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ZZ Polynomial of Regular m-tier Benzenoid Strips as Extended Strict Order Polynomials of Associated Posets Part 1. Proof of Equivalence

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Abstract

In Part 1 of the current series of papers, we demonstrate the equivalence between the Zhang-Zhang polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of a Kekuléan regular m-tier strip $\boldsymbol{S}$ of length n and the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ of a certain partially ordered set (poset) $\mathcal{S}$ associated with $\boldsymbol{S}$. The discovered equivalence is a consequence of the one-to-one correspondence between the set $\{K\}$ of Kekulé structures of $\boldsymbol{S}$ and the set $\{\mu : \mathcal{S} \supset \mathcal{A} \to [\,n\,]\}$ of strictly order-preserving maps from the induced subposets of $\mathcal{S}$ to the interval $[\,n\,]$. As a result, the problems of determining the Zhang-Zhang polynomial of $\boldsymbol{S}$ and of generating the complete set of Clar covers of $\boldsymbol{S}$ reduce to the problem of constructing the set $\mathcal{L}(\mathcal{S})$ of linear extensions of the corresponding poset $\mathcal{S}$ and studying their basic properties. In particular, the Zhang-Zhang polynomial of $\boldsymbol{S}$ can be written in a compact form as

$$\mathrm{ZZ}(\boldsymbol{S}, x) = \sum_{k=0}^{|\mathcal{S}|} \sum_{w \in \mathcal{L}(\mathcal{S})} \binom{|\mathcal{S}| - \mathrm{fix}_{\mathcal{S}}(w)}{k \;\; - \mathrm{fix}_{\mathcal{S}}(w)} \binom{n + \mathrm{des}(w)}{k} (1+x)^k \,,$$

where $\mathrm{des}(w)$ and $\mathrm{fix}_{\mathcal{S}}(w)$ denote the number of descents and the number of fixed labels, respectively, in the linear extension $w \in \mathcal{L}(\mathcal{S})$. A practical guide and a four-step, completely automatable algorithm for computing $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ of an arbitrary strip $\boldsymbol{S}$, followed by a complete account of ZZ polynomials for all regular m-tier benzenoid strips $\boldsymbol{S}$ with m = 1–6 and arbitrary n computed using the discovered

equivalence between $\mathrm{ZZ}(\boldsymbol{S}, x)$ and $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$, are presented in Parts 2 and 3, respectively, of the current series of papers.
We would like to stress that the pursued by us approach is unprecedented in the existing literature on chemical graph theory and therefore it seems to deserve particular attention of the community, despite of its quite difficult exposition and connection to advanced concepts in order theory.

1 General introduction

The theory of Clar covers of benzenoids dates back to the early seminal work of Clar [22], who suggested that the most chemically stable resonance structures of benzenoids are those with the maximal number of aromatic sextets. This maximal number of aromatic sextets that can be accommodated in a given benzenoid $\boldsymbol{B}$—referred to in the modern literature as the *Clar number* of $\boldsymbol{B}$ and denoted as Cl—constitutes an important topological invariant of $\boldsymbol{B}$. A considerable effort has been invested in the determination of Cl for various classes of benzenoids or generalized benzenoids [1–13,23,28,36,39,49,50,55,56,67–69]. In general, a *Clar structure* realizing the maximal number Cl of aromatic sextets is not unique; the number of Clar structures is denoted by c_{Cl} and constitutes yet another important topological invariant of $\boldsymbol{B}$. A related, well-established and thoroughly-studied concept is the Kekulé count $K\{\boldsymbol{B}\}$ denoting how many resonance structures of $\boldsymbol{B}$ can be constructed using only double bonds and no aromatic sextets [24,35]. These two numbers, $c_0 \equiv K\{\boldsymbol{B}\}$ and c_{Cl}, can be considered as the beginning and the end-point of a sequence $c_0, c_1, \ldots, c_{Cl}$ denoting the cardinalities of the sets of Clar covers of different order, with c_k corresponding to the number of generalized resonance structures of $\boldsymbol{B}$ constructed using exactly k aromatic sextets. The generating function $\mathrm{ZZ}(\boldsymbol{B}, x)$ for this sequence was introduced to chemical graph theory by Zhang and Zhang as the *Clar covering polynomial*, but in the modern literature it is more often referred to as the *Zhang-Zhang polynomial* or the *ZZ polynomial*. Zhang and Zhang showed [62–66] that $\mathrm{ZZ}(\boldsymbol{B}, x)$ has a number of inviting recurrence properties, which make its determination much easier than finding any single of the topological invariants of $\boldsymbol{B}$. These results stimulated Gutman, Furtula, and Balaban [27] and later Chou and Witek [17] to design an algorithm capable of fast and robust computation of $\mathrm{ZZ}(\boldsymbol{B}, x)$ using the concept of recursive decomposition. The resulting computer program (ZZCalculator) [16,17] for determination of Zhang-Zhang polynomials of arbitrary benzenoid structures has later been augmented with a graphical interface (ZZDecomposer) [20,70,71] allowing one for generation of benzenoid graphs, computation

of ZZ($\boldsymbol{B}, x$), and analysis of the recursive decomposition pathways. ZZDecomposer has been used in many applications [15, 18, 19, 21, 29–33, 37, 45, 46, 57–61] to discover and formally prove closed-form formulas of ZZ polynomials for various classes of elementary and composite benzenoids. At present, the most important unsolved problems in the theory of ZZ polynomials are the determination of ZZ($\boldsymbol{B}, x$) for oblate rectangles $Or\,(m, n)$ and hexagonal graphene flakes $O\,(k, m, n)$.

Completely new vistas in the Clar theory have been recently opened by the development of the interface theory of benzenoids [29, 38, 40, 41, 58]. It has been demonstrated that the description of resonance structures of a benzenoid $\boldsymbol{B}$ can be reduced to studying the covering characters of its interfaces. The number of covered edges in each interface and the relative distribution of the covered edges between the consecutive interfaces of $\boldsymbol{B}$ is regulated by the basic tenets of the interface theory (Theorems 11, 16, and 21 of [40]), allowing one to express uniquely each Clar cover of $\boldsymbol{B}$ as a sequence of covered interface bonds of $\boldsymbol{B}$. The generation of the full set of Clar covers can then be conveniently performed by considering all possible distributions of covered interface bonds in $\boldsymbol{B}$ that satisfy the interface theory requirements. In the current work, we communicate a very important connection discovered by us recently in this context. Namely, we show that the distribution of double interface bonds in Kekulé structures of regular benzenoid strips can be very naturally expressed using the formalism of partially ordered sets (posets). The existing language and the machinery of the poset theory allows us to articulate many concepts of the interface theory in a particularly natural and compact form. Before jumping into technicalities, we find it appropriate to outline our main findings here. For definitions of basic terms in the poset theory see Section 3.1 or Stanley's textbook [54].

2 Outline of the results

The main results obtained in the current work can be briefly summarized as follows.

- Every Kekuléan regular m-tier strip $\boldsymbol{S}$ of length n can be uniquely associated with a certain poset $\mathcal{S}$.

- Every Clar cover of $\boldsymbol{S}$ can be associated with a unique linear extension of an induced subposet $Q \subset \mathcal{S}$. The number of Clar covers associated with a linear extension v of Q is given by $2^{|Q|}\binom{n+\mathrm{des}(v)}{|Q|}$, where $\mathrm{des}(v)$ denotes the number of descents in v. Each

of these $2^{|Q|}\binom{n+\mathrm{des}(v)}{|Q|}$ Clar covers differs from each other by various distributions of covering characters (proper sextet ⏣ or aromatic sextet ◎) among available positions ($|Q|$ distinct entries selected from the sequence $1, 2, \ldots, n + \mathrm{des}(v)$).

- The set $\{K\}$ of Kekulé structures of $\boldsymbol{S}$ stands in a one-to-one relationship to the set $\{\mu : \mathcal{S} \supset \mathcal{A} \to [\,n\,]\}$ of strictly order-preserving maps from induced subposets of $\mathcal{S}$ to the interval $[\,n\,]$. This correspondence is established by a complementary pair of difficult and technical Lemmata 22 and 23.

- The ZZ polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of $\boldsymbol{S}$ is identical to the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1 + x)$ of $\mathcal{S}$ enumerating the strictly order-preserving maps from subposets of $\mathcal{S}$ to the interval $\{1, \ldots, n\}$:

$$\mathrm{ZZ}(\boldsymbol{S}, x) \equiv \mathrm{E}^{\circ}_{\mathcal{S}}(n, 1 + x). \tag{1}$$

  The equivalence between both polynomials is demonstrated by Theorem 24, which constitutes the main result of our paper.

3 Preliminaries

3.1 Poset theory

The poset terminology used here follows closely Stanley's book [54]. A *partially ordered set* P, or *poset* for short, is a set together with a binary relation $<_P$. In this manuscript, we are concerned with finite posets P with p elements and with strict partial orders, meaning that the relation $<_P$ is irreflexive, transitive and antisymmetric. We say that the element $t \in P$ covers the element $s \in P$ (denoted as $s \lessdot_P t$) if $s <_P t$ and there is no element $u \in P$ such that $s <_P u <_P t$. The relation $<_P$ of a finite poset P is entirely determined by its cover relation, which allows us to represent P graphically in the form of a *Hasse diagram*: The vertices of the Hasse diagram are the elements of P, and every cover relation $s \lessdot_P t$ is represented by an edge that is drawn upwards from s to t. An *induced subposet* $Q \subset P$ is a subset of P together with the order $<_Q$ inherited from P which is defined for any $s, t \in Q$ by $s <_P t \iff s <_Q t$. The usual symbol $<$ denotes the relation „larger than" in $\mathbb{N}$. The symbol $[\,n\,]$ stands for the set $\{1, 2, \ldots, n\}$, and $[\,n, m\,]$ stands for the set $\{n, n + 1, \ldots, m\}$. The symbol $\boldsymbol{n}$ represents the chain $1 < 2 < 3 < ... < n$. We say that a map $\phi : P \to \mathbb{N}$ is *order-preserving* if it satisfies $s <_P t \Rightarrow \phi(s) \leq \phi(t)$, and *strictly*

order-preserving if it satisfies $s <_P t \Rightarrow \phi(s) < \phi(t)$. A *natural labeling* of a poset P is an order-preserving bijection $\omega : P \to [\,p\,]$. A *linear extension* of P is an order-preserving bijection $\sigma : P \to \boldsymbol{p}$, which is often represented as a permutation $\omega \circ \sigma^{-1}$ expressed by the sequence $w = w_1 w_2 \ldots w_p$ with $w_i = \omega(\sigma^{-1}(i))$. The set of all such linear extensions w is denoted by $\mathcal{L}(P)$ and is usually referred to as the Jordan-Hölder set of P. If two subsequent labels w_i and w_{i+1} in w stand in the relation $w_i > w_{i+1}$, then the index i is called a *descent* of w. The total number of descents of w is denoted by $\mathrm{des}(w)$.

