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All-Benzenoid Systems: an Algebra of Invariants

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The current invariants of all-benzenoids (h, n, m, n_i, n_e, s – defined in the Introduction), in addition to the number of full and of empty hexagons (ν and ε), are studied. Their possible values are specified. Some of the relations between these invariants are summarized in a systematic way. The upper and lower bounds for all of them are accounted for as functions of any of these invariants.

INTRODUCTION

The fully benzenoid hydrocarbons are known to be of great importance in organic chemistry.[1–3] A citation from Randić[4] may serve as a definition of this class of molecules: »For these compounds one can write a valence structure in which a ring is either represented as an isolated sextet or is devoid of conjugation.« Here, we adhere to the term »all-benzenoid« as an abbreviation for all-benzenoid *systems*,[5,6] which, considered as chemical graphs, correspond to the fully benzenoid *hydrocarbons*, chemically known or unknown. The term »all-benzenoid« was adopted from the late Professor O. E. Polansky and his collaborators, who provided the first substantial graph-theoretical characterization of such systems.[7–9]

Studies of topological properties of all-benzenoids continue. The reader is referred to a series of eight articles[10] and some later works.[11] Extensive works on enumeration of all-benzenoids are also worth mentioning. They were foreshadowed by Dias,[12] while Knop *et al.*[13] reported the first of such results obtained by computer aid. In his later works, Dias[14] contributed to the enumeration of all-benzenoids with an emphasis on the strain-free systems. Other enumeration results from the above citations are available.[10(a),10(f),10(g)] Finally, some recent studies on all-benzenoid isomers should be mentioned.[15]

In the present work, the invariants of all-benzenoid systems are treated. Their upper and lower bounds are reported as functions of all the invariants that are currently taken into account. The results are presented in terms of inequalities of the

Harary-Harborth[16] type, referring to the classical treatment of »extremal animals« by these authors.

A LIST OF INVARIANTS

The adopted symbols for the main invariants of a benzenoid system are listed in the following; # means »number of«.

h = # hexagons; n = # vertices; m = # edges; n_i = # internal vertices; n_e = # external vertices; s = # vertices of degree two.

All these notions are immediately applicable to all-benzenoids as special cases of benzenoids. However, the values of the invariants are more restricted. Possible values of h are 1 (for the trivial case of benzene), 4 (triphenylene), and all integers $h \geq 6$ (see also Table I). Restrictions are more profound for most of the other main invariants and lead to introduction of certain *reduced invariants*, as explained in the following.

It was already noted, at least by Polansky and Rouvray,[8] that $n \equiv 0 \pmod 6$ for any all-benzenoid. Hence, it is reasonable to define as a reduced invariant

$$\nu = n/6; \ \nu = 1, \ \nu \geq 3. \tag{1}$$

Here, the given possible values of integer ν are consistent with possible n values specified in Table I.

The possible values of m for all-benzenoids (*cf.* Table I) are accounted for by the following scheme.

$$m = 6j_0; \qquad j_0 = 1,6,9,10,11, \quad j_0 \geq 13 \tag{2a}$$

$$m = 6j_1 + 1; \qquad j_1 = 6,10,11, \quad j_1 \geq 13 \tag{2b}$$

$$m = 6j_2 + 2; \qquad j_2 = 7,10,11,12, \quad j_2 \geq 14 \tag{2c}$$

$$m = 6j_3 + 3; \qquad j_3 = 3,7,8, \quad j_3 \geq 11 \tag{2d}$$

$$m = 6j_4 + 4; \qquad j_4 = 8,11,12,13, \quad j_4 \geq 15 \tag{2e}$$

$$m = 6j_5 + 5; \qquad j_5 = 4,8,9, \quad j_5 \geq 12 \tag{2f}$$

Furthermore, one has $n_i \equiv 0 \pmod 2$, $n_e \equiv 2 \pmod 4$ and $s \equiv 0 \pmod 2$. Hence, the following reduced invariants for all-benzenoids are defined.

$$\nu_i = n_i/2 \ ; \qquad \nu_i \geq 0 \tag{3}$$

$$\nu_e = (n_e - 2)/4 \qquad \nu_e = 1 \ , \ \nu_e \geq 4 \tag{4}$$

$$\sigma = s/2 \qquad \sigma = 3 \ , \ \sigma \geq 6 \tag{5}$$

The above equations (3) – (5) include the possible values for the reduced invariants in question. These specifications are consistent with those of Table I.

