structural constants m and n

$$\mathrm{ZZ}\left(O\left(2,m,n\right),x\right) = \begin{vmatrix} \sum_{i=0}^{\min(m,n)} \left[\binom{m}{i}\binom{n}{i}\right](1+x)^{i} & \sum_{i=0}^{n-1} \left[\binom{m-1}{i}\binom{n+1}{i+2}\right](1+x)^{i+1} \\ \sum_{i=0}^{m-1} \left[\binom{n-1}{i}\binom{m+1}{i+2}\right](1+x)^{i+1} & \sum_{i=0}^{\min(m,n)} \left[\binom{m}{i}\binom{n}{i}\right](1+x)^{i} \end{vmatrix} \tag{7}$$

In particular, Eq. (7) reproduces Eqs. (3) and (4) as special cases. The diagonal entries of the determinant (7) have the form of ZZ polynomials of the diagonal peak-valley paths, being a natural extension of the John-Sachs theory; the off-diagonal entries of the determinant have a rather surprising polynomial form, which at the moment cannot be connected in any respect to any natural extension of the John-Sachs theory and remains to be understood. It is important to emphasize that the determinantal formula for the ZZ polynomial of $O\left(2,m,n\right)$ given by Eq. (7) was given without a proof, so it should be treated as a conjecture until an extension of the John-Sachs theory to the world of Clar covers is formally formulated, fully studied, and properly understood, even though considerable numerical evidence accumulated using ZZDecomposer, together with the clear regularities and patterns observed in the process of deducing the result, leave no doubt for the validity of the obtained determinantal formula. The ZZ polynomial of $O\left(2,m,n\right)$ can be also obtained by generalizing the sequence of Eqs. (3), (4), and (5) to the following form

$$\mathrm{ZZ}\left(O\left(2,m,n\right),x\right)=\sum_{i=0}^{2m}\sum_{j=0}^{m-1}\frac{\binom{m-1}{j}\binom{m}{j}}{j+1}\binom{2m-2j}{i-2j}\binom{n+j}{i}\left(1+x\right)^{i},\tag{8}$$

where the sequences $(1,1)$, $(1,3,1)$, and $(1,6,6,1)$ in Eqs. (3), (4), and (5) are identified as members of the sequence A001263 in OEIS [79] representing Narayana numbers $T\left(m,j+1\right)=\frac{\binom{m-1}{j}\binom{m}{j}}{j+1}$ or consecutive rows of the Catalan triangle. The two equations (Eq. (7) and Eq. (8)) are consistent with each other.

3 New results

3.1 Road to the discovery

We explain in this subsection on the example of the hexagonal graphene flakes $O\left(3,5,n\right)$ how the formula given later by Eq. (26) has been discovered. In the first step, we have computed a collection of ZZ polynomials for the consecutive members of the $O\left(3,5,n\right)$ family of benzenoids for $n=1,\ldots,23$. These ZZ polynomials have a maximal order of $Cl=15$ and can be expressed in the basis of $\left(1+x\right)^{i}$ monomials in the following way

$$\mathrm{ZZ}\left(O\left(3,\,5\,,n\right),x\right)=\sum_{i=0}^{Cl}c_{i}\left(1+x\right)^{i}\tag{9}$$

with the coefficients c_i given in Table 1. For the first few structures $O\left(3,5,n\right)$, the highest coefficients vanish, as their Clar numbers are lower than 15; the corresponding zeros are not displayed in Table 1.

Our next task here is to understand what the dependence of the coefficients c_i on the flake width n and on the Clar cover order i is. A comparison of Eq. (9) with Eqs. (2)–(5), Eq. (8), and particularly Eq. (6) suggests that the dependence on n can be expressed *via* binomial coefficients $\binom{n+j}{i}$ with j assuming small integer values, and the dependence on i can be expressed by two binomial coefficients, $\binom{n+j}{i}$, mentioned already in the context of n, and $\binom{Cl-2j+s}{i-2j+t}$, with s and t assuming some small positive or negative integer values.

Table 1. Coefficients in Eq. (9) for the ZZ polynomial of hexagonal graphene flakes $O\,(3,5,n)$ expressed in the basis of the $(1+x)^i$ monomials.

n	c_0	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9
1	1	15	30	10						
2	1	30	195	440	380	120	10			
3	1	45	495	2155	4360	4360	2141	505	49	1
4	1	60	930	6020	19365	33600	32487	17694	5336	858
5	1	75	1500	12900	57025	141603	206448	180752	95385	30005
6	1	90	2205	23660	133175	431018	842499	1022424	778965	371888
7	1	105	3045	39165	267855	1069383	2624405	4080285	4078275	2626805
8	1	120	4020	60280	485310	2305128	6811882	12926220	16014348	13014482
9	1	135	5130	87870	813990	4483578	15499704	34741608	51394002	50485116
10	1	150	6375	122800	1286550	8062956	31925256	82555704	142027050	163700790
11	1	165	7755	165935	1939850	13630386	60824533	178264713	349730865	462804111
12	1	180	9270	218140	2814955	21917896	108836585	356549050	785707780	1174098640
13	1	195	10920	280280	3957135	33818421	184956408	669806280	1638109187	2728327173
14	1	210	12705	353220	5415865	50401806	301036281	1194217232	3209828583	5896149194
15	1	225	14625	437825	7244825	72930809	472335549	2037062781	5968794195	11987687855
16	1	240	16680	534960	9501900	102877104	718118852	3345408792	10613260200	23136639644
17	1	255	18870	645490	12249180	141937284	1062302800	5316276720	18154823940	42693416480
18	1	270	21195	770280	15552960	192048864	1534151094	8208417360	30022124916	75756120324
19	1	285	23655	910195	19483740	255406284	2169018093	12355805241	48188409729	129872834517
20	1	300	26250	1066100	24116225	334476912	3009140827	18182971158	75326375520	215953753950
21	1	315	28980	1238860	29529325	432017047	4104479456	26222290336	114993932845	349437067837
22	1	330	31845	1429340	35806155	551087922	5513606175	37133343720	171854757305	551758254300
23	1	345	34845	1638405	43034035	695071707	7304642565	51724469885	251937727635	852178545185

n	c_{10}	c_{11}	c_{12}	c_{13}	c_{14}	c_{15}
4	71	2				
5	5516	566	31	1		
6	109881	19532	1998	110	2	
7	1081287	278205	42962	3692	137	1
8	6896952	2338604	488891	58688	3365	56
9	32785104	13837382	3666349	570431	44632	1176
10	125974002	63710304	20487838	3930626	391038	14112
11	411945732	242987150	92000678	21024220	2541994	116424
12	1186979079	800318870	348893376	92609796	13190926	731808
13	3088572344	2343739892	1156511733	349860479	57386920	3737448
14	7389394727	6233536660	3435186677	1166920138	216653781	16195608
15	16478155083	15298661599	9313989581	3510958185	727915779	61408347
16	34612630728	35074477464	23381039110	9686069920	2218219906	208416208
17	69056497776	75846722980	54948397322	24816195502	6221692912	644195552
18	131742979476	155899844224	121970485616	59645600308	16248774080	1837984512
19	241645111440	306512029596	257561042384	135588246196	39882167892	4892876352
20	428075043759	579419616586	520467581020	293474329688	92699273888	12259074816
21	735183691044	1057695607834	1011410446839	608179695825	205321802768	29115302688
22	1227987633653	1871256849020	1897906264980	1212351518350	435642916640	65937597264
23	2000312898023	3218538393585	3451107444480	2333846757910	889376153085	143107211709

