

CONJUGATED CIRCUITS FOR POLYMERS

Hongyao Zhu and Douglas J. Klein

Texas A&M University at Galveston, Galveston, Texas 77553-1675, USA

(received: June 1994)

ABSTRACT: A new approach to treat the conjugated-circuit model on regular conjugated polymers is made with computational effort comparable to that for corresponding tight-binding models. First a translationally symmetric arrow assignment is used to construct an antisymmetrically signed "adjacency" matrix. Then symmetry blocking is used to manipulate this "adjacency" matrix, and make the associated conjugated-circuit computations. A consequent detailed description of π -electron resonance energy is presented for families of benzenoid and near-benzenoid polymers, including linear and zig-zag phenylene polymers, and so-called "azulenic" polymers.

1. INTRODUCTION

Clar's classically developed ideas concerning aromaticity of conjugated hydrocarbons ^[1] may be viewed ^[2] to have been given a quantitative realization through the work of Herndon ^[3] and of Randić ^[4]. Randić's description emphasizes the graph-theoretic aspects and has been

termed the conjugated-circuit model. This method has been successfully used to study both finite conjugated molecules ^[5] and extended systems ^[6]. Theoretical quantum-chemical foundations of the model have been derived from quantitative resonance-theoretic ideas via a so-called Simpson-Herndon model ^[7].

The concept of conjugated-circuit can be described clearly in a graph-theoretic manner in terms of Kekulé valence structures. A *conjugated n-circuit* in a Kekulé structure is an *n*-cycle of alternating single and double bonds. In his aromatic sextet structures, Clar ^[1] represented a conjugated sextet as implicating aromatic stability. A further stabilization was also viewed to arise from a mobility of the sextets, indicated by arrows over the spanned region. The correspondence between Clar's structures and conjugated (4*n*+2)-circuits is indicated in FIGURE 1. A 6-circuit relates to an aromatic sextet, while 10- and 14-circuits relate to their mobility. In general, the conjugated-circuit resonance energy is

$$RE = \sum_{m \geq 1} (Q_m \#_{4m} + R_m \#_{4m+2})/K \quad (1)$$

where $\#_n$ is the number of conjugated *n*-circuits summed over all Kekulé structures, Q_m and R_m are parametric values corresponding to 4*m*- and (4*m*+2)-circuits, respectively, and *K* denotes the count of Kekulé structures. The graph-theoretic counts in (1) have often been done by hand for various smaller benzenoids. A powerful algorithm for such counts via "transfer matrix" has been employed for the cases of regular polymers ^[6] and of those finite molecules comprised from several like "monomer" units.

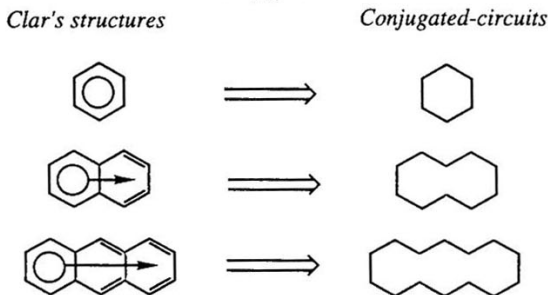


FIGURE 1 Correspondence between Clar's structures and conjugated circuit.

In the present paper, we develop another effective computational technique, which was introduced recently to study elemental carbon cages^[8] but which traces back to earlier work by Kasteleyn^[9] to count Kekulé structures for regular lattices. In this scheme, one assigns an arrow for every edge, so as to identify an antisymmetrically signed "adjacency" matrix S . The quantitative conjugated-circuit computational scheme we develop in the third section gives the desired ratios $\#_n/K$ in terms of the elements of suitable n by n submatrices of S^{-1} . With the achievement of translational symmetry for the arrow assignment the construction of these matrices for infinite polymers is accomplished by a transformation to wave-vector space where a numerical integration is performed. The consequent automated scheme has an advantage over the earlier transfer-matrix scheme: in the present scheme the size of the symmetry blocks to be manipulated grows linearly with the number of π -centers per unit cell (just as for Hückel theory), rather than exponentially with the number of links between unit cells. In the fourth section here, we use our present automated

method to treat about a dozen different benzenoid polymers as well as about a dozen near-benzenoid polymers, such as linear and zig-zag phenylene polymers, and certain "azulenic" polymers.