When we presently speak about invariants of all-benzenoids in general terms, then the reduced invariants are included.

RELATIONS BETWEEN INVARIANTS

Connections between the six main (not reduced) invariants (*cf.* Table I) for benzenoids are well known.[5,6,17] Any pair of them, except (n_e, s), for which $n_e = 2s - 6$, represents two independent invariants. Each of the other invariants can be expressed linearly in terms of the two invariants from such a pair.

Corresponding expressions are readily obtained, of course, for all-benzenoids when the reduced invariants are taken into account. Table II shows a collection of relations for (reduced) invariants in terms of selected pairs of quantities taken among the reduced invariants with h included.

TABLE I

Invariants of all-benzenoids and their possible values

Symbol	Possible integer value
h	1, 4, 6,7,8,9,...
$n = 6\nu$	6, 18, 24, 30, 36,...
m	6, 21, 29, 36,37, 44,45, 51,52,53,54, 59,60,61,62, 66,67,68,69,70, 74,75,76,77,78,79, 81,82,83,84,85,86,87, 89,90,91,92,...
$n_i = 2\nu i$	0, 2, 4, 6, ...
$n_e = 4\nu_e + 2$	6, 18, 22, 26, 30,...
$s = 2\sigma$	6, 12, 14, 16, 18, ...

TABLE II

Relations for invariants of all-benzenoids

(Reduced) invariant	(h, ν_i) (ν, ν_i)	(h, ν_e) (ν, σ)
h	h $(1/2)(3\nu+\nu_i-1)$	h $3\nu-\sigma+1$
ν	$(1/3)(2h-\nu_i+1)$ ν	$(1/3)(h+\nu_e+1)$ ν
m	$5h-2\nu_i+1$ $(1/2)(15\nu+\nu_i-3)$	$3h+2\nu_e+1$ $9\nu-\sigma$
ν_i	ν_i ν_i	$h-\nu_e$ $3\nu-2\sigma+3$
ν_e	$h-\nu_i$ $(1/2)(3\nu-\nu_i-1)$	ν_e $\sigma-2$
σ	$h-\nu_i+2$ $(1/2)(3\nu-\nu_i+3)$	ν_e+2 σ

Figure 1 shows a benzenoid ($C_{42}H_{18}$), well known to organic chemists as hexabenzo[*bc,ef,hi,kl,no,qr*]coronene and also studied by mathematical chemists as a chemical graph. The system has: $h = 13$, $\nu = 7$, $m = 54$, $\nu_i = 6$, $\nu_e = 7$, $\sigma = 9$.

FULL AND EMPTY HEXAGONS

Definitions and Relations

The notions of full and empty hexagons are specific for all-benzenoids.[8] Already Polansky and Rouvray, in the cited reference,[8] pointed out that the number of full hexagons is $n/6$, viz. equal to the reduced invariant that we call ν. Let us also introduce a symbol for the number of empty hexagons so that we have altogether:

ν = # full hexagons; ε = # empty hexagons.

All positive integer values, in addition to $\varepsilon = 0$ for benzene, are possible for all-benzenoids. One has

$$h = \nu + \varepsilon\,; \quad \varepsilon \geq 0 \tag{6}$$

Full hexagons may be identified as the aromatic sextets in 2^{ν} Kekulé (valence) structures. They are usually indicated by circles in the appropriate hexagons; see, *e.g.*, Figure 1. This particular example (hexabenzo[*bc,ef,hi,kl,no,qr*]coronene) has $\nu = 7$, $\varepsilon = 6$.