Since there exist many binomial identities and Eq. (6) can be expressed in many equivalent forms owing to these identities, in the first step we decided to assume that $s = t = l$, with l being some small positive or negative integer, and to test if the basis of binomial products $\binom{n+j}{i}\binom{Cl-2j-l}{i-2j-l}$ is sufficiently flexible to encode the n– and i–dependence of the coefficients c_i. It remained to be decided how large the basis actually needs to be by choosing a maximal value of j and minimal and maximal values of l. The form of the binomial basis functions suggests that $Cl-2j-l \geq 0$. The actual maximal values of j and l needed to be found experimentally. We have discovered that the choice of $0 \leq j \leq 8$ and $-3 \leq l \leq 3$ is sufficient to express all the coefficients c_i in question as linear combinations of binomial products $\binom{n+j}{i}\binom{Cl-2j-l}{i-2j-l}$, and at the same time such a choice of j and l recovers all the linear combination coefficients d_{lj} uniquely. Owing to these observations, the ZZ polynomials of the hexagonal flakes $O(3,\,5\,,n)$ could be represented using the following formula

$$\mathrm{ZZ}\left(O\left(3,\,5\,,n\right),x\right) = \sum_{i=0}^{Cl}\sum_{j=0}^{8}\sum_{l=-3}^{3} d_{lj}\binom{Cl-2j-l}{i-2j-l}\binom{n+j}{i}\left(1+x\right)^i \tag{10}$$

with the table of the coefficients d_{lj} given by the following matrix

$l \backslash j$	0	1	2	3	4	5	6	7	8
−3	0	0	0	0	0	0	1	2	1
−2	0	0	0	0	10	49	65	23	0
−1	0	0	10	120	415	505	202	15	0
0	1	30	260	871	1215	676	117	0	0
1	0	10	120	415	505	202	15	0	0
2	0	0	10	49	65	23	0	0	0
3	0	0	0	1	2	1	0	0	0

(11)

Since this formula was discovered by an empirical analysis based on a finite and rather small ($n = 1$–23) family of ZZ polynomials, it was important to confirm that it could be used to recover also the ZZ polynomials for $n > 23$. To this end, we computed with ZZDecomposer the ZZ polynomials $\mathrm{ZZ}\left(O\left(3,\,5\,,n\right),x\right)$ for $n = 1,\ldots,1000$ and confirmed that all of these polynomials can be reproduced by Eq. (10) with coefficients d_{lj} given by Eq. (11). This agreement provides quite strong evidence for the correctness of the conjectured Eq. (10), but of course it cannot replace a formal proof of this fact, which remains to be found. Similar considerations performed for the family of hexagonal flakes $O(3,3,n)$ show that their ZZ polynomials can be represented by the following formula

$$\mathrm{ZZ}\left(O\left(3,\,3\,,n\right),x\right) = \sum_{i=0}^{Cl}\sum_{j=0}^{4}\sum_{l=-1}^{1} d_{lj}\binom{Cl-2j-l}{i-2j-l}\binom{n+j}{i}\left(1+x\right)^i \tag{12}$$

with $Cl = 9$ and the table of the coefficients d_{lj} given by the following matrix

$l \backslash j$	0	1	2	3	4
−1	0	0	1	2	1
0	1	9	17	7	0
1	0	1	2	1	0

(13)

Note that Eqs. (12) and (13) provide yet another representation for the ZZ polynomials of the graphene flakes $O(3,3,n)$ equivalent to Eq. (6). Similar considerations performed for the family of hexagonal flakes $O(3,4,n)$ show that their ZZ polynomials can be represented by the following formula

$$\mathrm{ZZ}\left(O\left(3,\,4\,,n\right),x\right) = \sum_{i=0}^{Cl}\sum_{j=0}^{6}\sum_{l=-2}^{2} d_{lj}\binom{Cl-2j-l}{i-2j-l}\binom{n+j}{i}\left(1+x\right)^{i} \tag{14}$$

with $Cl = 12$ and the table of the coefficients d_{lj} given by the following matrix

$l \backslash j$	0	1	2	3	4	5	6
−2	0	0	0	0	1	2	1
−1	0	0	4	24	36	14	0
0	1	18	84	128	61	6	0
1	0	4	24	36	14	0	0
2	0	0	1	2	1	0	0

(15)

We have confirmed that Eqs. (12) and (13) reproduce the ZZ polynomials of hexagonal flakes $O(3,3,n)$ and that Eqs. (14) and (15) reproduce the ZZ polynomials of hexagonal flakes $O(3,4,n)$ computed in a brute-force manner using ZZDecomposer with $n = 1,\ldots,1000$.

The matrices of the coefficients d_{lj} given by Eqs. (13), (15), and (11) have similar structures and are characterized by a high degree of internal symmetry. The non-zero entries in rows $+l$ and $-l$ are identical, but are located in different columns. This symmetry can be utilized to discover even more compact representations of Eqs. (12), (14), and (10) given by

$$\mathrm{ZZ}\left(O\left(3,\,3\,,n\right),x\right) = \sum_{i=0}^{9}\sum_{j=0}^{3}\sum_{l=0}^{1}\sum_{h=0}^{l} c_{lj}\binom{l}{h}\binom{9-2j-l}{i-2j-l}\binom{n+j+h}{i}\left(1+x\right)^{i} \tag{16}$$

$$\mathrm{ZZ}\left(O\left(3,\,4\,,n\right),x\right) = \sum_{i=0}^{12}\sum_{j=0}^{5}\sum_{l=0}^{2}\sum_{h=0}^{l} c_{lj}\binom{l}{h}\binom{12-2j-l}{i-2j-l}\binom{n+j+h}{i}\left(1+x\right)^{i} \tag{17}$$

$$\mathrm{ZZ}\left(O\left(3,\,5\,,n\right),x\right) = \sum_{i=0}^{15}\sum_{j=0}^{6}\sum_{l=0}^{3}\sum_{h=0}^{l} c_{lj}\binom{l}{h}\binom{15-2j-l}{i-2j-l}\binom{n+j+h}{i}\left(1+x\right)^{i} \tag{18}$$

with the coefficients c_{lj} given by the following matrices

$l \backslash j$	0	1	2	3
0	1	9	17	7
1	0	1	2	1

for $O\,(3,3,n)\,,$ (19)