The strict order polynomial $\Omega^{\circ}_P(n)$ of a poset P [52–54] enumerates the strictly order-preserving maps $\phi : P \to [\,n\,]$ and can be expressed as

$$\Omega^{\circ}_P(n) = \sum_{w \in \mathcal{L}(P)} \binom{n + \mathrm{des}(w)}{p}. \tag{2}$$

The *extended strict order polynomial* $\mathrm{E}^{\circ}_P(n, z)$ of a poset P is formally defined [42] as

$$\mathrm{E}^{\circ}_P(n, z) = \sum_{Q \subset P} \Omega^{\circ}_Q(n) z^{|Q|}, \tag{3}$$

where the sum runs over the induced subposets Q of P. The theorem demonstrated recently by us (Theorem 2 of [42]) allows us to rewrite Eq. (3) in a more explicit form

$$\mathrm{E}^{\circ}_P(n, z) = \sum_{k=0}^{p} \sum_{w \in \mathcal{L}(P)} \binom{p - \mathrm{fix}_P(w)}{k - \mathrm{fix}_P(w)} \binom{n + \mathrm{des}(w)}{k} z^k, \tag{4}$$

where $\mathrm{fix}_P(w)$ denotes the number of fixed labels in the linear extension $w = w_1 w_2 \ldots w_p$ of P. A label w_i is *fixed* in w if at least one of the following two conditions is satisfied: (1) $i-1$ or i is a descent, or (2) the set $L(w_i) = \{l \,|\, l < i, w_l > w_i\}$ of positions of preceding larger labels and the set $J(w_i) = \{j \,|\, \omega^{-1}(w_j) <_P \omega^{-1}(w_i)\}$ of positions of necessarily preceding labels satisfy the following two conditions: $L(w_i) \neq \varnothing$ and $\max(L(w_i)) > \max(J(w_i))$.

3.2 Chemical graph theory

There are many non-equivalent definitions of a benzenoid in the literature [14, 25, 34, 65]. In the current paper, we aim at studying a specific family of benzenoids (regular m-tier benzenoid strips), so for our purpose it is sufficient to define a benzenoid $\boldsymbol{B}$ as a finite subgraph of the infinite hexagonal lattice L, obtained by choosing a cycle $C_{\boldsymbol{B}}$ in L and selecting all the vertices and edges of L that lie on or inside $C_{\boldsymbol{B}}$ [65]. We assume that the lattice L is oriented such that some of its edges are vertical. We say that a benzenoid $\boldsymbol{B}$ is a *regular 1-tier strip of length* n if it consists of n adjacent hexagons located in the

same horizontal row of L. A *regular m-tier strip* $\boldsymbol{S}$ is obtained by merging m consecutive regular 1-tier strips located in adjacent rows of L, in such a way that the following two conditions are satisfied: (*i*) Two adjacent strips differ at each end by $\pm\frac{1}{2}$ hexagon unit. (*ii*) The top and the bottom regular 1-tier strips are both of the same length n [60, 61]. Examples of regular m-tier strips are given in Figs. 1, 8, and 9.

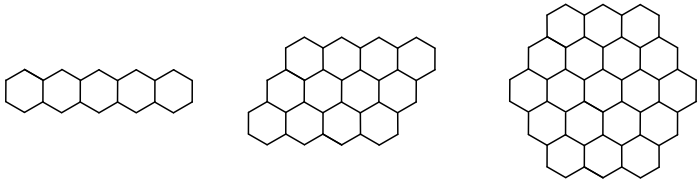

Figure 1. Examples of regular m-tier strips of length n, with $m = 1, 3, 5$ and $n = 5, 4, 3$, respectively.

A *Clar cover* is a spanning subgraph of B such that every one of its connected components is isomorphic to K_2 or C_6 [22, 69]. (K_2 denotes a complete graph on 2 vertices and C_6 denotes a cycle of girth 6.) A spanning subgraph of $\boldsymbol{B}$ consisting entirely of K_2 components is usually referred to as a *Kekulé structure* [25, 35], a perfect matching, or a 1-factor of $\boldsymbol{B}$. Both concepts, Kekulé structures and Clar covers, played very important roles in the early development stages of theoretical chemistry, when it seemed plausible that accurate predictions of energetic stability and reactivity of benzenoid hydrocarbons could be directly linked to the theory of chemical resonance [22, 48] based on topological invariants derived by analyzing Kekulé structures and Clar covers of a given benzenoid. Unfortunately, early quantum chemical methods based on these concepts, such as the Hückel method or the extended Hückel method, could not withstand the competition from much more accurate and sophisticated computational models of quantum chemistry, such as density functional theory and *ab initio* methods, and have been gradually sinking into oblivion. However, we see potential capabilities lying dormant in those graph-theoretical concepts, which might in the near future lead to a renaissance of Kekulé structure– or Clar cover–based novel techniques of quantum chemistry, using for example the set of Kekulé structures or Clar covers as a Hilbert space basis for valence bond configuration interaction (CI) or perturbation theory calculations. Such methods are yet to be developed, but their latent advantages rely on the efficient enumeration of Clar covers or Kekulé

structures and generation of Hamiltonian matrix elements in their basis using concepts similar to those used in the graphical unitary group approach (GUGA) to CI [47,51]. We hope that the research reported here will contribute to such a development.

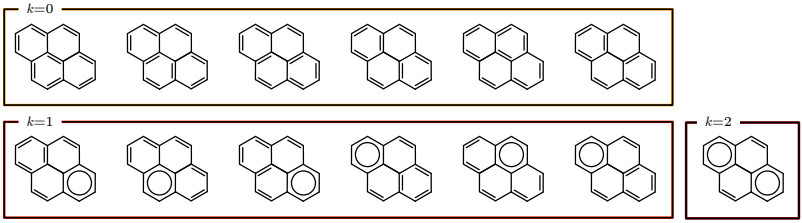

Figure 2. The parallelogram $M(2,2)$ has 6 possible Clar covers with no aromatic rings, 6 Clar covers with one aromatic ring, and one Clar cover with two aromatic rings. Therefore, $\mathrm{ZZ}(M(2,2)) = x^2 + 6x + 6$.

A Clar cover C of a benzenoid $\boldsymbol{B}$ with N vertices (atoms) consists of a certain number (say k) of hexagon (C_6) components and $\frac{N-6k}{2}$ edge (K_2) components. The number k is referred to as the *order* of the Clar cover C. As an example, we present in Fig. 2 all 13 possible Clar covers of the parallelogram $M(2,2)$ (i.e., the only regular 2-tier benzenoid strip of length 2). This set consists of six Clar covers of order 0 (coinciding with the Kekulé structures of $M(2,2)$), six Clar covers of order 1 and a single Clar cover of order 2. The maximal order Cl of the Clar covers of $\boldsymbol{B}$, naturally bounded from above by $\frac{N}{6}$, is referred to as the *Clar number* of $\boldsymbol{B}$ [22,26]. For $M(2,2)$ from Fig. 2, we have $Cl = 2$. Let us denote by c_k the number of Clar covers of $\boldsymbol{B}$ of order k. A generating function for the sequence $c_0, \ldots, c_{Cl}$

$$\mathrm{ZZ}(\boldsymbol{B}, x) \;=\; \sum_{k=0}^{Cl} c_k x^k \tag{5}$$

was introduced by Zhang and Zhang as the *Clar covering polynomial* [63–66], but is more commonly referred to in the modern literature as the *Zhang-Zhang polynomial* of $\boldsymbol{B}$ or simply the *ZZ polynomial* of $\boldsymbol{B}$. Zhang and Zhang demonstrated in Theorem 2 of [66] (see also Theorem 1 of [64]) that the ZZ polynomial of a benzenoid $\boldsymbol{B}$ can also be expressed as

$$\mathrm{ZZ}(\boldsymbol{B}, x) = \sum_{k=0}^{Cl} a(\boldsymbol{B}, k)(x+1)^k, \tag{6}$$

where $a(\boldsymbol{B}, k)$ denotes the number of Kekulé structures of $\boldsymbol{B}$ that have exactly k proper sextets, where a *proper sextet* is characterized by three edges of a Kekulé structure ar-

ranged within a hexagon as shown in the left panel of Fig. 3. The right panel of Fig. 3 gives a few examples of other coverings of a single hexagon that do not adhere to the definition of a proper sextet. Owing to Eq. (6), one can compute the ZZ polynomial of a benzenoid $\boldsymbol{B}$ from the analysis of the set of Kekulé structures of $\boldsymbol{B}$, which is substantially smaller than the set of Clar covers of $\boldsymbol{B}$. We heavily rely on this concept in the following.

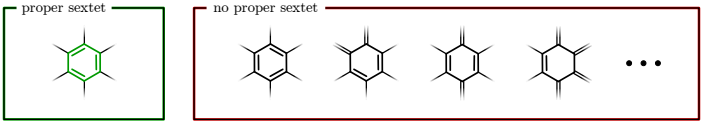

Figure 3. Left panel: Proper sextet. Right panel: Various coverings of a single hexagon that are not proper sextets.

3.3 Adaptation of the interface theory of benzenoids to the analysis of Kekulé structures of regular m-tier strips

Recently, we have developed a new theoretical framework for constructing, analyzing, and enumerating Kekulé structures and Clar covers of benzenoids, which is based on the concepts of fragments and interfaces. The resulting conceptual methodology was given the name of *interface theory of benzenoids* [40,41]. In this section, the main concepts and results of the interface theory of benzenoids are presented in a simplified form specialized for studying Kekulé structures of regular benzenoid strips. By virtue of Eq. (6), the presented formalism is sufficient to enumerate Clar covers of regular benzenoid strips and to compute their ZZ polynomials. In most cases, the presented theory is obviously consistent with the previous developments, but in situations when doubts might arise we give formal proofs of the presented facts.

We introduce the following linguistic equivalences to be used throughout this paper, which unify the terminologies typically used in the context of graph theoretical analysis of benzenoids by the mathematical and chemical communities: For a benzenoid $\boldsymbol{B}$ with a Kekulé structure K, a vertex in $\boldsymbol{B} \equiv$ an atom in $\boldsymbol{B}$, an edge in $\boldsymbol{B} \equiv$ a bond in $\boldsymbol{B}$, an edge covered by some K_2 in $K \equiv$ a double bond, and an edge in $\boldsymbol{B}$ that is not in $K \equiv$ a single bond.

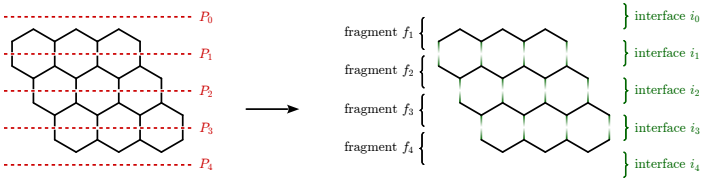

Figure 4. Dividing a regular m-tier strip of length n using $m+2$ horizontal partition lines $P_0, \ldots, P_{m+1}$ defines $m+1$ fragments $f_1, \ldots, f_{m+1}$ and $m+2$ interfaces $i_0, \ldots, i_{m+1}$. These concepts are illustrated here on the example of the parallelogram $M(m, n)$ with $m = 3$ and $n = 3$.

Consider a regular m-tier strip $\boldsymbol{S}$ with $m+2$ horizontal partition lines $P_0, \ldots, P_{m+1}$ along each row, as shown on the left side of Fig. 4. The vertical bonds of $\boldsymbol{S}$ crossed by the partition lines are called *interface bonds*, and the slanted bonds between the partition lines are called *spine bonds*. The set of bonds and atoms which are (at least partially) between the lines P_{k-1} and P_k is called the *fragment* f_k of $\boldsymbol{B}$. The set of interface bonds crossed by the line P_k is called the *interface* i_k of $\boldsymbol{B}$. The interfaces i_{k-1} and i_k above and below the fragment f_k are called the *upper and lower interfaces of* f_k, respectively. Each fragment is assigned a shape, as depicted in Fig. 5, in the following way.

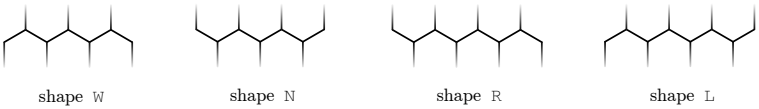

Figure 5. Fragments can have four possible shapes: `W` (wide), `N` (narrow), `R` (right), or `L` (left).