Numbers ν and ε constitute a pair of independent invariants (ν, ε) for all-benzenoids. Thus, all the other invariants considered above can be expressed linearly in terms of the pair (ν, ε) or other pairs containing ε. Table III shows a selection of such relations. They are consistent with Eq. (6) and with[10(b)] $\varepsilon = (1/4)(2\nu + n_i - 2)$.

Extremal All-Benzenoid

To every extremal benzenoid A, except for naphthalene, a unique all-benzenoid S can be constructed. If A has h(A) hexagons and n_i(A) internal vertices, then S should have h(A) full hexagons (ν) and n_i(A) empty hexagons (ε). The ν full hexagons should be arranged in the same way as the h(A) hexagons in the initial benzenoid. This is the one-to-one correspondence between the extremal benzenoids and certain all-benzenoids which was described by Dias.[15,(a),15(b)] It is said that the all-benzenoid S is as-

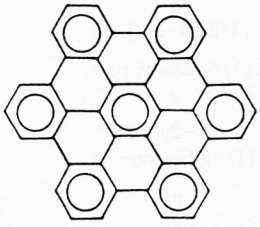

Figure 1. A fully benzenoid hydrocarbon $C_{42}H_{18}$ or an all-benzenoid system with $h = 13$, $n = 42$, $m = 54$, $n_i = 12$, $n_e = 30$, $s = 18$.

sociated with A.[15(c),15(e)] As an example, the system of Figure 1 is associated with coronene: the 7 hexagons and 6 internal vertices of coronene match the 7 full hexagons and 6 empty hexagons, respectively, of hexabenzo[*bc,ef,hi,kl,no,qr*]coronene. An all-benzenoid which is associated with an extremal benzenoid is called an *extremal all-benzenoid.* Also, as a degenerate case, the non-benzenoid biphenyl is usually said to be associated with naphthalene. It should be noted that the extremal all-benzenoids, except benzene (which is associated with benzene), are *not* extremal benzenoids.

An extremal benzenoid is defined as having the maximum number of internal vertices (n_i) for a given number of hexagons (h),$n_i = (n_i)_{max}(h)$, and the expression for this maximum is known:[16,18] $(n_i)_{max}(h) = 2h + 1 - \lceil(12h - 3)^{1/2}\rceil$.

From the above considerations it can be deduced by analogy that

$$\varepsilon_{max}(\nu) = 2\nu + 1 - \lceil(12h - 3)^{1/2}\rceil \ . \tag{7}$$

It is reasonable to assume that Eq. (7) applies to all-benzenoids in general. Hence, an extremal all-benzenoid can also be defined as having the maximum number of empty hexagons (ε) for a given number of full hexagons (ν). This maximum is given by Eq. (7).

From (7), since $\varepsilon \leq \varepsilon_{max}$, it is obtained

$$2\nu - \varepsilon + 1 \geq \lceil(12\nu - 3)^{1/2}\rceil \ . \tag{8}$$

Since $\lceil (12\nu-3)^{1/2}\rceil \geq (12\nu - 3)^{1/2}$, it follows that

$$2\nu - \varepsilon + 1 \geq (12\nu - 3)^{1/2} \ . \tag{9}$$

Furthermore,

$$(2\nu - \varepsilon + 1)^2 \geq 12\nu - 3 \ , \tag{10}$$

$$4\nu^2 - 4(\varepsilon + 2)\nu + (\varepsilon - 2)^2 \geq 0 \ . \tag{11}$$

Herefrom, the sign of equality gives

$$\nu_{\pm} = (1/2)\ (\varepsilon + 2 \pm 6^{1/2}\varepsilon^{1/2}) \ . \tag{12}$$

Consequently, $\nu \geq \nu_+$ or $\nu \leq \nu_-$. However, the solution with ν_- can be ruled out because $\nu > (1/2)(\varepsilon+2)$. This fact emerges from Eq. (8) when it is observed that $\lceil(12\nu - 3)^{1/2}\rceil > 2$. As a net result one obtains the minimum number of full hexagons (ν) for a given number of empty hexagons (ε) as:

$$\nu_{min}(\varepsilon) = \lceil(1/2)(\varepsilon + 2 + 6^{1/2}\varepsilon^{1/2}\rceil = 1 + \lceil(1/2)\ (\varepsilon + 6^{1/2}\varepsilon^{1/2})\rceil \ . \tag{13}$$

This relation is consistent with $\nu \geq \nu_+$, but does not follow immediately from it. However, a closer inspection verified the correctness of (13).