$l \backslash j$	0	1	2	3	4	5
0	1	18	84	126	57	4
1	0	4	24	36	14	0
2	0	0	1	2	1	0

for $O\,(3,4,n)$, $O\,(4,3,n)$, (20)

and

$l \backslash j$	0	1	2	3	4	5	6
0	1	30	260	851	1117	546	71
1	0	10	120	415	502	196	12
2	0	0	10	49	65	23	0
3	0	0	0	1	2	1	0

for $O\,(3,5,n)$, $O\,(5,3,n)$. (21)

Immediate generalization of these investigations to $O\,(3,6,n)$ and $O\,(3,7,n)$ yields readily the following matrices of the coefficients c_{lj}

$l \backslash j$	0	1	2	3	4	5	6	7	8
0	1	45	625	3583	9355	11249	5820	1045	29
1	0	20	400	2524	6418	6882	2858	322	0
2	0	0	50	468	1330	1379	473	25	0
3	0	0	0	20	86	104	34	0	0
4	0	0	0	0	1	2	1	0	0

for $O\,(3,6,n)$, $O\,(6,3,n)$ (22)

and

$l \backslash j$	0	1	2	3	4	5	6	7	8	9
0	1	63	1281	11375	49515	110139	124349	67182	14942	907
1	0	35	1050	10545	46330	96819	96448	42478	6608	159
2	0	0	175	2685	13566	28627	26209	9477	934	0
3	0	0	0	175	1374	3377	3100	953	44	0
4	0	0	0	0	35	137	154	47	0	0
5	0	0	0	0	0	1	2	1	0	0

for $O\,(3,7,n)$, $O\,(7,3,n)$. (23)

The isostructural form of Eqs. (16 – 18) allows us to conjecture that the ZZ polynomial of a general hexagonal graphene flake $O\,(k,m,n)$ can be expressed as

$$\mathrm{ZZ}\,(O\,(k,\,m\,,n)\,,x) \;=\; \sum_{i=0}^{k\cdot m}\sum_{j=0}^{j_{\max}}\sum_{l=0}^{l_{\max}}\sum_{h=0}^{l} c_{lj}\binom{l}{h}\binom{k\cdot m-2j-l}{i-2j-l}\binom{n+j+h}{i}(1+x)^i \qquad (24)$$

with the structural constants c_{lj} specified separately for each k and m (but being independent of n) and with the upper summation limits $j_{\max}$ and $l_{\max}$ given as a function of the parameters k and m. (Note that the values of $j_{\max}$ and $l_{\max}$ for $O\,(3,6,n)$ and $O\,(3,7,n)$ in Eq. (24) are implicitly defined through the vertical and horizontal dimensions of the tables of structural constants c_{lj} given in Eqs. (22) and (23).) To discover the actual functional dependence of $j_{\max}$ and $l_{\max}$ on the parameters k and m, we have computed explicitly ZZ polynomials of hexagonal graphene flakes with $k, m = 2, \ldots, 7$ and $n = 1, \ldots, 100$ and used them to find the values of $j_{\max}$ and $l_{\max}$ matching Eq. (24). The results of this investigation

$j_{\max}$

$k \backslash m$	2	3	4	5	6	7
2	1	2	3	4	5	6
3	2	3	5	6	8	9
4	3	5	7	9	11	13
5	4	6	9	11	14	16
6	5	8	11	14	17	20
7	6	9	13	16	20	23

and

$l_{\max}$

$k \backslash m$	2	3	4	5	6	7
2	0	0	0	0	0	0
3	0	1	2	3	4	5
4	0	2	4	6	8	10
5	0	3	6	9	12	15
6	0	4	8	12	16	20
7	0	5	10	15	20	25

(25)

allow us to decipher the k– and m–dependence of $j_{\max}$ and $l_{\max}$ to be $j_{\max} = \left\lfloor \frac{k \cdot m}{2} \right\rfloor - 1$ and $l_{\max} = (k-2)(m-2)$.

3.2 Compilation of additional results

In the previous subsection we have conjectured that the ZZ polynomial of a hexagonal graphene flake $O(k, m, n)$ with general values of indices $k, m \geq 2$ can be expressed using a single equation given by

$$\mathrm{ZZ}\left(O\left(k,\ m\,,n\right),x\right) = \sum_{i=0}^{k \cdot m} \sum_{j=0}^{\left\lfloor \frac{k \cdot m}{2} \right\rfloor - 1} \sum_{l=0}^{(k-2)(m-2)} \sum_{h=0}^{l} c_{lj} \binom{l}{h} \binom{k \cdot m - 2j - l}{i - 2j - l} \binom{n+j+h}{i} (1+x)^i \quad (26)$$

with some appropriately selected coefficients c_{lj}, depending parametrically on k and m but not on n. In this section, we proceed to test this hypothesis by determination of structural constants c_{lj} which satisfy Eq. (26) for various values of the indices k, m, and n. This task is achieved by taking a large collection of ZZ polynomials of hexagonal graphene flakes $O(k,\ m\,,n)$ with indices $2 \leq k, m \leq 7$ and $1 \leq n \leq 100$ and solving an overdetermined system of linear equations for the coefficients c_{lj}. In every case studied here, we have been able to reach the solution in the form of a unique set of structural constants c_{lj} satisfying these equations. Detailed tables of these constants corresponding to all choices of the indices $2 \leq k, m \leq 7$ are presented later in this section. Clearly, the solutions obtained by us are formally valid only for $n \leq 100$. To further test their legitimacy and plausibility of correctness for a general value of n, we have computed a larger collection of ZZ polynomials for hexagonal graphene flakes $O(k,\ m\,,n)$ with indices

$2 \leq k, m \leq 7$ and n up to 1000. (The reader should be aware that the largest of these ZZ polynomials, $\mathrm{ZZ}\left(O\left(7,\ 7\,,1000\right), x\right)$, is a real numerical monster, with the largest coefficient (corresponding to x^{24}) equal to 50 909 322 696 394 350 082 772 496 801 903 352 514 969 943 953 390 091 610 237 817 825 177 029 987 781 807 068 252 953 119 773 192 428 410 207 708 792 804 942 850 $\approx 5{\cdot}10^{122}$ and that it takes a few days to compute these results with our new implementation of ZZCalculator.) The formula given by Eq. (26)—with the structural constants c_{lj} determined as described above and given in tables below—is able to reproduce all these ZZ polynomials with $n \leq 1000$. The fact that a single formula with a handful of coefficients c_{lj} is capable of reproducing dozens of coefficients in thousands of ZZ polynomials strongly suggests that Eq. (26) is valid for an arbitrary value of n, but since we cannot offer a formal proof of this fact, it remains for the time being a conjecture until such a proof is furnished. Unfortunately, the structural constants c_{lj} do not display too many clear patterns in their evolution with k and m (for details, see the discussion in Section 4), and at the moment their only way of determination is finding them directly from ZZ polynomials. A promising path of evaluation of the structural constants c_{lj} might be offered by the connection to the generalized strict order polynomial $\mathrm{E}^{\circ}_{P}(n, 1+x)$ in poset theory [80], but research along this line is too preliminary at the moment to be reported here.