Let f_k be a fragment of a regular strip. Denote the leftmost interface bond of f_k by b_{first} and the rightmost interface bond of f_k by b_{last}. The *shape* of f_k is

$$\begin{array}{lll} \texttt{W} \quad \text{(wide)} & \text{if } b_{\text{first}} \in i_k & \text{and } b_{\text{last}} \in i_k, \\ \texttt{N} \quad \text{(narrow)} & \text{if } b_{\text{first}} \in i_{k-1} & \text{and } b_{\text{last}} \in i_{k-1}, \\ \texttt{R} \quad \text{(right)} & \text{if } b_{\text{first}} \in i_{k-1} & \text{and } b_{\text{last}} \in i_k, \\ \texttt{L} \quad \text{(left)} & \text{if } b_{\text{first}} \in i_k & \text{and } b_{\text{last}} \in i_{k-1}, \end{array}$$

where i_{k-1} is the upper interface of f_k and i_k is the lower interface of f_k. For example, in the parallelogram shown in Fig. 4, the fragment f_1 has shape `W`, f_2 and f_3 have shape `R`, and f_4 has shape `N`. It is clear that the sequence $[\texttt{W}, \texttt{R}, \texttt{R}, \texttt{N}]$ and the length $n = 3$ fully specify the geometry of this particular regular strip.

The bonds within each interface are numbered from the left to the right: The j^{th} bond in the interface i_k is denoted by $e_{k,j}$. Note that this differs from the bond notation

in the previous papers [40, 41]; it is however the most convenient naming system for the following derivations. The cardinality of a set J of edges will be denoted by $|J|$.

Definition 1. Consider a regular strip $\boldsymbol{S}$ and one of its Kekulé structures K. The *set K_I of double interface bonds* in K is defined as

$$K_I = E(K) \cap \bigcup_{k=1}^{m} i_k.$$

Any Kekulé structure K is uniquely determined by its set K_I:

Lemma 2 (Lemma 8 of [40])**.** *Let $\boldsymbol{S}$ be a regular strip, and consider two Kekulé structures K and K' of $\boldsymbol{S}$. If their sets of double interface bonds coincide, i.e., $K_I = K'_I$, then $K = K'$.*

Proof. The set K_I specifies the covering character of all interface bonds: those in K_I are double bonds, and the remaining ones are single bonds. According to Lemma 8 of [40], the interface bond covering characters fully determine the entire Clar cover (here K). Therefore, $K_I = K'_I$ implies $K = K'$. ■

Definition 3. Consider a regular strip $\boldsymbol{S}$ and one of its Kekulé structures K. The *order* of an interface i of $\boldsymbol{S}$ is defined as the number of edges of K located in i:

$$\mathrm{ord}(i) = |K_I \cap i|\,.$$

Theorem 4 (First Rule: Interface order criterion (Theorem 11 of [40]))**.** *Consider a regular m-tier strip $\boldsymbol{S}$ of length n with a Kekulé structure K. Let i be an interface of $\boldsymbol{S}$. Then,*

$$ord(i) = |i| - n. \tag{7}$$

Proof. According to Theorem 11 of [40] and the definition of regular strips,

$$\mathrm{ord}(i_k) = \begin{cases} \mathrm{ord}(i_{k-1}) + 1 & \text{if shape}(f_k) = \texttt{W}, \\ \mathrm{ord}(i_{k-1}) - 1 & \text{if shape}(f_k) = \texttt{N}, \\ \mathrm{ord}(i_{k-1}) & \text{if shape}(f_k) = \texttt{R or L}, \end{cases} \quad \text{and} \quad |i_k| = \begin{cases} |i_{k-1}| + 1 & \text{if shape}(f_k) = \texttt{W}, \\ |i_{k-1}| - 1 & \text{if shape}(f_k) = \texttt{N}, \\ |i_{k-1}| & \text{if shape}(f_k) = \texttt{R or L}. \end{cases}$$

The empty interface i_0 naturally has $\mathrm{ord}(i_0) = 0$. The first fragment f_1 of a regular strip always has the shape W, thus the first interface i_1 has $\mathrm{ord}(i_1) = \mathrm{ord}(i_0)+1 = 1$. In a regular strip of length n, the interface i_1 has $|i_1| = n + 1$ bonds, and therefore $|i_1| - \mathrm{ord}(i_1) = n$. Owing to the recursive properties of $\mathrm{ord}(i_k)$ and $|i_k|$ specified a few lines above, for every fragment shape, we find $|i_k| - \mathrm{ord}(i_k) = |i_{k-1}| - \mathrm{ord}(i_{k-1})$. It follows by induction that $|i_k| - \mathrm{ord}(i_k) = n$ for all $k = 1, 2, \ldots, m$. ■

Remark 5. We see from Theorem 4 that $\mathrm{ord}(i) = |i| - n$, and since $|i|$ and n are both independent of K, so is $\mathrm{ord}(i)$. This signifies that the interface orders $\mathrm{ord}(i_1), \ldots, \mathrm{ord}(i_m)$ are identical for all Kekulé structures K of $\boldsymbol{S}$ and constitute yet another topological invariant of $\boldsymbol{S}$. We will in the following take advantage of this fact, and understand the order $\mathrm{ord}(i)$ of an interface i of $\boldsymbol{S}$ to be equal to $|i| - n$, even when no Kekulé structure is specified.

Theorem 6 (Second Rule: Double interface bonds alternate (Theorem 16 of [40]))**.** *Let $\boldsymbol{S}$ be a regular strip with a Kekulé structure K. Let f be a fragment of $\boldsymbol{S}$. The double interface bonds of K belonging to f (i.e., edges in $K_I \cap f$) are, from left to right, distributed as follows.*

(a) *The first interface bond and the first double interface bond in f belong to the same interface.*

(b) *The last interface bond and the last double interface bond in f belong to the same interface.*

(c) *If there is a double bond in the upper (lower) interface, then the next double bond can only belong to the lower (upper) interface.*

Proof. Since a regular strip $\boldsymbol{S}$ is a benzenoid and since its Kekulé structure K is a Clar cover, all assumptions of Theorem 16 of [40] are satisfied and we know from the statements (a) and (b) of the reformulation of Theorem 16 of [40] given by Theorem 4 of [41] that the statements (a) and (b) of the current theorem are true, because in a regular strip $\boldsymbol{S}$ the first (last) atom of f is connected to the first (last) interface bond of f. The statement (c) of the current theorem is a direct consequence of the statement (c') of Theorem 16 of [40]. ■

Theorem 7 (Third Rule: Construction of Clar covers (Theorem 21 of [40]))**.** *Consider a regular m-tier strip $\boldsymbol{S}$. Define a set K_v of double interface bonds in $\boldsymbol{S}$ satisfying for every $k \in [\,m\,]$ the following conditions:*

(a) $|K_v \cap i_k| = ord(i_k)$

(b) *The set $K_v \cap f_k$ satisfies the statements (a)–(c) of Theorem 6.*

Then, there is exactly one Kekulé structure K with $K_I = K_v$.

Proof. The present theorem is a direct consequence of Theorem 5 of [41] applied to Kekulé structures (i.e., Clar covers of order 0) of regular strips. Reinterpreting the set K_v in the language used in [41] corresponds to assigning double bond covering character to all the interface bonds in K_v, and single bond covering character to all the interface bonds in $\bigcup_{k=1}^{m} i_k \setminus K_v$. Condition (a) of Theorem 5 of [41] is vacuously satisfied since none of the interface bonds in $\boldsymbol{S}$ have aromatic covering character. Condition (a) of the present Theorem implicitly defines interface orders $\mathrm{ord}(i_k)$ satisfying—by the arguments presented in the proof of Theorem 4 above—the conditions (a)–(c) of Theorem 3 of [41], which in turn implies the validity of condition (b) of Theorem 5 of [41]. The proof of Theorem 6 shows that a set of double interface bonds $K_v \cap f_k$ which satisfies condition (b) of the present theorem also satisfies condition (c) of Theorem 5 of [41]. Therefore, all the conditions of Theorem 5 of [41] are satisfied, meaning that there exists exactly one Clar cover with the double interface bonds specified by K_v. Since none of the interface bonds are aromatic, this unique Clar cover is a Kekulé structure K with $K_I = K_v$. ■

4 Derivation of the main results

We always assume in the following that $\boldsymbol{S}$ is a regular m-tier strip of length n with at least one Kekulé structure.

4.1 Partially ordered set of DIBs

Consider an arbitrary Kekulé structure K of the regular strip $\boldsymbol{S}$ and the corresponding set of double interface bonds K_I. We will see in the following that the set K_I can be naturally extended to a poset, whose structure is completely determined by the First and Second Rule of interface theory, and thus identical for every Kekulé structure K.

Let us first analyze the structure of K_I. The number of bonds of K_I located in any interface i_k of $\boldsymbol{S}$, $|K_I \cap i_k|$, is, by Theorem 4, equal to $\mathrm{ord}(i_k) = |i_k| - n$. Since $|i_k| - n$ is independent of K, the numbers of double bonds in the interfaces $i_1, \ldots, i_m$ are the same for every choice of K. Let us refer to the j^{th} element of $K_I \cap i_k$ from the left as $d^K_{k,j}$. Then, we can express the set K_I as

$$K_I \;=\; \bigcup_{k=1}^{m} \bigcup_{j=1}^{\mathrm{ord}(i_k)} \left\{ d^K_{k,j} \right\}. \tag{8}$$

It is clear that the structure of the set K_I given by Eq. (8) is identical for every Kekulé structure K.

We can introduce now a strict partial order $<_K$ on the set K_I via an appropriate cover relation $\lessdot_K$:

Definition 8. Consider two double interface bonds $d^K_{k,j}, d^K_{k',j'} \in K_I \subset E(K)$ and denote $\kappa = \max(k, k')$. We say that $d^K_{k,j}$ and $d^K_{k',j'}$ stand in the cover relation $d^K_{k,j} \lessdot_K d^K_{k',j'}$ if and only if

- $|k' - k| = 1$ and
- $j' - j = \begin{cases} 0 & \text{when the first interface bond of } f_\kappa \text{ belongs to } i_k, \\ 1 & \text{when the first interface bond of } f_\kappa \text{ belongs to } i_{k'}. \end{cases}$

The first condition, $|k' - k| = 1$, indicates that $d^K_{k,j}$ and $d^K_{k',j'}$ belong to the same fragment f_κ of $\boldsymbol{S}$, and the second condition effectively stipulates that $d^K_{k',j'}$ is the next double interface bond in f_κ to the right from $d^K_{k,j}$:

Theorem 9 (DIB Reformulation of the Second Rule)**.** *Consider a fragment f and a Kekulé structure K of $\boldsymbol{S}$. Consider further two double interface bonds $d^K_{k,j}, d^K_{k',j'} \in K_I \cap f$ which stand in the relation $d^K_{k,j} \lessdot_K d^K_{k',j'}$. Then, $d^K_{k,j}$ is located to the left of $d^K_{k',j'}$, and all the interface bonds of f between $d^K_{k,j}$ and $d^K_{k',j'}$ are single bonds.*

Proof. Denote by i_l the interface of f which contains the first interface bond of f, and by i_r the other interface of f. According to condition (a) of the Second Rule (given in Theorem 6), the first double interface bond $d^K_{l,1}$ of f is in i_l. According to condition (c) of Theorem 6, a double bond in i_l (i_r) is followed by a double bond in i_r (i_l). Therefore, the double interface bonds of f are alternating between the interfaces i_l and i_r and are given, from left to right, by the sequence $d^K_{l,1}, d^K_{r,1}, d^K_{l,2}, d^K_{r,2}, d^K_{l,3}, \ldots$

For two double interface bonds of the fragment f standing in the relation $d^K_{k,j} \lessdot_K d^K_{k',j'}$, we need to consider two possibilities: (i) $k' = r$ or (ii) $k' = l$. In case (i), the first condition of Definition 8 tells us that $k = l$ and the second condition of Definition 8 tells us that $j' = j$. A comparison with the sequence specified at the beginning of this proof shows that $d^K_{k,j} = d^K_{l,j'}$ is indeed located to the left of $d^K_{k',j'} = d^K_{r,j'}$. Similarly, in case (ii), we have $k = r$ and $j' = j + 1$. Again, a comparison with the sequence specified at the beginning of this proof shows that $d^K_{k,j} = d^K_{r,j'-1}$ is indeed located to the left of $d^K_{k',j'} = d^K_{l,j'}$. Since $d^K_{l,j'}$ and $d^K_{r,j'}$ in case (i) and $d^K_{r,j'-1}$ and $d^K_{l,j'}$ in case (ii) are consecutive pairs of double interface

bonds in the above sequence, no double interface bonds are located between them and all interface bonds (if any) located between $d^K_{k,j}$ and $d^K_{k',j'}$ are single bonds. ■

Definition 10. The transitive closure of the relation $\lessdot_K$ shall be denoted by $<_K$.