Upper and Lower Bounds for ν and ε

The analysis of the preceding section gives the upper bound of ε in terms of ν and the lower bound of ν in terms of ε for all-benzenoids. It is also of interest to determine the lower bound of ε and the upper bound of ν.

The lower bound of ε for a given value of ν is realized in catacondensed systems ($n_i = \nu_i = 0$) when ν is odd and in systems with two internal vertices ($n_i = 2$, $\nu_i = 1$) when ν is even. Elucidating examples are found in Figure 2. In general, one has (*cf.* Table III)

$$\varepsilon = (1/2)\ (\nu + \nu_i - 1). \tag{14}$$

Now, in the former case (ν odd) $\nu_i = 0$ gives $\varepsilon_{\min} = (\nu - 1)/2$, while $\nu_i = 1$ gives $\varepsilon_{\min} = \nu/2$ in the latter case (ν even). Altogether:

$$\varepsilon_{\min}(\nu) = \lfloor \nu/2 \rfloor \tag{15}$$

The upper bound of ν for a given ε is obtained quite straightforwardly: $\nu_{\max}$ is realized in the catacondensed systems (see the left-hand part of Figure 2 for an example) for every ε value. From Table III or Eq. (14) one has now

$$\nu = 2\varepsilon - \nu_i + 1 \tag{16}$$

which for $\nu_i = 0$ gives

$$\nu_{\max}(\varepsilon) = 2\varepsilon + 1\ . \tag{17}$$

The findings of the two preceding sections are summarized in the following inequalities for all-benzenoids.

$$\lfloor \nu/2 \rfloor \leq \varepsilon \leq 2\nu + 1 - \lceil (12\nu - 3)^{1/2} \rceil \tag{18}$$

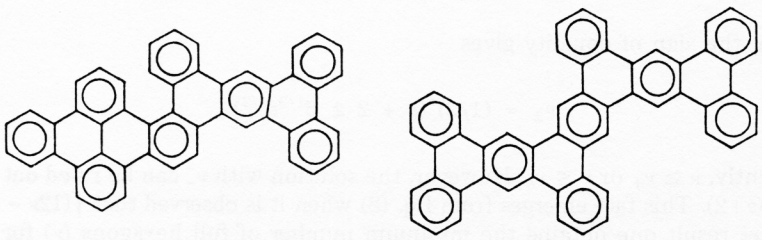

Figure 2. Two all-benzenoids with the minimum number of empty hexagons, $\varepsilon_{\min}(\nu) = 4$, for the given numbers of full hexagons. In the left-hand system, ν (the number of full hexagons) = 9, while $\nu = 8$ in the right-hand system.

$$\lceil (1/2)(\varepsilon + 2 + 6^{1/2}\varepsilon^{1/2}) \rceil \leq \nu \leq 2\varepsilon + 1 \tag{19}$$

Here, as well as in all inequalities of this type in subsequent sections, the upper and lower bounds are always realized for all-benzenoids. In the present cases of Eqs. (18) and (19), also all intermediate values, between an upper and a lower bound, are realized (in steps of one unit) among the all-benzenoids.