In Tables 2–11, we report the structural constants c_{lj} for Eq. (26) for $3 \leq k, m \leq 7$. Note that when one of these two indices is equal to 1, then Eq. (26) is not valid (due to the negative upper summation limit) and the ZZ polynomials of the $O\left(1,\ m\,,n\right)$ and $O\left(k,\ 1\,,n\right)$ families of hexagonal graphene flakes are given by Eq. (2) (or its equivalent with m replaced by k). Similarly, when one of these indices is equal to 2, then the ZZ polynomial $O\left(2,\ m\,,n\right)$ (or $O\left(k,\ 2\,,n\right)$) is given by Eq. (8) (or its equivalent with m replaced by k, respectively). This equation is structurally similar to Eq. (26) and we could possibly give the tables of structural constants c_{lj} also for these cases. However, for $k = 2$ (or $m = 2$), the structural constants can be actually expressed in a closed form related to Narayana numbers as described in Eq. (8) above. Structural constants c_{lj} for ($k = 3, m =$ 3–7) and ($k =$ 3–7$, m = 3$) are given by Eqs. (19 – 23). Therefore, the tabulation below reports only the structural constants c_{lj} for the remaining cases. We would be happy to present the results even for a larger collection of hexagonal graphene flakes $O\left(k,\ m\,,n\right)$, but unfortunately, MATCH does not support supplementary materials

Table 2. $O\,(4,4,n)$ $\Longrightarrow$

$l \backslash j$	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**
0	1	36	395	1732	3253	2524	671	28
1	0	16	252	1192	2124	1392	248	0
2	0	1	43	256	456	261	25	0
3	0	0	2	22	42	22	0	0
4	0	0	0	1	2	1	0	0

$l \backslash j$	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
0	1	90	2835	42106	330696	1444370	3557648	4863646	3505103	1191712	148567	2926
1	0	80	3900	68112	562134	2413114	5548332	6730646	4038766	1028034	73566	0
2	0	15	1750	40272	367650	1593298	3462420	3727373	1829197	325812	9321	0
3	0	0	300	11118	120770	546472	1138102	1085616	423740	46418	0	0
4	0	0	15	1510	21932	108131	218754	183945	54456	2637	0	0
5	0	0	0	86	2238	12934	25750	18892	3868	0	0	0
6	0	0	0	1	122	947	1878	1184	131	0	0	0
7	0	0	0	0	2	40	82	44	0	0	0	0
8	0	0	0	0	0	1	2	1	0	0	0	0

$\Uparrow$

Table 3. $O\,(4,6,n)$ $O\,(6,4,n)$

Table 4. $O\,(4,5,n)$ $O\,(5,4,n)$ $\Longrightarrow$

$l \backslash j$	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
0	1	60	1195	10557	45799	100479	108946	53396	9391	260
1	0	40	1200	12074	52986	108740	102328	39166	4178	0
2	0	5	370	4803	22491	44241	36268	10408	486	0
3	0	0	40	846	4572	8856	6346	1258	0	0
4	0	0	1	71	502	972	604	65	0	0
5	0	0	0	2	30	60	32	0	0	0
6	0	0	0	0	1	2	1	0	0	0

Table 5. $O\,(5,5,n)$

$\Downarrow$

$l \backslash j$	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**
0	1	100	3575	61498	570996	3014170	9210008	16151778	15663239	7753602	1658789	100360
1	0	100	5598	114502	1129524	5932174	17166844	27228706	22636108	8877682	1284814	29808
2	0	25	3060	81528	890668	4753620	13152024	18858772	13264624	3957229	335046	0
3	0	1	720	28802	368514	2050898	5479194	7083750	4133562	877247	30370	0
4	0	0	69	5484	88929	532296	1385033	1603484	752781	100206	0	0
5	0	0	2	566	13090	88088	224382	229494	82350	4982	0	0
6	0	0	0	31	1191	9714	24012	21101	5291	0	0	0
7	0	0	0	1	66	744	1714	1221	172	0	0	0
8	0	0	0	0	2	39	80	43	0	0	0	0
9	0	0	0	0	0	1	2	1	0	0	0	0

Tables 2 – 5. Structural constants c_{lj} of hexagonal graphene flakes $O\,(k,m,n)$.

Table 6. $O(4,7,n)$ $O(7,4,n)$ ⟹

$l \backslash j$	0	1	2	3	4	5	6	7	8	9	10	11	12	13
0	1	126	5761	129276	1606995	11748122	51965874	140079872	227463265	215255744	111295513	27810631	2578865	37865
1	0	140	10080	271480	3632662	26881096	115274542	290520968	425358576	347680482	146071040	26609756	1369106	0
2	0	35	5950	214290	3244678	24981230	105482287	250347508	330378638	230928351	76632505	9386697	183614	0
3	0	0	1400	81410	1496238	12411132	52557378	118392482	140623876	82877584	20815706	1475346	0	0
4	0	0	105	15666	390197	3653311	15863562	34201095	36447695	17743523	3144693	89649	0	0
5	0	0	0	1374	58494	665628	3051792	6353974	6041550	2354970	257874	0	0	0
6	0	0	0	35	4800	75780	382757	777182	653637	193959	9395	0	0	0
7	0	0	0	0	164	5210	31344	62800	46150	9478	0	0	0	0
8	0	0	0	0	1	198	1649	3306	2089	231	0	0	0	0
9	0	0	0	0	0	2	52	108	58	0	0	0	0	0
10	0	0	0	0	0	0	1	2	1	0	0	0	0	0

Table 7. $O(5,6,n)$ $O(6,5,n)$ ⟱

$l \backslash j$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	150	8425	239124	3868493	37902272	232022586	898378195	2193419840	3314585382	2983771265	1494055599	366934090	33854828	499908
1	0	200	17988	622624	11013356	111019348	670815138	2479667056	5602783156	7576978488	5854650932	2367904136	421261918	21404754	0
2	0	75	14200	647860	12993730	137480443	829115485	2940756853	6147625801	7393875651	4830038995	1526161135	180496959	3441045	0
3	0	6	5200	351518	8381778	95348670	581153418	1987787446	3839361696	4070916080	2202052850	517421048	34772252	0	0
4	0	0	885	108604	3284990	41377680	258489770	856666286	1524079881	1407261358	612156479	98820457	2596492	0	0
5	0	0	60	19512	820852	11887630	77372212	249489092	406531396	321261160	107621012	10315654	0	0	0
6	0	0	1	1998	133461	2334649	16147135	50790698	75051270	49507545	11918995	475337	0	0	0
7	0	0	0	110	14168	319256	2406882	7373148	9715430	5155158	786548	0	0	0	0
8	0	0	0	2	965	30540	261107	769923	880739	355160	25076	0	0	0	0
9	0	0	0	0	40	2004	20904	57508	54844	15398	0	0	0	0	0
10	0	0	0	0	1	86	1234	2997	2232	361	0	0	0	0	0
11	0	0	0	0	0	2	50	104	56	0	0	0	0	0	0
12	0	0	0	0	0	0	1	2	1	0	0	0	0	0	0

Tables 6 – 7. Structural constants c_{lj} of hexagonal graphene flakes $O(4,7,n)$, $O(7,4,n)$, $O(5,6,n)$ and $O(6,5,n)$.