Lemma 11. *The relation $<_K$ is a strict partial order.*

Proof. We have to show that $<_K$ is irreflexive, transitive and antisymmetric. Transitivity is clear from Def. 10. It follows from Theorem 9 that, whenever $d^K_{k,j} <_K d^K_{k',j'}$, the double interface bond $d^K_{k,j}$ is located to the left of $d^K_{k',j'}$; consequently, $<_K$ is antisymmetric and irreflexive. ■

Fact 12. *Consider a fragment f of $\boldsymbol{S}$ and its Kekulé structure K. Denote by i_u the upper interface of f and by i_l the lower interface of f. It follows from Def. 8 that the set $\mathscr{C}_K(f)$ of cover relations $\lessdot_K$ between the double interface bonds of f (i.e., between the elements of $K_I \cap (i_u \cup i_l) = \left\{d^K_{u,1}, \ldots, d^K_{u,ord(i_u)}, d^K_{l,1}, \ldots, d^K_{l,ord(i_l)}\right\}$) is completely specified by the following chain of inequalities*

$$\begin{cases} d^K_{u,1} \lessdot_K d^K_{l,1} \lessdot_K d^K_{u,2} \lessdot_K d^K_{l,2} \lessdot_K \ldots \lessdot_K d^K_{l,ord(i_l)} \lessdot_K d^K_{u,ord(i_u)} & \text{if } shape(f) = \texttt{W} \\ d^K_{l,1} \lessdot_K d^K_{u,1} \lessdot_K d^K_{l,2} \lessdot_K d^K_{u,2} \lessdot_K \ldots \lessdot_K d^K_{u,ord(i_u)} \lessdot_K d^K_{l,ord(i_l)} & \text{if } shape(f) = \texttt{N} \\ d^K_{l,1} \lessdot_K d^K_{u,1} \lessdot_K d^K_{l,2} \lessdot_K d^K_{u,2} \lessdot_K \ldots \lessdot_K d^K_{l,ord(i_l)} \lessdot_K d^K_{u,ord(i_u)} & \text{if } shape(f) = \texttt{R} \\ d^K_{u,1} \lessdot_K d^K_{l,1} \lessdot_K d^K_{u,2} \lessdot_K d^K_{l,2} \lessdot_K \ldots \lessdot_K d^K_{u,ord(i_u)} \lessdot_K d^K_{l,ord(i_l)} & \text{if } shape(f) = \texttt{L} \end{cases} \tag{9}$$

The structure of the set $\mathscr{C}_K(f)$ is independent of the Kekulé structure K used for its construction and depends only on the structural parameters of $\boldsymbol{S}$: the shape of a given fragment f of $\boldsymbol{S}$ is obviously independent of K and the orders of its both interfaces, $ord(i_u)$ and $ord(i_l)$, are independent of K by Remark 5.

Fact 13. *Consider a regular benzenoid strip $\boldsymbol{S}$ and its Kekulé structure K. The complete set $\mathscr{C}_K(\boldsymbol{S})$ of cover relations $\lessdot_K$ that can be constructed for $\boldsymbol{S}$ is given by*

$$\mathscr{C}_K(\boldsymbol{S}) = \bigcup_{k=2}^{m} \mathscr{C}_K(f_k) \tag{10}$$

Again, following the discussion at the end of Fact 12, the structure of the set $\mathscr{C}_K(\boldsymbol{S})$ given by Eq. (10) is identical for every Kekulé structure K and thus independent of K. Note that the fragments f_1 and f_{m+1} can be excluded from the sum in Eq. (10), because they contain only one non-empty interface each and consequently do not contribute any cover relations to $\mathscr{C}_K(\boldsymbol{S})$.

Below, in Examples 14 and 15, we construct the Hasse diagram corresponding to the poset generated by the complete set of cover relations $\mathscr{C}_K(\boldsymbol{S})$ for two regular strips, $\boldsymbol{S} = M(3,2)$ and $\boldsymbol{S} = O(3,2,3)$.

Example 14. Consider the two distinct Kekulé structures of the parallelogram $M(3,2)$ shown in Figures 6(a) and (b). Each interface of $M(3,2)$, i_1 and i_2, has order one and contains one double bond, denoted as $d^K_{1,1}$ and $d^K_{2,1}$, respectively. The set K_I thus contains two elements, $K_I = \{d^K_{1,1}, d^K_{2,1}\}$. Definition 8 allows us to establish one cover relation, $d^K_{1,1} \lessdot_K d^K_{2,1}$, which is identical for each selected Kekulé structure—in fact, since Definition 8 relies only on the indices of the elements of K_I, this cover relation holds for every Kekulé structure of $M(3,2)$. According to Theorem 9, the relation $d^K_{1,1} \lessdot_K d^K_{2,1}$ implies that $d^K_{1,1}$ is located to the left of $d^K_{2,1}$; this is easily verified for any given Kekulé structure such as the ones given in Fig. 6(a) and (b). The resulting Hasse diagram for $M(3,2)$ for the posets K_I with the derived relation $<_K$ is shown in Figure 6(c).

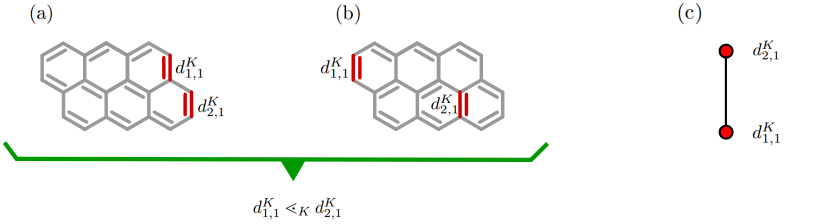

Figure 6. The double interface bonds $d^K_{1,1}$ and $d^K_{2,1}$ in two distinct Kekulé structures (a) and (b) of the parallelogram $M(3,2)$ are related by the same cover relation $d^K_{1,1} \lessdot_K d^K_{2,1}$, which indicates that $d^K_{1,1}$ must be located to the left of $d^K_{2,1}$. In (c) we show the resulting Hasse diagram (identical for every Kekulé structure of $M(3,2)$) corresponding to the cover relation $d^K_{1,1} \lessdot_K d^K_{2,1}$.

Example 15. Consider two distinct Kekulé structures of the hexagonal graphene flake $O(3,2,3)$ shown in Figures 7(a) and (b). The orders of the interfaces $i_1, \ldots, i_4$ are $1,2,2,1$, respectively. The set K_I contains thus six elements, $K_I = \{d^K_{1,1}, d^K_{2,1}, d^K_{2,2}, d^K_{3,1}, d^K_{3,2}, d^K_{4,1}\}$. Definition 8 allows us to establish seven cover relations (for the detailed list, see Figure 7). It can be verified that these cover relations are identical for every Kekulé structure of $O(3,2,3)$, and that Theorem 9 holds for each of these Kekulé structures. The Hasse diagram corresponding to the posets K_I of $O(3,2,3)$ is shown in Figure 7(c).

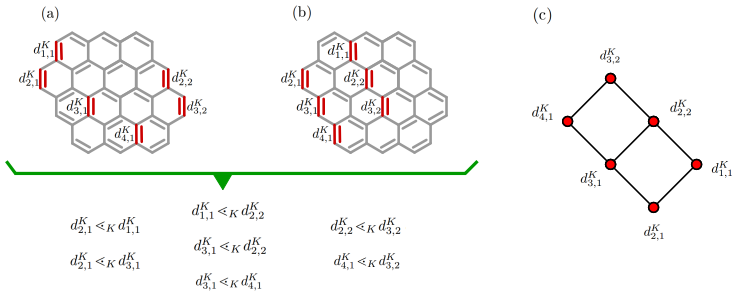

Figure 7. (a) and (b) Two distinct Kekulé structures of the hexagonal graphene flake $O(3,2,3)$. The cover relations determined from Definition 8 are the same for both Kekulé structures. (c) The resulting Hasse diagram for the partial order $<_K$ induced on the set $K_I = \{d^K_{1,1}, d^K_{2,1}, d^K_{2,2}, d^K_{3,1}, d^K_{3,2}, d^K_{4,1}\}$ by the seven listed cover relations is identical for every Kekulé structure of $O(3,2,3)$.

We have demonstrated before that the structure of the set K_I given by Eq. (8) is identical for every Kekulé structure K of $\boldsymbol{S}$. Similarly, we have demonstrated that the structure of the set of cover relations $\mathscr{C}_K(\boldsymbol{S})$ given by Eq. (10) is identical for every Kekulé structure K of $\boldsymbol{S}$. This shows that the corresponding Hasse diagrams (for example those constructed in Examples 14 and 15) are also independent of the choice of Kekulé structure K used for their construction; the only difference between two Hasse diagrams constructed using two distinct Kekulé structures is that the corresponding poset elements (i.e., the Hasse diagram vertices) $d^K_{k,j}$ and $d^{K'}_{k,j}$ may stand for different interface edges of $\boldsymbol{S}$. This notion can be further formalized by introducing a poset $\mathcal{S}$ which is isomorphic to all the posets K_I of $\boldsymbol{S}$.

Definition 16. Consider a regular benzenoid strip $\boldsymbol{S}$ with m interfaces $i_1, \ldots, i_m$ of orders $\mathrm{ord}(i_1), \ldots, \mathrm{ord}(i_m)$, respectively. We define the poset $\mathcal{S}$ as

$$\mathcal{S} = \bigcup_{k=1}^{m} \bigcup_{j=1}^{\mathrm{ord}(i_k)} \{s_{k,j}\}$$

together with the partial order $<_{\mathcal{S}}$ defined via its cover relations: Two elements $s_{k,j}, s_{k',j'} \in \mathcal{S}$ stand in the cover relation $s_{k,j} \lessdot_{\mathcal{S}} s_{k',j'}$ if and only if

- $|k' - k| = 1$ and
- $j' - j = \begin{cases} 0 & \text{when the first interface bond of } f_\kappa \text{ belongs to } i_k, \\ 1 & \text{when the first interface bond of } f_\kappa \text{ belongs to } i_{k'}, \end{cases}$

where $\kappa = \max(k, k')$. The elements $s_{k,j}$ of $\mathcal{S}$ are called the *double interface bonds of* $\boldsymbol{S}$, or DIBs for short. The set $\mathcal{S}$ will be referred to as the *set of* DIBs.

Examples of posets $\mathcal{S}$ for nine classes of regular benzenoid strips are shown in Figure 8.

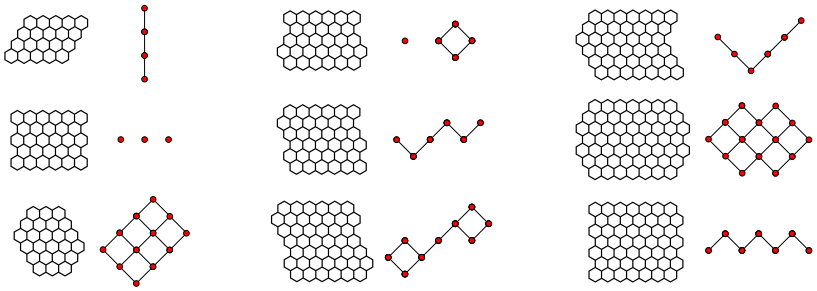

Figure 8. Examples of posets $\mathcal{S}$ constructed for nine selected regular benzenoid strips $\boldsymbol{S}$.