Other Inequalities in Terms of ν and ε

Inequalities of type (18) are readily obtained for all the other invariants considered here. One only has to substitute ε by the appropriate expression in terms of ν and the invariant in question. The expressions are easily found from Table III. The resulting inequalities for h, m, ν_i, ν_e and σ are listed in Table IV. Here, a small complication occurs for ν_i since $2\varepsilon = \nu_i + \nu - 1$. Hence, (18) should first be multiplied by 2 throughout, and then 2ε should be inserted. Again, the upper and lower bounds, viz. $(\nu_i)_{\max}(\nu)$ and $(\nu_i)_{\min}(\nu)$, are always realized in all-benzenoids (*cf.* also above). But, now one has $(\nu_i)_{\max}(\nu) \equiv (\nu_i)\min(\nu)$ (mod 2), and the possible intermediate values of ν_i should be taken in steps of 2 units. This is indicated in Table IV by number 2 in the column labelled Interval. Example: for $\nu = 8$, $1 \leq \nu_i \leq 7$; the possible values are $\nu_i = 1, 3, 5, 7$.

The inequalities for σ in terms of ν (see Table IV) were deduced previously[15e] using a somewhat different approach from that of the present work.

The inequalities in terms of ε listed in Table IV were obtained from (19) in a quite analogous way as those of ν. For m in particular (number 7 under Interval), one has $m_{\max}(\varepsilon) \equiv m_{\min}(\varepsilon)$ (mod 7), and the intermediate m values should be taken in steps of 7 units. Example: for $\varepsilon = 4$, $45 \leq m \leq 66$; the possible values are $m = 45, 52, 59, 66$.

TABLE III

Relations for all-benzenoid invariants which include the number of empty hexagons (ε)

(Reduced) invariant	(h, ε) (ε, ν_i)	(ν, ε) (ε, σ)
h	h $3\varepsilon-\nu_i+1$	$\nu+\varepsilon$ $(1/2)(3\varepsilon+\sigma-1)$
ν	$h-\varepsilon$ $2\varepsilon-\nu_i+1$	ν $(1/2)(\varepsilon+\sigma-1)$
m	$7h-6\varepsilon-1$ $15\varepsilon-7\nu_i+6$	$7\nu+\varepsilon-1$ $(1/2)(9\varepsilon+7\sigma-9)$
ν_i	$3\varepsilon-h+1$ ν_i	$2\varepsilon-\nu+1$ $(1/2)(3\varepsilon-\sigma+3)$
ν_e	$2h-3\varepsilon-1$ $3\varepsilon-2\nu_i+1$	$2\nu-\varepsilon-1$ $\sigma-2$
σ	$2h-3\varepsilon+1$ $3\varepsilon-2\nu_i+3$	$2\nu-\varepsilon+1$ σ

TABLE IV

Invariants of all-benzenoids in terms of ν and ε; see also Eq. (18) and Eq. (19)

Inequalities	Interval
$\nu+\lfloor\nu/2\rfloor \le h \le 3\nu+1-\lceil(12\nu-3)^{1/2}\rceil$	1
$7\nu-1+\lfloor\nu/2\rfloor \le m \le 9\nu-\lceil(12\nu-3)^{1/2}\rceil$	1
$1-\nu+2\lfloor\nu/2\rfloor \le \nu_i \le 3\nu+3-2\lceil(12\nu-3)^{1/2}\rceil$	2
$\lceil(12\nu-3)^{1/2}\rceil-2 \le \nu_e \le 2\nu-1-\lfloor\nu/2\rfloor$	1
$\lceil(12\nu-3)^{1/2}\rceil \le \sigma \le 2\nu+1-\lfloor\nu/2\rfloor$	1
$\varepsilon+\lceil(1/2)(\varepsilon+2+6^{1/2}\varepsilon^{1/2})\rceil \le h \le 3\varepsilon+1$	1
$\lceil(1/2)(\varepsilon+2+6^{1/2}\varepsilon^{1/2})\rceil \le \nu \le 2\varepsilon+1$	1
$\varepsilon+6+7\lceil(1/2)(\varepsilon+6^{1/2}\varepsilon^{1/2})\rceil \le m \le 15\varepsilon+6$	7
$0 \le \nu_i \le 2\varepsilon-\lceil(1/2)(\varepsilon+6^{1/2}\varepsilon^{1/2})\rceil$	1
$1-\varepsilon+2\lceil(1/2)(\varepsilon+6^{1/2}\varepsilon^{1/2})\rceil \le \nu_e \le 3\varepsilon+1$	2
$3-\varepsilon+2\lceil(1/2)(\varepsilon+6^{1/2}\varepsilon^{1/2})\rceil \le \sigma \le 3\varepsilon+3$	2