$l \backslash j$	0	1	2	3	4	5	6	7	8	9
0	1	210	17045	722330	18076201	285015882	2938557748	20224054068	93752453027	292531274982
1	0	350	46158	2424890	67579452	1119416400	11672185260	78966919980	351362307430	1029040647372
2	0	175	47740	3335890	107065128	1898998264	20257968347	135641596569	581152336272	1597596351492
3	0	21	23800	2459540	94936330	1844710338	20398946742	136171608941	563540516222	1453296510734
4	0	0	5845	1064550	52387509	1146766565	13345121449	89523915924	358932553176	867172813463
5	0	0	630	277680	18898076	482735323	6018192938	40930310622	159425569562	359969463019
6	0	0	21	42962	4551346	141976340	1937323697	13490759263	51171633187	107557978358
7	0	0	0	3692	733698	29664436	454914996	3280414879	12137489356	23601984544
8	0	0	0	137	77917	4427852	78955993	597543734	2157231314	3843369719
9	0	0	0	1	5222	469498	10194948	82373408	289454304	465513505
10	0	0	0	0	198	34672	977706	8650064	29352204	41682975
11	0	0	0	0	2	1698	68502	694530	2232824	2714607
12	0	0	0	0	0	51	3372	42634	124852	124571
13	0	0	0	0	0	1	110	1970	4946	3787
14	0	0	0	0	0	0	2	63	132	71
15	0	0	0	0	0	0	0	1	2	1

$l \backslash j$	10	11	12	13	14	15	16
0	608117552346	824530964465	703467308379	356238139706	97031394599	11812503473	412271170
1	1961796549598	2375258256881	1749385464792	728721105272	150742710368	11804801291	148583978
2	2783833344176	2986902757162	1872158258963	624532990872	92648414388	3943961256	0
3	2304159869580	2169447542000	1135940101580	292403300304	28408270800	445429994	0
4	1243363043837	1014313703827	432812936091	81423290041	4397338695	0	0
5	462962649848	321818319511	108132859166	13637408557	279104576	0	0
6	122727195702	71086372435	17888421428	1292574725	0	0	0
7	23539545686	11015769269	1917171112	54667709	0	0	0
8	3283065683	1187053783	123549993	0	0	0	0
9	331156480	86302783	3774288	0	0	0	0
10	23736499	3940951	0	0	0	0	0
11	1168218	90985	0	0	0	0	0
12	37284	0	0	0	0	0	0
13	668	0	0	0	0	0	0
14	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0

Table 8. Structural constants c_{lj} of hexagonal graphene flakes $O(5,7,n)$ and $O(7,5,n)$.

$l \backslash j$	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
0	1	225	19775	916223	25301701	444342631	5151950473	40290605845	214711769549	780585516377
1	0	400	57428	3315700	102492388	1900685508	22407714064	173268558356	892081378672	3067336666628
2	0	225	65247	4998960	178236618	3550482707	43003466765	330794187292	1650189102054	5366956149129
3	0	36	36950	4120050	176037868	3843833760	48391994142	372723845630	1806618440688	5555342174336
4	0	1	10925	2044661	110057847	2699070472	35789764732	277947056664	1312450971092	3811442182539
5	0	0	1600	633824	45937260	1303280408	18480518612	145808734404	672322335232	1840166999100
6	0	0	101	123330	13156625	447719184	6909866830	55842390272	251934557620	647722324530
7	0	0	2	14814	2617652	111716812	1915574920	15998758660	70712852724	169877083036
8	0	0	0	1046	361954	20508106	400095065	3487266139	15101521897	33622067327
9	0	0	0	42	34378	2792900	63661220	585497920	2478718612	5049357408
10	0	0	0	1	2185	284321	7777827	76461594	314280122	574389951
11	0	0	0	0	88	21798	733448	7828776	30737720	48990150
12	0	0	0	0	2	1252	53294	631231	2291019	3068439
13	0	0	0	0	0	50	2908	39854	126476	136024
14	0	0	0	0	0	1	108	1906	4943	3977
15	0	0	0	0	0	0	2	62	130	70
16	0	0	0	0	0	0	0	1	2	1

$l \backslash j$	**10**	**11**	**12**	**13**	**14**	**15**	**16**
0	1921494348645	3148551612905	3335550606803	2180193810463	814834545229	152422345585	10844827896
1	6988936769912	10348980994736	9621475143560	5304482438536	1573691730016	209115511048	8000025160
2	11287524974811	15009166986900	12106786912724	5517087418959	1249374951631	107424113482	1492504600
3	10743639663274	12725720417294	8777254118240	3218423735264	525500520358	24727069342	0
4	6743483064467	7042208799621	4075591021979	1158725917640	124657502886	2177618656	0
5	2958341271012	2687699574100	1272861982108	265844878980	16014545752	0	0
6	937586575243	728250366046	272664450229	38407783534	884915810	0	0
7	218693148206	141891928526	39953554160	3250265412	0	0	0
8	37855680891	19875858691	3891049807	126349943	0	0	0
9	4860402604	1973880618	233062534	0	0	0	0
10	458344467	134426857	6773139	0	0	0	0
11	31067384	5847300	0	0	0	0	0
12	1457419	131730	0	0	0	0	0
13	44764	0	0	0	0	0	0
14	799	0	0	0	0	0	0
15	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0

$l \backslash j$	**17**
0	124219818
1	0

Table 9. Structural constants c_{lj} of hexagonal graphene flakes $O(6, 6, n)$.