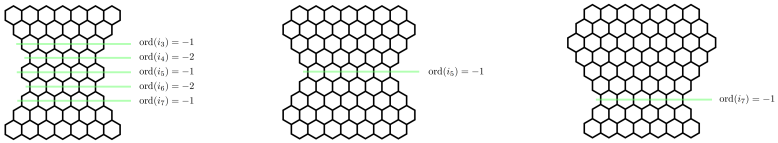

Figure 9. Not every regular strip $\boldsymbol{S}$ can be associated with a poset $\mathcal{S}$. The three regular strips shown above contain at least one interface with a negative order (marked in green online). Consequently, by Example 11 of [41], all the three structures are non-Kekuléan, there is no poset associated with them, and their ZZ polynomials are identically equal to 0.

It is now straightforward to construct an obvious isomorphism τ_K between $\mathcal{S}$ and any K_I:

Definition 17. Consider a Kekulé structure K of $\boldsymbol{S}$. Then the map $\tau_K : \mathcal{S} \to K_I \subset E(K)$ is defined by

$$\tau_K : s_{k,j} \mapsto d^K_{k,j} \text{ for every } k \in [\,m\,], j \in [\,\mathrm{ord}(i_k)\,].$$

Lemma 18. *If two* DIBs *stand in the relation* $s_{k,j} \lessdot_{\mathcal{S}} s_{k',j'}$*, then for any Kekulé structure* K *of* $\boldsymbol{S}$ *we have* $\tau_K(s_{k,j}) \lessdot_K \tau_K(s_{k',j'})$.

Proof. This fact is a direct consequence of the similarity between Definitions 8 and 16 of the relations $\lessdot_K$ and $\lessdot_{\mathcal{S}}$. If $s_{k,j} \lessdot_{\mathcal{S}} s_{k',j'}$, then the indices k, k', j and j' satisfy the two

conditions in Def. 16, which are identical to the two conditions in Def. 8, meaning that $\tau_K(s_{k,j}) = d^K_{k,j} \preccurlyeq_K d^K_{k',j'} = \tau_K(s_{k',j'})$. ■

Remark 19. Before continuing the exposition, let us summarize briefly the structure of the studied regular benzenoid strip $\boldsymbol{S}$. We recollect that $\boldsymbol{S}$ contains m interfaces $i_1, \ldots, i_m$. The interface i_k consists of $n+\mathrm{ord}(i_k)$ edges, out of which n have single covering character and $\mathrm{ord}(i_k)$ have double covering character in every Kekulé structure K of $\boldsymbol{S}$. The j^{th} bond in the interface i_k (with $j \in [\, n + \mathrm{ord}(i_k)\,]$) is denoted by $e_{k,j}$, regardless of its covering character. Additionally, for each Kekulé structure K, the j^{th} double interface bond in the interface i_k (with $j \in [\, \mathrm{ord}(i_k)\,]$) is denoted by $d^K_{k,j}$. Consequently, for each $d^K_{k,j}$ there exists an index $\tilde{j} = \tilde{j}\,(K,k,j) \in [\, n + \mathrm{ord}(i_k)\,]$ such that $d^K_{k,j} \equiv e_{k,\tilde{j}}$. Combining this fact with the definition of τ_K, we can see that for each $s_{k,j}$ there exists an index $\tilde{j} = \tilde{j}\,(K,k,j) \in [\, n + \mathrm{ord}(i_k)\,]$ such that $\tau_K(s_{k,j}) = e_{k,\tilde{j}}$. We use this fact in Definition 20 to define a new (K-dependent) property of $s_{k,j}$.

Definition 20. Let $\mathrm{pos}_K : \mathcal{S} \to \mathbb{N}$ be the map which assigns to each $s_{k,j}$ a number $\mathrm{pos}_K\,(s_{k,j})$ such that $\tau_K(s_{k,j}) = e_{k,\mathrm{pos}_K(s_{k,j})}$. This number $\mathrm{pos}_K\,(s_{k,j})$ is called the *position* of $s_{k,j}$ in K.

It is now clear that we can define any Kekulé structure K of $\boldsymbol{S}$ simply by specifying $\mathcal{S}$ and the corresponding map $\mathrm{pos}_K\,(s_{k,j})$: The set $K_I = \left\{ e_{k,\mathrm{pos}_K(s_{k,j})} \,|\, s_{k,j} \in \mathcal{S} \right\}$ uniquely determines K by Lemma 2.

4.2 Equivalence between the extended strict order polynomial and the ZZ polynomial

We have seen in the previous subsection that the set $\mathcal{S}$ together with the relation $<_{\mathcal{S}}$ constitutes a partially ordered set. The pair $(\mathcal{S}, <_{\mathcal{S}})$—denoted concisely also as $\mathcal{S}$—encodes the relative positions of double interface bonds within all Kekulé structures of a given regular strip. The absolute positions of the elements of K_I in a given Kekulé structure K are encoded by the triple $(\mathcal{S}, <_{\mathcal{S}}, \mathrm{pos}_K)$. We will show in the following that, in order to define K, it is sufficient to specify $\mathrm{pos}_K\,(s_{k,j})$ not for all elements of $\mathcal{S}$, but only for the elements of the subposet $\mathcal{A}_K \subset \mathcal{S}$ defined as follows.

Definition 21. Let K be a Kekulé structure of $\boldsymbol{S}$. Then, we denote by $\mathcal{A}_K$ the induced subposet of $\mathcal{S}$ given by

$$\mathcal{A}_K = \{ s_{k,j} \in \mathcal{S} \,|\, \tau_K(s_{k,j}) \text{ participates in a proper sextet of } K \}\,.$$

We will in the following Lemmata 22 and 23 establish a one-to-one correspondence between Kekulé structures of $\boldsymbol{S}$ and certain order-preserving maps from the elements of subposets $\mathcal{A}_K \subset \mathcal{S}$ to the numbers encoding the absolute positions of DIBs in K. This will allow us to establish, in Theorem 24, the equivalence between the ZZ polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ of a Kekuléan regular m-tier strip $\boldsymbol{S}$ and the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ of the corresponding poset $\mathcal{S}$.

Lemma 22. *Let $\boldsymbol{S}$ be a regular m-tier strip of length n with the poset of* DIB*s $\mathcal{S}$, and let K be a Kekulé structure of $\boldsymbol{S}$. Then, there is exactly one strictly order-preserving map $\mu : \mathcal{A}_K \to [\,n\,]$ such that*

1. $\mathrm{pos}_K(s_{k,j}) = \mu(s_{k,j}) + j$ *for every* $s_{k,j} \in \mathcal{A}_K$ *and*
2. $\mathrm{pos}_K(s_{k,j}) = \max(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}) + j$ *for every* $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$.

Lemma 23. *Let $\boldsymbol{S}$ be a regular m-tier strip of length n with the poset of* DIB*s $\mathcal{S}$. Let further $\mathcal{A} \subset \mathcal{S}$ be an induced subposet of $\mathcal{S}$, and let $\mu : \mathcal{A} \to [\,n\,]$ be a strictly order-preserving map. Then, there exists exactly one Kekulé structure K such that*

1. $\mathrm{pos}_K(s_{k,j}) = \mu(s_{k,j}) + j$ *for every* $s_{k,j} \in \mathcal{A}$,
2. $\mathrm{pos}_K(s_{k,j}) = \max(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}) + j$ *for every* $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}$,
3. $\mathcal{A}_K = \mathcal{A}$.

The proofs of Lemmata 22 and 23, being rather long and technical, are exiled to the Appendix.

Lemmata 22 and 23 are complementary. Together they establish a one-to-one correspondence between the set $\{K\}$ of Kekulé structures of $\boldsymbol{S}$ and the set $\{\mu : \mathcal{S} \supset \mathcal{A} \to [\,n\,]\}$ of strictly order-preserving maps from the induced subposets of $\mathcal{S}$ and the interval $[\,n\,]$. In particular, the pair $(\mathcal{A}, \mu)$ completely determines the corresponding Kekulé structure K in the following way. The cardinality of the set $\mathcal{A}$ determines the number of proper sextets in K; the positions of double interface bonds participating in the proper sextets are fully and uniquely determined by the map μ using condition 1 of Lemma 23. The positions of the double interface bonds not participating in proper sextets are fully and uniquely

determined by the map μ using condition 2 of Lemma 23. Both sets of double interface bonds define the set K_I and—by Lemma 2—uniquely determine the corresponding Kekulé structure K. This one-to-one correspondence is used to conclude our investigations with

Theorem 24. *Let $\boldsymbol{S}$ be a regular m-tier strip of length n with the poset of* DIBs *$\mathcal{S}$, and consider an integer k. Then the number $a(\boldsymbol{S}, k)$ of Kekulé structures with exactly k proper sextets is given by*

$$a(\boldsymbol{S}, k) = \sum_{\substack{\mathcal{A}\subset\mathcal{S} \\ |\mathcal{A}|=k}} \Omega^{\circ}_{\mathcal{A}}(n), \tag{11}$$

and the ZZ polynomial of $\boldsymbol{S}$ is given by the extended strict order polynomial of $\mathcal{S}$

$$\mathrm{ZZ}(\boldsymbol{S}, x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1). \tag{12}$$

Proof. For every $\mathcal{A} \subset \mathcal{S}$, Lemmata 22 and 23 establish a one-to-one correspondence between the sets $\mathcal{M} = \{\mu : \mathcal{A} \to [\,n\,] \mid \mu \text{ is strictly order-preserving}\}$ and $\mathcal{K} = \{K \mid K \text{ is a Kekulé structure with } \mathcal{A}_K{=}\mathcal{A}\}$, implying that $|\mathcal{M}| = |\mathcal{K}|$. The cardinality of $\mathcal{M}$ is, by Eq. (2), given by $\Omega^{\circ}_{\mathcal{A}}(n)$. In other words, there are $\Omega^{\circ}_{\mathcal{A}}(n)$ Kekulé structures K with $\mathcal{A}_K = \mathcal{A}$, which directly proves Eq. (11). Then, by Eqs. (6) and (3), we have

$$\begin{aligned} \mathrm{ZZ}(\boldsymbol{S}, x) &= \sum_{k=0}^{Cl} a(\boldsymbol{S}, k)(x+1)^k = \sum_{k=0}^{Cl} \sum_{\substack{\mathcal{A}\subset\mathcal{S} \\ |\mathcal{A}|=k}} \Omega^{\circ}_{\mathcal{A}}(n)(x+1)^k \\ &= \sum_{\mathcal{A}\subset\mathcal{S}} \Omega^{\circ}_{\mathcal{A}}(n)(x+1)^{|\mathcal{A}|} = \mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)\ . \end{aligned} \tag{13}$$

■

5 Applications

Practical application of Theorem 24 to the determination of ZZ polynomials of regular strips is presented in Parts 2 and 3 in this series of papers [43, 44], where we give a practical guide to computation of the extended strict order polynomials $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ together with a complete account of ZZ polynomials $\mathrm{ZZ}(\boldsymbol{S}, x)$ of regular m-tier benzenoid strips $\boldsymbol{S}$ with m = 1–6 and an arbitrary value of n determined as the extended strict order polynomials $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ of the corresponding posets $\mathcal{S}$. It would be inconvenient to present this collection of results here owing to its somewhat bulky volume. However, in order to foreshadow the forthcoming results, we illustrate very briefly the process of

determination of $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ using Eq. (4) for the two families of benzenoids, $M(2,n)$ and $O(3,2,n)$, for which we constructed the corresponding posets $\mathcal{S}$ in Examples 14 and 15. (Note that the poset $\mathcal{S}$ is independent of the structural parameter n, allowing us to compute $\mathrm{E}^{\circ}_{\mathcal{S}}(n, 1+x)$ for the whole families of structures simultaneously.)