INEQUALITIES IN TERMS OF INVARIANTS OTHER THAN ν AND ε

Introductory Remarks

It is of interest to deduce inequalities of type (18) and (19) for the invariants of all-benzenoids as functions of other variables than ν and ε. Assume that we have found such inequalities for a certain invariant in terms of another invariant, for instance $\nu_{\min}(h) \le \nu \le \nu_{\max}(h)$. Then, the upper and lower bounds for all the other invariants (different from ν) are easily obtained as functions of h by means of the known relations between the different invariants (Tables II and III). The methods are basically the same as described above for the functions of ν and ε. Therefore, it should not be necessary to go into details on the derivations of most of the results in the following.

Functions of h

The inequalities for ν in terms of h are given at the top of Table V. Throughout this table, particular invariants (as ν in the present case) are chosen so that the intervals, in the sense of Table IV are constantly 1.

The upper bound $\nu_{\max}(h)$ was found through $(\nu_i)_{\min}(h) \in \{0, 1, 2\}$. Let $h_o \in \{0, 1, 2\}$ be defined by

$$h_o = h - 3\lfloor h/3\rfloor \tag{20}$$

Then

$$(\nu_i)_{\min}(h) = 2h_o + 1 - 3j \tag{21}$$

where

TABLE V

Inequalities for selected invariants of all—benzenoids in terms of h, m, ν_i, ν_e *and* σ *(Intervals equal 1 throughout)*

$$\lceil (1/3)[h+1+(4h-3)^{1/2}] \rceil \leq \nu \leq 2\lfloor h/3 \rfloor + \lfloor (1/2)(h+1-3\lfloor h/3 \rfloor) \rfloor$$

$$\lceil (1/27)[3m+2+(12m-23)^{1/2}] \rceil \leq \nu$$

$$\nu \leq 2\lfloor m/15 \rfloor + \lfloor (1/8)(m+2-15\lfloor m/15 \rfloor) \rfloor$$

$$\lceil (1/3)[2\nu_i+1+(4\nu_i+1)^{1/2}] \leq \varepsilon < \infty$$

$$\nu_e+1-\lfloor (1/3)(\nu_e+2) \rfloor \leq \nu \leq \lfloor (1/12)(\nu_e^2+4\nu_e+7) \rfloor$$

$$\sigma-1-\lfloor \sigma/3 \rfloor \leq \nu \leq \lfloor (1/12)(\sigma^2+3) \rfloor$$

$$j = \lfloor (1/2)((h_o + 1) \rfloor . \tag{22}$$

The net result is

$$(\nu_i)_{\min} = 2h + 1 - 6\lfloor h/3 \rfloor - 3\lfloor (1/2)(h + 1 - 3\lfloor h/3 \rfloor) \rfloor \tag{23}$$

Then, simply $\nu_{\max}(h) = (1/3)[2h + 1 - (\nu_i)_{\min}]$, which gives the expression of Table V. In this expression, as well as in Eq. (23), it is seen that a floor function inside another floor function occurs. This feature is not present in the equivalent expression below.

$$\nu_{\max}(h) = \lfloor (2/3)(h + 1) \rfloor + \lceil (1/3)(h + 1) \rceil - \lfloor (1/3)(h + 1) \rfloor - 1 \tag{24}$$

For the sake of completeness, we give here the inequalities for ν_i in terms of h:

$$(\nu_i)_{\min} \leq \nu_i \leq 2h + 1 - 3\lceil (1/3)[h + 1 + (4h + 3)^{1/2}] \rceil \tag{25}$$

In this case $(\nu_i)_{\max}(h) \equiv (\nu_i)_{\min}(h) \pmod 2$; the interval is 2, which is to say that the intermediate values of ν_i should be taken in steps of 2 units.