$l \backslash j$	0	1	2	3	4	5	6	7	8
0	1	315	39900	2741312	115619085	3200545485	60547174862	802958088186	7582941537662
1	0	700	146748	12742260	610784900	18152004834	355619053850	4760516794778	44482637606502
2	0	525	218029	25271985	1413768423	45810239049	938529310832	12761899828692	118446588956866
3	0	126	167580	28120400	1898944000	68323253908	1479975815726	20581890045694	190508445131382
4	0	7	70875	19404636	1651828743	67443080003	1564036321310	22411986925648	207760863373860
5	0	0	16100	8659650	983129862	46756826664	1177553409530	17530042490992	163473895939488
6	0	0	1806	2529004	412332947	23575046875	655469952118	10229939125732	96417125433884
7	0	0	84	478970	123665442	8832634744	276320659280	4567160349196	43720902444914
8	0	0	1	57088	26633471	2491398393	89658553306	1587247724515	15513423262724
9	0	0	0	4080	4100288	532979100	22641007566	434753814854	4362003810852
10	0	0	0	160	445429	86747948	4484041470	94699189202	980855401177
11	0	0	0	2	33382	10732808	700399502	16512283314	177569589112
12	0	0	0	0	1667	1002134	86661070	2315553100	26005011410
13	0	0	0	0	52	69182	8520674	261898966	3090551422
14	0	0	0	0	1	3384	665757	23903097	298459222
15	0	0	0	0	0	110	40988	1753178	23392302
16	0	0	0	0	0	2	1924	101784	1479922
17	0	0	0	0	0	0	62	4482	74512
18	0	0	0	0	0	0	1	134	2873
19	0	0	0	0	0	0	0	2	76
20	0	0	0	0	0	0	0	0	1

$l \backslash j$	9	10	11	12	13	14
0	51431577028397	251192160398133	880930702343267	2199803333462914	3853933803675767	4629921474321523
1	293505014794562	1373056462262628	4542499997618460	10530090335370208	16819210122229138	18026578499381300
2	761791995302759	3414574532836667	10642084518884548	22828299911634660	33061425759524632	31340480550125909
3	1196568577598148	5138934064281532	15060710116138884	29777270758668844	38843382831000674	32224393093584590
4	1276657136028943	5251781003656878	14437870843425034	26182689799160757	30514305632338964	21866887078332722
5	984396120342872	3875983728633532	9963901113135848	16473690889319768	16982564346318076	10342008335782660
6	569819470795733	2144796361775145	5134705296907224	7682008667738465	6918843029088176	3506618448607463
7	253910136776956	911859845213542	2022376813993720	2712418180161016	2101391716321996	862425610009426
8	88613352763881	302770288474317	617883914408759	734211473621015	479664214028454	153567521115802
9	24515557098560	79367046034342	147726440803158	153211910497118	82244539112608	19465060910518
10	5421751286253	16533259301773	27744015958759	24636935482589	10492621581275	1687256088043
11	963723147422	2744651836258	4089457694486	3032807128154	974987559186	91464118114
12	138064567908	362708016509	470344173015	281852616345	63341196004	2408559608
13	15937879366	37938386052	41722828664	19305360346	2644559386	0
14	1475934244	3104326412	2800983356	936279591	55942219	0
15	108414286	194926116	138184224	29912436	0	0
16	6175173	9130827	4791039	515853	0	0
17	262252	305780	110488	0	0	0
18	7871	6743	1565	0	0	0
19	160	86	0	0	0	0
20	2	1	0	0	0	0

Table 10. Structural constants c_{lj} of hexagonal graphene flakes $O(6,7,n)$ and $O(7,6,n)$.

$l \backslash j$	**15**	**16**	**17**	**18**	**19**	**20**
0	3686454978107086	1848482761458848	538713170609607	79523271157898	4497148465196	41067694904
1	12452473455697436	5209247569658264	1191416942928128	123323715383098	3691738921634	0
2	18527690659925310	6321248539795586	1087796818948664	71636225780052	763364349513	0
3	16026896573520322	4328413468915142	527323327050874	18589012621784	0	0
4	8951855531531266	1837116519450524	144022564250079	1831746511722	0	0
5	3386224483533170	497715712557694	21178401473078	0	0	0
6	882906905723331	84691389320826	1322636077996	0	0	0
7	157747254252450	8359247357508	0	0	0	0
8	18659078297839	371169332401	0	0	0	0
9	1337128041426	0	0	0	0	0
10	44882012644	0	0	0	0	0
11	0	0	0	0	0	0

Table 10 (continued). Structural constants c_{lj} of hexagonal graphene flakes $O\left(6,7,n\right)$ and $O\left(7,6,n\right)$.

and such results cannot be announced here. The future plan involves extending the presented here tabulations to hexagonal graphene flakes with $k+m \leq 20$ and announcing these results in some other media in the form of accompanying electronic text files, which should facilitate using these results in practice.

$l \backslash j$	0	1	2	3	4	5	6	7	8	9	10	11
0	1	441	80360	8150464	520808637	22437241151	679656432876	14881651014624	239965363556414	2885013842370396	26058155106531840	177468914708263294
1	0	1225	373968	48547984	3572763520	167584767539	5336698988308	119893492761912	1947644661551236	23244477621238072	205793234434476988	1358105698387760194
2	0	1225	725788	126286464	10949209234	566730866907	19138287487654	443740526285678	7290821428209344	86596956573629380	752559218860053710	4814413307639683052
3	0	441	755968	188993290	19873201716	1153233204177	41705090058292	1004373113724334	16760910472623340	198643550400106376	1696789549215747844	10525504682797558140
4	0	49	455637	180497321	23876405663	1582747248456	61979173081760	1561255902694988	26581041242006710	315186168071337346	2649718662276938660	15939191447012524592
5	0	1	159110	115323885	20101128412	1556286549800	66826521199836	1774366661284632	30967794585803876	368407333821713550	3051930105264218048	17801150028875397528
6	0	0	30961	50265085	12244539248	1136740559008	54294337197416	1532502794501292	27558806457153080	329872132188694396	2695906171770534162	15241983044101694724
7	0	0	3108	14975095	5494946992	631106568398	34080215323244	1032227232004410	19231629687266828	232302572446135254	1874907135308226412	10268721034752605110
8	0	0	139	3015409	1832776102	270298580180	16812407161898	552130652113492	10721016199663830	131084540140411416	1045773353367718204	5543237668207083028
9	0	0	2	401743	455233666	90139947980	6597002500100	237629374273856	4839655537134586	60084924318361900	474159480450250792	2429095400398641944
10	0	0	0	34320	83894425	23530686562	2076474746315	83092121061548	1787156874442529	22600934557267322	176505770113936401	872253653132026878
11	0	0	0	1784	11369156	4819758796	527414877626	23778369830936	544046125691768	7030441213437840	54341922597705450	258373098724163130
12	0	0	0	55	1116519	774706811	108544060615	5600049781570	137346705415634	1819150748983754	13911494841263800	63412896520968831
13	0	0	0	1	77676	97555805	18148681464	1090267727298	28888383241678	393260566589146	2972189785676140	12926977326521745
14	0	0	0	0	3703	9598240	2468751787	176161336625	5080746000259	71249561085992	531131869122746	2189937301225826
15	0	0	0	0	114	735928	273232702	23714955985	749276872872	10840639822676	79446379336036	307815810438614
16	0	0	0	0	2	43816	24558040	2670988460	92830729232	1386352895048	9938003028327	35749130585369
17	0	0	0	0	0	1988	1781656	252594370	9668128510	148934647412	1036514039010	3404617662879
18	0	0	0	0	0	63	102619	20055191	845097197	13407414288	89602634689	262657603771
19	0	0	0	0	0	1	4494	1322839	61658882	1006351396	6353131530	16114853731
20	0	0	0	0	0	0	134	70260	3707684	62486564	362873859	766258553
21	0	0	0	0	0	0	2	2814	178910	3175264	16189310	27322377
22	0	0	0	0	0	0	0	75	6554	129942	536493	699463
23	0	0	0	0	0	0	0	1	162	4126	12358	11707
24	0	0	0	0	0	0	0	0	2	91	192	103
25	0	0	0	0	0	0	0	0	0	1	2	1

Table 11. Structural constants c_{lj} of hexagonal graphene flakes $O(7,7,n)$.