- For $M(2,n)$, the poset $\mathcal{S}$ with $p = 2$ vertices in Fig. 6 allows only a single linear extension, $\mathcal{L}(\mathcal{S})$=$\{12\}$. The number of descents and the number of fixed elements in this extension are both zero, $\mathrm{des}(12) = 0$ and $\mathrm{fix}_{\mathcal{S}}(12) = 0$. Consequently, the ZZ polynomial of $M(2,n)$ is given by

$$\begin{aligned}\mathrm{ZZ}(M(2,n),x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x) &= \sum_{k=0}^{p} \binom{p-\mathrm{fix}_{\mathcal{S}}(12)}{k-\mathrm{fix}_{\mathcal{S}}(12)} \binom{n+\mathrm{des}(12)}{k} (1+x)^k \\ &= \sum_{k=0}^{2} \binom{2-0}{k-0} \binom{n+0}{k} (1+x)^k \\ &= \sum_{k=0}^{2} \binom{2}{k} \binom{n}{k} (1+x)^k\end{aligned}$$

  in agreement with, for example, Eq. (4) of [18].

- For $O(3,2,n)$, the poset $\mathcal{S}$ with $p = 6$ vertices in Fig. 7 allows five linear extensions, $\mathcal{L}(\mathcal{S})$=$\{123456,\ 123546, 132456, 135246, 132546\}$. The numbers of descents for these extensions are 0, 1, 1, 1, and 2, respectively, and the numbers of fixed elements are 0, 2, 2, 2, and 4, respectively. Consequently, the ZZ polynomial of $O(3,2,n)$ is given by

$$\mathrm{ZZ}(O(3,2,n),x) = \mathrm{E}^{\circ}_{\mathcal{S}}(n,1+x) = \sum_{k=0}^{6} \left(\tbinom{6}{k}\tbinom{n}{k} + 3\tbinom{4}{k-2}\tbinom{n+1}{k} + \tbinom{2}{k-4}\tbinom{n+2}{k} \right) (1+x)^k$$

  in agreement with, for example, Eq. (25b) of [61].

Further examples with more details were given previously in Examples 4 and 5 and Section 5.1 of [42].

6 Conclusions

We have demonstrated that for any Kekuléan regular m-tier strip $\boldsymbol{S}$ of length n, its Zhang-Zhang polynomial $\mathrm{ZZ}(\boldsymbol{S}, x)$ can be computed as the extended strict order polynomial $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ [42] from the poset $\mathcal{S}$ associated with $\boldsymbol{S}$. The equivalence between

$\mathrm{ZZ}(\boldsymbol{S}, x)$ and $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ given by Theorem 24 exists owing to the one-to-one correspondence between the set $\{K\}$ of Kekulé structures of $\boldsymbol{S}$ and the set $\{\mu : \mathcal{S} \supset \mathcal{A} \to [\,n\,]\}$ of strictly order-preserving maps from the induced subposets of $\mathcal{S}$ to the interval $[\,n\,]$ established by the complementary Lemmata 22 and 23. The determination of the poset $\mathcal{S}$ is straightforward and can be performed directly from the geometrical parameters of $\boldsymbol{S}$ for any Kekuléan regular strip; for non-Kekuléan strips, there is no poset associated with them, and consequently their ZZ polynomials are identically equal to 0. Owing to the fact that $\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1)$ of a p-element poset $\mathcal{S}$ can be written in a compact form as

$$\mathrm{E}^{\circ}_{\mathcal{S}}(n, x+1) = \sum_{w \in \mathcal{L}(\mathcal{S})} \sum_{k=0}^{p} \binom{p - \mathrm{fix}_{\mathcal{S}}(w)}{k - \mathrm{fix}_{\mathcal{S}}(w)} \binom{n + \mathrm{des}(w)}{k} (1+x)^k \,, \tag{14}$$

the process of determination of $\mathrm{ZZ}(\boldsymbol{S}, x)$ can be completely automatized for any regular m-tier strip $\boldsymbol{S}$. The corresponding algorithm, whose details are elaborated in Part 2 of the current series of papers [43] (see also [42] for mathematical details), can be summarized by the following steps: (*i*) Construct the poset $\mathcal{S}$ corresponding to $\boldsymbol{S}$. (*ii*) Construct the set $\mathcal{L}(\mathcal{S})$ of linear extensions of $\mathcal{S}$. (*iii*) For each linear extension $w \in \mathcal{L}(\mathcal{S})$, compute $\mathrm{des}(w)$ and $\mathrm{fix}_{\mathcal{S}}(w)$. (*iv*) Compute the sum in Eq. (14). An associated algorithm for generating the complete set of Clar covers of $\boldsymbol{S}$ could proceed as follows: (1) Construct the poset $\mathcal{S}$ corresponding to $\boldsymbol{S}$. (2) Construct all induced subposets $\mathcal{A} \subset \mathcal{S}$. (3) For each induced subposet $\mathcal{A}$, construct a set $\{v\}$ of its linear extensions. (4) For each linear extension v of $\mathcal{A}$, construct $2^{|\mathcal{A}|} \binom{n+\mathrm{des}(v)}{|\mathcal{A}|}$ Clar covers by selecting numbers $1 \le k_1 < k_2 < \ldots < k_{|\mathcal{A}|} \le n + \mathrm{des}(v)$ and assigning to each of the positions k_i the covering character ⬡ or ◎. The complete account of ZZ polynomials of regular m-tier benzenoid strips $\boldsymbol{S}$ with $m = 1$–6 and an arbitrary value of n using the corresponding posets $\mathcal{S}$ and Eq. (14) is presented in Part 3 of the current series of papers [44].

Summarizing the development presented in the current paper, we want to stress that the path pursued by us here is unprecedented in the existing literature on chemical graph theory. We are aware that the presented results rely heavily on quite advanced concepts in poset theory and might be difficult to be fully grasped and appreciated in the first reading. However, in our personal opinion the quite revolutionary character of our findings deserves particular attention of the community and should not be overlooked.

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Appendix

A.1 Proof of Lemma 22

During this subsection, let $\boldsymbol{S}$ be a regular m-tier strip of length n with the poset of DIBs $\mathcal{S}$ and a Kekulé structure K. In order to prove Lemma 22, we have to demonstrate that there is exactly one strictly order-preserving map $\mu : \mathcal{A}_K \to [\,n\,]$ that satisfies the two conditions

1. $\mathrm{pos}_K(s_{k,j}) = \mu(s_{k,j}) + j$ for every $s_{k,j} \in \mathcal{A}_K$ and
2. $\mathrm{pos}_K(s_{k,j}) = \max(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}) + j$ for every $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$.

We will show this by explicitly constructing such a map—first on the domain $\mathcal{S}$ and later restricted to the domain $\mathcal{A}_K$—and then by demonstrating its uniqueness.

Definition 25. Let μ_K be the map which assigns to each element of $\mathcal{S}$ a number depending on its position in K as follows.

$$\mu_K : \mathcal{S} \to \mathbb{N}, s_{k,j} \mapsto \mathrm{pos}_K(s_{k,j}) - j.$$

For a given Kekulé structure K, we will during this subsection often denote the number $\mu_K(s_{k,j})$ by $m^K_{k,j}$, or, since the considered Kekulé structure is clear, simply by $m_{k,j}$.

The following lemmata will show that μ_K is an order-preserving map $\mathcal{S} \to [\,0, n\,]$, and that the restriction $\mu_K|_{\mathcal{A}_K}$ is a strictly order-preserving map $\mathcal{A}_K \to [\,n\,]$ which is unique for every Kekulé structure.

Lemma 26. *Consider two* DIBs $s_{k,j}, s_{k',j'} \in \mathcal{S}$ *in a fragment* f *with* $s_{k',j'} \lessdot_{\mathcal{S}} s_{k,j}$*. Then,* $\tau_K(s_{k',j'})$ *is located to the left of* $\tau_K(s_{k,j})$*, and the number of interface bonds in* f *that are located between* $\tau_K(s_{k',j'})$ *and* $\tau_K(s_{k,j})$ *is given by*

$$b_K(s_{k',j'}, s_{k,j}) = 2\,(m_{k,j} - m_{k'j'})\,. \tag{15}$$

Proof. From $s_{k',j'} \lessdot_{\mathcal{S}} s_{k,j}$ it follows according to Lemma 18 that $\tau_K(s_{k',j'}) \lessdot_K \tau_K(s_{k,j})$, and it is then clear from Theorem 9 that $\tau_K(s_{k',j'})$ must be located to the left of $\tau_K(s_{k,j})$. Denote by i_l the interface of f which contains the first interface bond of f, and by i_r the other interface of f. Let further $p = \mathrm{pos}_K\,(s_{k,j}) = m_{k,j}+j$ and $p' = \mathrm{pos}_K\,(s_{k',j'}) = m_{k',j'}+j'$, meaning that $\tau_K(s_{k,j}) = e_{k,p}$ and $\tau_K(s_{k',j'}) = e_{k',p'}$. Following the definition of the bond names, the relevant interface bonds in f are $\ldots, e_{l,p'}, e_{r,p'}, e_{l,p'+1}, e_{r,p'+1}, \ldots, e_{l,p-1}, e_{r,p-1}, e_{l,p}, e_{r,p}, \ldots$. There are two possibilities:

$k = r$: According to Def. 16, this implies $j' = j$ and $k' = l$. Thus, the number of interface bonds between $e_{k'p'} \equiv e_{l,p'}$ and $e_{k,p} \equiv e_{r,p}$ is $2(p - p') = 2(p - p' - j + j') = 2\,(m_{k,j} - m_{k',j'})$.

$k = l$: According to Def. 16, this implies $j' = j - 1$ and $k' = r$. Thus, the number of interface bonds between $e_{k',p'} \equiv e_{r,p'}$ and $e_{k,p} \equiv e_{l,p}$ is $2(p - p' - 1) = 2(p - p' - j + j') = 2\,(m_{k,j} - m_{k',j'})$.

In either case, Eq. (15) is true. ∎

Lemma 27. *The map* μ_K *is order-preserving.*

Proof. Consider two DIBs $s_{k,j}$ and $s_{k',j'}$ with $s_{k',j'} <_{\mathcal{S}} s_{k,j}$. We have to show that the numbers $m_{k,j}$ and $m_{k',j'}$ satisfy the condition

$$m_{k',j'} \leq m_{k,j}. \tag{16}$$

Assume first that $s_{k',j'} \lessdot_{\mathcal{S}} s_{k,j}$. Then, according to Lemma 18 we have $\tau_K(s_{k',j'}) \lessdot_K \tau_K(s_{k,j})$, meaning that $\tau_K(s_{k',j'})$ and $\tau_K(s_{k,j})$ must belong to the same fragment f. The number $b_K(s_{k',j'}, s_{k,j})$ of interface bonds in f between $\tau_K(s_{k',j'})$ and $\tau_K(s_{k,j})$ is, according to Lemma 26, given by $b_K(s_{k',j'}, s_{k,j}) = 2m_{k,j} - 2m_{k',j'}$. Since $b_K(s_{k',j'}, s_{k,j})$ is non-negative, it is clear that $m_{k',j'} \leq m_{k,j}$.