Functions of m

Table V includes the inequalities for ν in terms of m. Here, the upper bound $\nu_{\max}(m)$ was found through $(\nu_i)_{\min}(m) \in \{0, 1, 2, \cdots, 14\}$. An analysis corresponding to the one for $(\nu_i)_{\min}(h)$ led to

$$(\nu_i)_{\min}(m) = 2m_o + 3 - 15j \tag{26}$$

where

$$m_o = m - 15\lfloor m/15 \rfloor \tag{27}$$

and

$$j = \lfloor (1/8)(m_o + 2) \rfloor . \tag{28}$$

The net result is $(\nu_i)_{\min}(m) = 2m + 3 - 15\nu_{\max}(m)$, where the last function ($\nu_{\max}$) is found in Table V. For the upper and lower bounds of ν_i one has $(\nu_i)_{\max}(m) \equiv (\nu_i)_{\min}(m)$ (mod 15), and for a given m the possible ν_i values between these bounds should be taken in steps of 15 units.

It appears that the m value in many cases determines all the other invariants of an all-benzenoid. Firstly, this is the case for all $m < 96$. The smallest m value that is compatible with more than one value for one of the other invariants is 96. In this case, $\nu = 12$ ($h = 13$) or $\nu = 13$ ($h = 6$).

Functions of ν_i

For given values of ν_i the invariant ε has no upper bound, as indicated in Table V. This is also true of all the other invariants of interest.

Functions of ν_e *and* σ

Finally, in Table V, the inequalities for ν in terms of ν_e and of σ are given. The inherent upper and lower bounds in the latter case, viz. $\nu_{\max}(\sigma)$ and $\nu_{\min}(\sigma)$, have been published previously.[15(c)]

CONCLUSION

The studies of upper and lower bounds for invariants in benzenoids were initiated by Harary and Harborth[16] and pursued in several later works.[6,18,19] In the present work, the corresponding problem for the important subclass of benzenoids called all-benzenoids was tackled. A complete solution is presented inasmuch as the upper and lower bounds of all the current invariants are accounted for as functions of any of these invariants, viz. h, n, m, n_i, n_e, s and ε. For the sake of brevity, all versions of the pertinent inequalities have not been given, and many results have been formulated in terms of certain reduced invariants (ν, ν_i, ν_e, σ). However, all the desired versions of inequalities in terms of the seven current invariants, which are listed above, are accessible from the reported formulas by simple substitutions. An illustrative example is given below.

Stojmenović *et al.*[20] used n_e (the perimeter length) as the leading parameter for their computerized enumerations of benzenoids. For each n_e, they found »empirically« a range of h. The analytical expression of this range has not been given explicitly before, but is easily obtained from the known formulas[19] as:

$$\lceil (1/4)(n_e - 2) \rceil \leq h \leq \lfloor (1/48)(n_e^2 + 12) \rfloor \tag{29}$$

The corresponding inequalities for all-benzenoids are now found from the formula apparatus of the present work with the result:

$$(1/2)(n_e + 2) - 3\lfloor (1/12)(n_e + 6) \rfloor \leq h$$

$$h \leq 3\lfloor (1/192)(n_e^2 + 12n_e + 84) \rfloor - (1/4)(n_e + 2). \tag{30}$$

Here, the intermediate values of h should be taken in steps of 3 units.

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SAŽETAK

Potpuno benzenoidni sustavi: Algebra invarijanti

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Osim broja praznih i punih šesterokuta u potpunim benzenoidima, proučavane su i neke recentne invarijante u tim sustavima. Specificirane su moguće vrijednosti i sustavno su navedene veze među ovim invarijantama. Za svaku invarijantu dane su gornje i donje ocjene u ovisnosti o svakoj preostaloj invarijanti.