$l \backslash j$	12	13	14	15	16	17	18
0	911470508686101510	3518698753460601390	10140590421889372336	21579866258058851370	33378189408954187379	36698505658882611953	27802031686120975632
1	6684876574594220052	24459565779274980334	66030328257321967708	129924110611295515006	183023508561667423460	179933735420151003389	119043145539032009116
2	22698800752831606638	78596256414520969524	198221594314975628056	359175895084465790318	458143366678479988556	399395867474450102013	227949905747899938718
3	47496034860451524524	155337272092974688312	364843562529362132364	605926338114738578566	695060158791591108208	531997537114570107433	258051074564456863164
4	68765504809917757560	211937737624428210662	461847401959122689734	699125174645244597706	715410820786466298808	475054787413989639265	192245144810438020253
5	73322590558324889888	212367736719420883326	427482179972162121632	585960210306393325006	529764975853714292068	300784014746757665497	99190355776225921198
6	59833883563660846084	162315303666342689604	300227745653887373240	369752300645079121378	291947832043821636558	139196256146405068880	36272990045501098529
7	38332809639894609128	97005685485614900078	163846743089540806968	179622411048867234824	122122932674468010524	47790311588830413242	9436934188366282036
8	19622639809399170258	46098795258132983326	70571688036821668590	68097518066820483036	39175083946883295754	12212425240939160320	1720229531807243299
9	8125869479719105182	17617798968307540450	24225637248120092772	20295219200007826452	9662756798849662570	2304080236028996140	210626121214089694
10	2745454757143109941	5454182287947398804	6663079565074199475	4764714794989687822	1824152014374156955	313797585757566012	15725986236778869
11	761024033464160400	1373165400816215134	1470462139838937614	878550829313892738	260111977139741688	29453049697938498	548397072463682
12	173587260824166855	281401195979295623	259786261159730147	126144599308367172	27309876424785040	1726978182295326	0
13	32600160391532320	46842312345365173	36511172648243620	13883540749419448	2013692329288290	48493259225882	0
14	5031045541204183	6300262824894348	4037062052925481	1140486687013223	94666599026841	0	0
15	634959718294026	678519896357356	345093588642326	66758946395647	2185176586504	0	0
16	64998533041466	57719976135906	22194139147705	2539889709911	0	0	0
17	5329897109338	3802460975470	1027515464062	48873714759	0	0	0
18	343981927437	188489091665	31524420976	0	0	0	0
19	17053766738	6735743295	510248644	0	0	0	0
20	627466675	162260859	0	0	0	0	0
21	16270036	2219363	0	0	0	0	0
22	281359	0	0	0	0	0	0
23	3252	0	0	0	0	0	0
24	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0

Table 11 (continued). Structural constants c_{lj} of hexagonal graphene flakes $O(7,7,n)$.

$l \backslash j$	**19**	**20**	**21**	**22**	**23**
0	13880775404349086642	4273960604525412735	729601219978707461	56900039937466224	1289252390888310
1	50250484386833471802	12463707878932390612	1579418503155938033	77152179492049624	611127372372622
2	79826013746631666354	15445030308636725698	1362992141581876377	34956741961396772	0
3	73185665015864931548	10572976639801015196	588325587660613823	5315574136983444	0
4	42786331366207114817	4333561663344472403	127600108827417774	0	0
5	16595699143936303485	1068251482039364696	11183843627712094	0	0
6	4288585003767876393	147457700969953378	0	0	0
7	715817996324929761	8850979884217732	0	0	0
8	70508785212273313	0	0	0	0
9	3149065545571691	0	0	0	0
10	0	0	0	0	0

Table 11 (continued). Structural constants c_{lj} of hexagonal graphene flakes $O\,(7, 7, n)$.

4 Discussion

The structural constants c_{lj} of hexagonal graphene flakes $O\,(k,\, m\,, n)$ tabulated in Eqs. (19 – 23) and in Tables 2–11 have a rather complicated k– and m–dependent form, which might prove difficult to recognize and understand. Nevertheless, some of the regularities appearing in the constants c_{lj} are obvious and easy to notice. The values of structural constants c_{lj} in the following columns and rows could be identified:

- In the column $j = 0$ the only non-vanishing structural constant is $c_{00} = 1$.

- The entries c_{lj} in the column $j = 1$ could be identified as

$$c_{l1} = \binom{k}{l+2}\binom{m}{l+2}. \tag{27}$$

  Only the entries with $l = 0, \ldots, \min\,(k, m) - 2$ have non-zero values. These entries seem to appear in various combinatorial problems (see the sequences A008459, A062145, A124428, A132813, A062196, and A062264 in OEIS [79]).

- In the row $l = l_{\max} = (k-2)\,(m-2)$ the only three non-zero structural constants c_{lj} are $c_{(k-2)(m-2),k+m-5} = 1$, $c_{(k-2)(m-2),k+m-4} = 2$, and $c_{(k-2)(m-2),k+m-3} = 1$.

In addition, we have been able to characterize the position l_{last} of the last non-vanishing element $c_{l_{\text{last}},j}$ in every column $j = 0, \ldots, j_{\max} = \left\lfloor \frac{k \cdot m}{2} \right\rfloor - 1$

$$l_{\text{last}} = \begin{cases} j \cdot \min(k, m) - 2j & \text{for } j \leq |m-k| + 1 \\ k \cdot m - 2j - 2 & \text{for } j \geq m + k - 3 \\ k \cdot m - 2j - \left\lfloor \left(\frac{k+m-j}{2}\right)^2 \right\rfloor & \text{otherwise} \end{cases} \tag{28}$$

and in some cases to identify the value of $c_{l_{\text{last}},j}$

$$c_{l_{\text{last}},j} = \begin{cases} \det(\mathbb{M}(k,m,j)) & \text{for } j \leq |m-k| + 1 \\ \text{not identified} & \text{for } j \geq m + k - 3 \\ 1 & \text{otherwise for } m + k + j \text{ odd} \\ 2 & \text{otherwise for } m + k + j \text{ even} \end{cases} \tag{29}$$

where the matrix $\mathbb{M}(k,m,j)$ with the entries $\mathbb{M}_{\alpha\beta} = \binom{|m-k|+1}{j-\alpha+\beta}$ has the size of $\min(k,m) \times \min(k,m)$. The last identifications have been possible owing to (i) an observation that the convex hull of the non-vanishing portion of the table of the structural constants c_{lj} for $O(k,\, m\,, n)$ is delimited in a large part by a superposition of triples $(1, 2, 1)$ and (ii) the following series of discoveries:

- The values $c_{l_{\text{last}},j}$ in the columns $j = 0, \ldots, m-2$ for hexagonal graphene flakes $O(3,\, m\,, n)$ could be identified as members of the sequence A056939 in OEIS [79] corresponding to the number of antichains (or order ideals) in the poset $\mathbf{3} \times (\boldsymbol{m} - \mathbf{2} - \boldsymbol{j}) \times \boldsymbol{j}$. (For all the basic terminology and concepts in poset theory, one might want to consult Stanley's classical text [81]. For example, $\boldsymbol{a} \times \boldsymbol{b} \times \boldsymbol{c}$ denotes a poset obtained as a Cartesian product of three linear chains $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ (pages 246 and 244 of [81]).) It is well-known (sequence A056939 in OEIS [79]) that these numbers can be computed as

$$c_{l_{\text{last}},j} = \begin{vmatrix} \binom{m-2}{j} & \binom{m-2}{j+1} & \binom{m-2}{j+2} \\ \binom{m-2}{j-1} & \binom{m-2}{j} & \binom{m-2}{j+1} \\ \binom{m-2}{j-2} & \binom{m-2}{j-1} & \binom{m-2}{j} \end{vmatrix} \tag{30}$$

- The values $c_{l_{\text{last}},j}$ in the columns $j = 0, \ldots, m-3$ for hexagonal graphene flakes $O(4,\, m\,, n)$ could be identified as members of the sequence A056940 in OEIS [79] corresponding to the number of antichains (or order ideals) in the poset $\mathbf{4} \times (\boldsymbol{m} - \mathbf{3} - \boldsymbol{j}) \times \boldsymbol{j}$. (When $j = 0$ or $m - j = 2$, the poset is empty with one (empty) ideal.) Again, it is well-known that these numbers can be computed as

$$c_{l_{\text{last}},j} = \begin{vmatrix} \binom{m-3}{j} & \binom{m-3}{j+1} & \binom{m-3}{j+2} & \binom{m-3}{j+3} \\ \binom{m-3}{j-1} & \binom{m-3}{j} & \binom{m-3}{j+1} & \binom{m-3}{j+2} \\ \binom{m-3}{j-2} & \binom{m-3}{j-1} & \binom{m-3}{j} & \binom{m-3}{j+1} \\ \binom{m-3}{j-3} & \binom{m-3}{j-2} & \binom{m-3}{j-1} & \binom{m-3}{j} \end{vmatrix} \tag{31}$$

- These two discoveries seem to be extendable to a general hexagonal flake $O(k,\ m\,,n)$. In this case, the position l_{last} of the last non-zero structural constants $c_{l_{\text{last}},j}$ in the columns $j = 0, \ldots, |m-k|+1$ for hexagonal graphene flakes $O(k,\ m\,,n)$ is equal to $l_{\text{last}} = j \cdot \min(k,m) - 2j$. Moreover, numerical experiments show that the values of $c_{(\min(k,m)-2)\cdot j,j}$ are given by the determinant of a $\min(k,m) \times \min(k,m)$ matrix $\mathbb{M}(k,m,j)$ with the entries $\mathbb{M}_{\alpha\beta} = \binom{|m-k|+1}{j-\alpha+\beta}$.
- It is possible to confirm that the structural constants $c_{(\min(k,m)-2)\cdot j,j}$ with $j = 0, \ldots, |m-k|+1$ for hexagonal graphene flakes $O(k,\ m\,,n)$ enumerate the number of antichains in the poset $\mathbf{min\,(}\boldsymbol{k,m}\mathbf{)} \times \mathbf{(}|\boldsymbol{m}-\boldsymbol{k}|\mathbf{+1-}\boldsymbol{j}\mathbf{)} \times \boldsymbol{j}$. The resulting sequences of values for $k = 3$, 4, and 5 are given by the sequences A056939, A056940, and A056941 in OEIS [79], respectively. For larger values of k, the sequences can be computed with MAPLE by, for example, the Stembridge's Maple Package for Posets [82] using the following short code

```
read "posets2.4v.txt":
withposets():
for k from 3 to 7 do
  for m from k to 7 do
    [seq(chain(k) &* chain(j) &* chain(m-k-j+1),j=1..m-k)]:
    map(nops@antichains,%):
    print(1,op(%),1):
  end do:
end do:
```

The remaining structural constants c_{lj} have a rather involved structure that escapes our attempts of identification at the moment. Factorization of c_{lj} often involves large primes, which might suggest that those coefficients are obtained from (multiple) summations.

An important direction aiming at further characterization of the structural constants c_{lj} comes from the poset theory, which appeared in this article already in two different contexts. We have been in the past few months working on finding a new method to compute ZZ polynomials of benzenoid strips and we have noticed that the recently developed interface theory of benzenoids offers the possibility of computing the values of c_{lj} by drawing an analogy between the Clar theory of benzenoids and the theory of strict order polynomials used in the poset theory to enumerate certain order-preserving maps from a poset P to an interval $[\,n\,] = \{1, \ldots, n\}$. To be more precise, the structural parameters k and m corresponding to a hexagonal graphene flake $O\,(k,\ m\,, n)$ uniquely define a poset $P = \boldsymbol{k} \times \boldsymbol{m}$, for which one can define the generalized strict order polynomial $\mathrm{E}^{\circ}_{P}(n, 1+x)$ [80], which coincides with the ZZ polynomial of $O\,(k,\ m\,, n)$. This correspondence allows to reinterpret the structural constants c_{lj} in the language of poset theory as the number of certain classes of linear extensions of the poset $P = \boldsymbol{k} \times \boldsymbol{m}$. Work on this topic is in progress and we hope to shed some more light on the transcendental meaning of the structural constants c_{lj} in the near future.

5 Conclusion

We have presented a compilation of structural constants c_{lj} that, used together with Eq. (26), allow to compute in a fast manner the ZZ polynomials of hexagonal graphene flakes $O\,(k, m, n)$ with $k, m = 3, \ldots, 7$ and $n = 1, \ldots, 1000$. We conjecture that the presented results are valid for an arbitrary value of n. This conclusion is strongly supported by the methodology of determination of c_{lj}, which were extracted from the ZZ polynomials of hexagonal graphene flakes $O\,(k, m, n)$ with $n = 1, \ldots, 100$ and then subsequently tested for $n = 101, \ldots, 1000$. We hope that the presented collection of numerical results will be helpful in discovering the general closed-form formula for the ZZ polynomials of hexagonal graphene flakes $O\,(k, m, n)$ valid for arbitrary structural parameters k, m, and n. The closed-form formula for the ZZ polynomial of hexagonal graphene flakes $O\,(k, m, n)$ with general values of the structural parameters k, m, and n constitutes perhaps the most difficult challenge of the Clar theory of benzenoids.

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