Assume now that $s_{k',j'} \not\lessdot_{\mathcal{S}} s_{k,j}$. Then, there must exist DIBs s_{k_q,j_q} such that $s_{k',j'} \equiv s_{k_1,j_1} \lessdot_{\mathcal{S}} s_{k_2,j_2} \lessdot_{\mathcal{S}} \ldots \lessdot_{\mathcal{S}} s_{k_r,j_r} \equiv s_{k,j}$. Since Eq. (16) is true for all cover relations, it follows that $m_{k',j'} \leq m_{k_2,j_2} \leq \ldots \leq m_{k_{r-1},j_{r-1}} \leq m_{k,j}$. ∎

Lemma 28. *The map μ_K has the codomain $[\,0, n\,]$.*

Proof. Consider a DIB $s_{k,j} \in \mathcal{S}$. We have to show that its image $\mu_K(s_{k,j})$ satisfies $0 \leq \mu_K(s_{k,j}) \leq n$. Assume $\tau_K(s_{k,j}) = e_{k,p}$. In i_k, to the left of $\tau_K(s_{k,j})$, there are $j-1$ distinct double interface bonds $\tau_K(s_{k,1}), \ldots, \tau_K(s_{k,j-1})$. In other words, in i_k there are at least $j-1$ bonds to the left of $e_{k,p}$, meaning $p \geq j$ and thus $\mu_K(s_{k,j}) = p - j \geq 0$. To the right of $\tau_K(s_{k,j})$, in i_k, there are $\mathrm{ord}(i_k) - j$ double interface bonds $\tau_K(s_{k,j+1}), \ldots, \tau_K(s_{k,\mathrm{ord}(i_k)})$. With Theorem 4, it follows that $p \leq |i_k| - (\mathrm{ord}(i_k) - j) = n + j$ and thus $\mu_K(s_{k,j}) = p - j \leq n$. ∎

Lemma 29. *Let $s_{k,j} \in \mathcal{S}$. The following statements are equivalent:*

(i) $\quad m_{k,j} = max(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\})$

(i') $\quad m_{k,j} = max(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\})$

(ii) $\quad s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$.

Proof. Assume first that $\tau_K(s_{k,j}) = e_{k,1}$, which implies $m_{k,j} + j = \mathrm{pos}_K(s_{k,j}) = 1$. There is no space to the left of $e_{k,1}$ that could accommodate a proper sextet which has $\tau_K(s_{k,j})$ as its double interface bond. Therefore, statement (ii) is true. Simultaneously, due to the naming convention of the DIBs, we have $j = 1$ and thus $m_{k,j} = 1 - j = 0$. Since μ_K is order-preserving and maps to $[\,0, n\,]$, it is clear that $0 \leq \max\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \leq m_{k,j} = 0$, which ensures that the right-hand sides of statements (i') and (i) are also equal to zero. Therefore, statements (i), (i') and (ii) are simultaneously true.

Assume now that $\tau_K(s_{k,j}) = e_{k,p}$ with $p > 1$. This implies that there is a hexagon H of $\boldsymbol{S}$ to the left of $\tau_K(s_{k,j})$, as shown on the left side of Fig. 10. It is easy to verify that in any Kekulé structure, there are only five possible coverings of the bonds in and around H, which are depicted on the right side of Fig. 10.

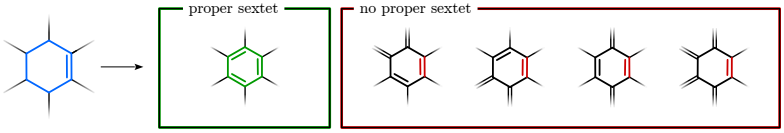

Figure 10. All possible coverings of the bonds in and around a hexagon H directly to the left of a double bond $s_{k,j}$.

Only in one of the five possible cases we find that the covering of H forms a proper sextet. This is the case exactly if none of the interface bonds connected to the top and bottom corner of H are double bonds. In the other four cases, at least one these bonds is a double bond, and $\tau_K(s_{k,j})$ is not part of a proper sextet, meaning that $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$. As a result, the following statements are equivalent.

(ii) $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$.

$\Updownarrow$ (according to Fig. 10)

(b) There is a double bond connected to the top or bottom corner of H.

$\Updownarrow$

(c) At least one of the following is true:

- (c') In the fragment f_k, there is a DIB $s_{k-1,j'} \lessdot_{\mathcal{S}} s_{k,j}$ such that there are no interface bonds of f_k between $\tau_K(s_{k-1,j'})$ and $\tau_K(s_{k,j})$.
- (c'') In the fragment f_{k+1}, there is a DIB $s_{k+1,j''} \lessdot_{\mathcal{S}} s_{k,j}$ such that there are no interface bonds of f_{k+1} between $\tau_K(s_{k+1,j''})$ and $\tau_K(s_{k,j})$.

$\Updownarrow$ (by Lemma 26)

(d) At least one of the following is true:

- (d') In the fragment f_k, there is a DIB $s_{k-1,j'} \lessdot_{\mathcal{S}} s_{k,j}$ such that $m_{k-1,j'} = m_{k,j}$.
- (d'') In the fragment f_{k+1}, there is a DIB $s_{k+1,j''} \lessdot_{\mathcal{S}} s_{k,j}$ such that $m_{k+1,j''} = m_{k,j}$.

$\Updownarrow$ (since $0 \leq m_{k'j'} \leq m_{kj}$ for all $s_{k',j'} \in \mathcal{S}$ with $s_{k',j'} <_{\mathcal{S}} s_{k,j}$)

(i')
$$\begin{aligned} m_{k,j} &= \max\{m_{k',j'} \mid s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \\ &= \max(\{m_{k',j'} \mid s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}). \end{aligned}$$

It remains to be shown that statements (i') and (i) of the lemma are equivalent. The implication $(i) \Rightarrow (i')$ is obvious from the inclusion $\mathcal{A}_K \subset \mathcal{S}$ together with the fact that

μ_K is order-preserving. We still have to show $(i') \Rightarrow (i)$, i.e., that for the considered above element $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$, we have

$$m_{k,j} = \max\left(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right). \tag{17}$$

We distinguish two cases: $m_{k,j} = 0$ and $m_{k,j} > 0$. Keep in mind that we know from Lemmata 27 and 28 that

$$m_{k,j} \geq \max\left(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right). \tag{18}$$

In the case $m_{k,j} = 0$, it follows from Eq. (18) that Eq. (17) is trivially true.

In the case $m_{k,j} > 0$, consider the set $M_{k,j} = \{s_{k',j'} \in \mathcal{S} \,|\, m_{k',j'} = m_{k,j}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\}$. Statement (i') together with $m_{k,j} > 0$ implies that $M_{k,j}$ is non-empty, and thus contains at least one minimal (w.r.t. $<_{\mathcal{S}}$) element $s_{\tilde{k},\tilde{j}}$. We will show that $s_{\tilde{k},\tilde{j}} \in \mathcal{A}_K$. Clearly, we have $m_{\tilde{k},\tilde{j}} = m_{k,j} > 0$. Furthermore, by choice of $s_{\tilde{k},\tilde{j}}$ as a minimal element of $M_{k,j}$, for any $s_{k',j'} \in \mathcal{S}$ with $s_{k',j'} <_{\mathcal{S}} s_{\tilde{k},\tilde{j}}$, we must have $m_{k',j'} < m_{\tilde{k},\tilde{j}}$. It follows that $m_{\tilde{k},\tilde{j}} > \max\left(\left\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{\tilde{k},\tilde{j}}\right\} \cup \{0\}\right)$, which means, due to the equivalence of the statements (ii) and (i'), that $s_{\tilde{k},\tilde{j}} \in \mathcal{A}_K$. We have shown that there exists an element $s_{\tilde{k},\tilde{j}} \in \mathcal{A}_K$ with $s_{\tilde{k},\tilde{j}} <_{\mathcal{S}} s_{k,j}$ and $m_{\tilde{k},\tilde{j}} = m_{k,j}$; thus it follows together with Eq. (18) that $m_{k,j} = \max\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\}$, which shows that Eq. (17) holds. Therefore, in either case, it follows from statement (i') that statement (i) is true. ■

Lemma 30. *The restriction of the map μ_K to the subposet $\mathcal{A}_K \subset \mathcal{S}$ is a strictly order-preserving map $\mu_K|_{\mathcal{A}_K} : \mathcal{A}_K \to [\,n\,]$.*

Proof. Consider an element $s_{k,j} \in \mathcal{A}_K$. We know from the order-preserving nature and the codomain of μ_K that $m_{k,j} \geq \max\left(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right)$ and from Lemma 29 that $m_{k,j} \neq \max\left(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right)$; thus $m_{k,j} > \max\left(\{m_{k',j'} \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right)$ is the only remaining possibility. This implies two facts: Firstly, $m_{k,j} > 0$, meaning that the codomain of $\mu_K|_{\mathcal{A}_K}$ does not contain zero and is therefore restricted to $[\,n\,]$. Secondly, $m_{k,j} > m_{k',j'}$ for every $s_{k',j'} \in \mathcal{S}$ with $s_{k',j'} <_{\mathcal{S}} s_{k,j}$—and thus in particular for every such $s_{k',j'} \in \mathcal{A}_K$. Since $\mu_K(s_{k',j'}) \equiv m_{k',j'} < m_{k,j} \equiv \mu_K(s_{k,j})$ for every $s_{k',j'} \in \mathcal{A}_K$ with $s_{k',j'} <_{\mathcal{S}} s_{k,j}$, the restricted map $\mu_K|_{\mathcal{A}_K}$ is strictly order-preserving. ■

Lemma 31. *Let μ be a strictly order-preserving map $\mu : \mathcal{A}_K \to [\,n\,]$ which satisfies conditions* 1 *and* 2 *of Lemma 22. Then, $\mu = \mu_K|_{\mathcal{A}_K}$.*

Proof. The maps μ and $\mu_K|_{\mathcal{A}_K}$ have the same domain $\mathcal{A}_K$. For every $s_{k,j} \in \mathcal{A}_K$, condition 1 of Lemma 22 fully determines the value of $\mu(s_{k,j})$ to be $\mu(s_{k,j}) = \mathrm{pos}_K(s_{k,j}) - j = \mu_K(s_{k,j})$. ∎

Proof. (of Lemma 22) The map $\mu_K|_{\mathcal{A}_K}$ is, according to Lemma 30, a strictly order-preserving map $\mu_K|_{\mathcal{A}_K} : \mathcal{A}_K \to [n]$. It satisfies condition 1 of Lemma 22 by construction. Furthermore, this map satisfies condition 2 of Lemma 22 according to Lemma 29. Finally, Lemma 31 demonstrates that $\mu_K|_{\mathcal{A}_K}$ is the only strictly order-preserving map $\mathcal{A}_K \to [n]$ which satisfies both conditions. ∎

A.2 Proof of Lemma 23

The purpose of the present subsection is to prove Lemma 23. During this subsection, let $\boldsymbol{S}$ be a Kekuléan regular m-tier strip of length n with the set of DIBs $\mathcal{S}$. Let further $\mathcal{A} \subset \mathcal{S}$ be an induced subposet of $\mathcal{S}$, and let $\mu : \mathcal{A} \to [n]$ be a strictly order-preserving map. Recall that $\mu_K(s_{k,j}) = \mathrm{pos}_K(s_{k,j}) - j$ for every $s_{k,j} \in \mathcal{S}$. We have to show that there exists exactly one Kekulé structure K of $\boldsymbol{S}$ such that

1. $\mu_K(s_{k,j}) = \mu(s_{k,j})$ for every $s_{k,j} \in \mathcal{A}$,
2. $\mu_K(s_{k,j}) = \max(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\})$ for every $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}$,
3. $\mathcal{A}_K = \mathcal{A}$.

The proof of Lemma 23 proceeds by explicitly constructing the Kekulé structure in question. The following Lemma 32 will be used to demonstrate the uniqueness of such a Kekulé structure.

Lemma 32. *Consider two Kekulé structures K and K' of $\boldsymbol{S}$ with $\mathcal{A}_K = \mathcal{A}_{K'}$ and $\mu_K|_{\mathcal{A}_K} = \mu_{K'}|_{\mathcal{A}_{K'}}$. Then, $K = K'$.*

Proof. For every $s_{k,j} \in \mathcal{A}_K$, we know that $\mu_K(s_{k,j}) = \mu_{K'}(s_{k,j})$. For every $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$, we know from the assumptions and Lemma 29 that

$$\begin{aligned}\mu_K(s_{k,j}) &= \max(\{\mu_K(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}_K, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}) \\ &= \max(\{\mu_{K'}(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}_{K'}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}) \quad = \quad \mu_{K'}(s_{k,j}).\end{aligned}$$

Therefore, we have $\mu_K(s_{k,j}) = \mu_{K'}(s_{k,j})$ for every $s_{k,j} \in \mathcal{S}$, which means that the double interface bonds in K and K' are identical, and thus

$$K_I = \left\{ e_{k,\mu_K(s_{k,j})+j} \,|\, s_{k,j} \in \mathcal{S} \right\} = \left\{ e_{k,\mu_{K'}(s_{k,j})+j} \,|\, s_{k,j} \in \mathcal{S} \right\} = K'_I.$$

It follows from Lemma 2 that $K = K'$. ■

Proof. (of Lemma 23) We will first construct a set $K_v \subset \bigcup_k i_k$ of interface bonds of $\boldsymbol{S}$ that corresponds to $\mathcal{A}$ and μ. Then, we show that the third rule of interface theory given in Theorem 7 can be applied to prove that there exists a Kekulé structure K with $K_I = K_v$.

Let us consider the auxiliary map $\tilde{\mu} : \mathcal{S} \to [\,0, n\,]$ constructed as follows.

$$\tilde{\mu}(s_{k,j}) = \begin{cases} \mu(s_{k,j}) & \text{if } s_{k,j} \in \mathcal{A} \\ \max\left(\{\mu(s_{k',j'}) \,|\, s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right) & \text{if } s_{k,j} \in \mathcal{S} \setminus \mathcal{A} \end{cases} \tag{19}$$

During this subsection, let us for all $s_{k,j} \in \mathcal{S}$ denote the value $\tilde{\mu}(s_{k,j})$ by $\tilde{m}_{k,j}$. Clearly, the map $\tilde{\mu} : \mathcal{S} \to [\,0, n\,]$, $s_{k,j} \mapsto \tilde{m}_{k,j}$ is order-preserving. For every $s_{k,j} \in \mathcal{S}$, let $n_{k,j} = \tilde{m}_{k,j} + j$.

The numbers $n_{k,j}$ specify distinct, well-defined interface bonds $e_{k,n_{k,j}}$: For any given $k \in [\,m\,]$, the set $\{s_{k',j} \in \mathcal{S} \,|\, k' = k\}$ contains, by construction, $\mathrm{ord}(i_k)$ elements $s_{k,1} <_{\mathcal{S}} s_{k,2} <_{\mathcal{S}} \ldots <_{\mathcal{S}} s_{k,\mathrm{ord}(i_k)}$. Since $\tilde{\mu}$ is order-preserving and has the codomain $\tilde{\mu} : \mathcal{S} \to [\,0, n\,]$, it follows that the corresponding numbers $\tilde{m}_{k,j}$ satisfy $0 \leq \tilde{m}_{k,1} \leq \tilde{m}_{k,2} \leq \ldots \leq \tilde{m}_{k,\mathrm{ord}(i_k)} \leq n$, and consequently we have $0 < n_{k,1} < n_{k,2} < \ldots < n_{k,\mathrm{ord}(i_k)} \leq n + \mathrm{ord}(i_k)$. The interface i_k contains, according to Theorem 4, $|i_k| = n + \mathrm{ord}(i_k)$ bonds $e_{k,1}, \ldots, e_{k,n+\mathrm{ord}(i_k)}$. Therefore, for every $s_{k,j}$, the bond $e_{k,n_{k,j}}$ is an element of i_k and is different from all other $e_{k,n_{k,j'}}$ with $j \neq j'$.

Let us now set $K_v = \left\{ e_{k,n_{k,j}} \,|\, s_{k,j} \in \mathcal{S} \right\}$. We have ensured by construction that every interface i_k contains exactly $\mathrm{ord}(i_k)$ elements of K_v: $|K_v \cap i_k| = \mathrm{ord}(i_k)$, meaning that *the set K_v satisfies condition (a) of the Third Rule of interface theory given in Theorem 7.*

Next, we need to show that *the set K_v satisfies conditions (a) – (c) of the Second Rule of interface theory given in Theorem 6 (and consequently condition (b) of the Third Rule):* Consider an arbitrary fragment f of $\boldsymbol{B}$, denote by i_l the interface of f which contains the first interface bond of f, and denote by i_r the other interface of f. According to Def. 16, the DIBs of f satisfy, for applicable values of $j = 1, 2, \ldots$, the cover relations $s_{l,j} \lessdot_{\mathcal{S}} s_{r,j}$ and $s_{r,j} \lessdot_{\mathcal{S}} s_{l,j+1}$. Since $\tilde{\mu}$ is order-preserving, it follows that $\tilde{m}_{l,j} \leq \tilde{m}_{r,j}$ and $\tilde{m}_{r,j} \leq \tilde{m}_{l,j+1}$, and therefore $n_{l,j} \leq n_{r,j}$ and $n_{r,j} < n_{l,j+1}$. Note now that the interface bond $e_{l,p}$ is located to the left of the interface bond $e_{r,p}$, which in turn is located to the left of $e_{l,p+1}$; therefore,

$n_{l,j} \leq n_{r,j}$ ensures that $e_{l,n_{l,j}}$ is located to the left of $e_{r,n_{r,j}}$, and $n_{r,j} < n_{l,j+1}$ ensures that $e_{r,n_{r,j}}$ is located to the left of $e_{l,n_{l,j+1}}$. Thus, the sequence of double interface bonds of the fragment f, from left to right, is given by

$$e_{l,n_{l,1}}, e_{r,n_{r,1}}, e_{l,n_{l,2}}, e_{r,n_{r,2}}, \ldots, \begin{cases} e_{r,n_{r,\mathrm{ord}(i_r)}} & \text{if } \mathrm{ord}(i_l) + \mathrm{ord}(i_r) \text{ is even,} \\ e_{l,n_{l,\mathrm{ord}(i_l)}} & \text{if } \mathrm{ord}(i_l) + \mathrm{ord}(i_r) \text{ is odd.} \end{cases}$$

Comparison to the sequence of interface bonds of f

$$e_{l,1}, e_{r,1}, e_{l,2}, e_{r,2}, \ldots, \begin{cases} e_{r,\mathrm{ord}(i_r)} & \text{if } \mathrm{ord}(i_l) + \mathrm{ord}(i_r) \text{ is even,} \\ e_{l,\mathrm{ord}(i_l)} & \text{if } \mathrm{ord}(i_l) + \mathrm{ord}(i_r) \text{ is odd,} \end{cases}$$

shows that all the conditions of the Second Rule, Theorem 6 are satisfied.

With this, we have seen that the two conditions (a) and (b) of the Third Rule of interface theory given in Theorem 7 are satisfied; consequently, Theorem 7 states there exists exactly one Kekulé structure K with $K_I = K_v$.

It remains to show that this Kekulé structure K indeed satisfies conditions 1–3 of Lemma *23*. It is clear from the construction of K_v and the fact that $K_I = K_v$ that $\tilde{\mu} = \mu_K$ (because $\mu_K(s_{k,j}) = \mathrm{pos}_K(s_{k,j}) - j = n_{k,j} - j = \tilde{m}_{k,j} = \tilde{\mu}(s_{k,j})$ for all $s_{k,j} \in \mathcal{S}$ and the domains of both maps are identical). First, we show condition 3 by demonstrating that $\mathcal{A} = \mathcal{A}_K$:

By construction of μ and $\tilde{\mu}$, for all $s_{k,j} \in \mathcal{A}$, we have $\tilde{\mu}(s_{k,j}) = \mu(s_{k,j}) \in [\, n \,]$ and

$$\tilde{\mu}(s_{k,j}) > \max\left(\{\tilde{\mu}(s_{k',j'}) \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right) \tag{20}$$

for the following reason: For every $s_{k',j'} \in \mathcal{A}$, we have $\tilde{\mu}(s_{k',j'}) = \mu(s_{k',j'}) < \mu(s_{k,j}) = \tilde{\mu}(s_{k,j})$ since μ is strictly order-preserving. For every $s_{k',j'} \in \mathcal{S} \setminus \mathcal{A}$, by Eq. (19) there are two possibilities: $\tilde{\mu}(s_{k',j'}) = 0 < \mu(s_{k,j}) = \tilde{\mu}(s_{k,j})$, or there exists an element $s_{k'',j''} \in \mathcal{A}$ with $s_{k'',j''} <_{\mathcal{S}} s_{k',j'}$ for which $\tilde{\mu}(s_{k',j'}) = \mu(s_{k'',j''})$. Since $s_{k'',j''} \in \mathcal{A}$ and since μ is strictly order-preserving, we have $\tilde{\mu}(s_{k',j'}) = \mu(s_{k'',j''}) < \mu(s_{k,j}) = \tilde{\mu}(s_{k,j})$. It follows from Eq. (20) and $\tilde{\mu} = \mu_K$ that statement (i') of Lemma 29 is not satisfied for $s_{k,j}$, which shows that $s_{k,j} \in \mathcal{A}_K$, demonstrating that $\mathcal{A} \subset \mathcal{A}_K$.

On the other hand, for every $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}$, we have by construction in Eq. (20)

$$\tilde{\mu}(s_{k,j}) = \max\left(\{\mu(s_{k',j'}) \,|\, s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right). \tag{21}$$

Since $\tilde{\mu}$ is order-preserving, any $s_{k',j'} \in \mathcal{S}$ with $s_{k',j'} <_{\mathcal{S}} s_{k,j}$ must satisfy $\tilde{\mu}(s_{k',j'}) \leq \tilde{\mu}(s_{k,j})$, and therefore it is clear that

$$\tilde{\mu}(s_{k,j}) = \max\left(\{\tilde{\mu}(s_{k',j'}) \,|\, s_{k',j'} \in \mathcal{S}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right). \tag{22}$$

It follows from Eq. (22) and $\tilde{\mu} = \mu_K$ that statement (i') of Lemma 29 is satisfied for $s_{k,j}$, which shows that $s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K$, demonstrating that $\mathcal{S} \setminus \mathcal{A} \subset \mathcal{S} \setminus \mathcal{A}_K$ and consequently $\mathcal{A}_K \subset \mathcal{A}$.

This shows that $\mathcal{A} = \mathcal{A}_K$, demonstrating correctness of statement 3 of Lemma 23.

It is now obvious that

$$\mu_K(s_{k,j}) = \tilde{\mu}(s_{k,j}) \tag{23}$$

$$= \begin{cases} \mu(s_{k,j}) & \text{if } s_{k,j} \in \mathcal{A} \\ \max\left(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right) & \text{if } s_{k,j} \in \mathcal{S} \setminus \mathcal{A} \end{cases} \tag{24}$$

$$= \begin{cases} \mu(s_{k,j}) & \text{if } s_{k,j} \in \mathcal{A}_K \\ \max\left(\{\mu(s_{k',j'}) \mid s_{k',j'} \in \mathcal{A}, s_{k',j'} <_{\mathcal{S}} s_{k,j}\} \cup \{0\}\right) & \text{if } s_{k,j} \in \mathcal{S} \setminus \mathcal{A}_K \end{cases} \tag{25}$$

which demonstrates correctness of statements 1 and 2 of Lemma 23.

Every Kekulé structure K' satisfying conditions 1–3 has to satisfy $\mu_{K'}|_{\mathcal{A}} = \mu = \mu_K|_{\mathcal{A}}$, and thus according to Lemma 32 is identical to K, ensuring that there is only one such Kekulé structure, concluding the proof. ■