2. SIGNED ADJACENCY MATRIX AND CONJUGATED-CIRCUIT COUNT

The use of a signed adjacency matrix to obtain conjugated-circuit counts has been formulated in detail [8]. The standard adjacency matrix A for a graph G reads as:

$$A_{ij} = \begin{cases} 1 & , i \sim j \text{ in } G \\ 0 & , i \not\sim j \text{ in } G \end{cases} \quad (2)$$

where $i \sim j$ denotes bonded vertices in G . The *signed* adjacency matrix S derives from A with matrix elements

$$S_{ij} = \pm A_{ij} \quad (3)$$

where the sign is decided as indicated by Kasteleyn [9]. Alternatively, we express this signing process by making the graph directed: each edge $\{i, j\}$ has an orientation (indicated by \longrightarrow) such that

$$i \longrightarrow j \iff S_{ij} = -1 \text{ and } S_{ji} = +1 \quad (4)$$

In Kasteleyn's method which applies for any planar graph G , an S is constructed with the *independent* rings odd-oriented in the sense that around the periphery of each such ring there are an odd number of arrows in the clockwise direction. Then [9]

$$\det S = \{ K(G) \}^2 \quad (5)$$

Now a further graph-theoretic result is

$$\frac{\#_n(G)}{K(G)} = \sum_{G \supseteq C}^{n\text{-cycle}} 2 f_C(G) \quad (6)$$

where the sum is over all n -cycles of G , and $f_C(G)$ denotes the fraction of Kekule structures containing a given conjugated circuit around a cycle C of G . Next it turns out [8] that a further evaluation gives us our desired result

$$f_C(G) = \{ \det (S^{-1})_{C;C} \}^{1/2} \quad (7)$$

where $(S^{-1})_{C;C}$ denotes the submatrix obtained from S^{-1} by collecting the rows and columns of C . The odd-oriented assignments for finite planar graphs, especially for elemental carbon cages have been described and programmed [8].

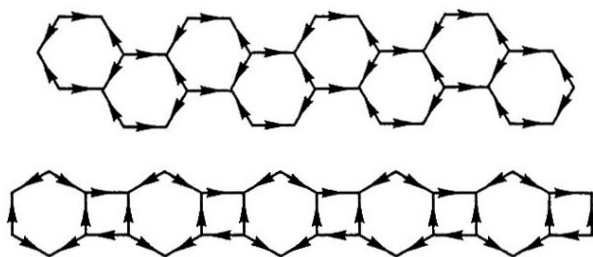


FIGURE 2 Polymers with odd-oriented rings constructed so as to retain translational symmetry.

The arrow assignment problem is more severe if we demand that it preserve (e.g., space-group) symmetry. That it can be done (sometimes at least) is indicated in the two examples of FIGURE 2. For regular polymer chains such assignments are in fact usually relatively easy to realize. Ordinarily unit cells (i.e., monomer units) may be chosen to consist of whole rings some edges of which are *free* in the sense that they are contained in no more than one ring. For a translationally symmetric assignment one need only properly correlate the arrows on the corresponding edges adjoining (say by fusion) to adjacent cells, and the free edges may be assigned last in any way to achieve odd orientation. See, e.g., FIGURE 3. If some rings contain no free edges (as can occur for wider polymer strips), then: first imagine the free edges of a unit cell erased, whence a "new" polymer cell with new free edges appears; second make arrow assignments for this "new" polymer to achieve odd orientations for its rings; and third add back in the original free edges making a suitable assignment to odd-orient the remaining rings they give rise to.

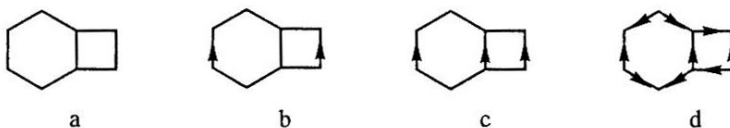


FIGURE 3 A unit cell in (a) for the second polymer of FIGURE 2. In (b) one (of two) correlated assignments of the two edges fused to adjacent cells is made, and in (c) one of two assignments of the remaining non-free edge is made. Of the 16 (and 4) ways to assign the 4 (and 2) free edges in the hexagon (and square) half must be odd-oriented and half must be even-oriented, the final choice of (d) being one of the 16 making both the hexagon and square odd oriented.

If instead of linear chains one deals with 2-dimensional networks, the constraint of 2-dimensional translational symmetry is even more severe. Though there are no free edges in such circumstances, one still can often find ^[10] a solution, but we do not go into this problem here.

3. SYMMETRY BLOCKING

Here we develop the computational method involving the antisymmetrically signed "adjacency" matrix S which has translational symmetry. Granted such a translationally symmetric arrow assignment, we define *intracellular* and *intercellular* signed *local* "adjacency" matrices Z and X , with elements

$$Z_{mn} = \begin{cases} +1 & , m \leftarrow n \text{ within unit cell} \\ -1 & , m \rightarrow n \text{ within unit cell} \\ 0 & , \text{otherwise} \end{cases} \quad (8)$$

$$X_{mn} = \begin{cases} +1 & , m \leftarrow n \text{ with } m \in (a) \text{ and } n \in (a+1) \\ -1 & , m \rightarrow n \text{ with } m \in (a) \text{ and } n \in (a+1) \\ 0 & , \text{otherwise} \end{cases} \quad (9)$$

where (a) labels the a th unit cell (or monomer unit) along the length of the polymer and m, n label π -centers within each unit cell. The signed matrix S for the full polymer is given as

$$S_{a,m; b,n} = \delta_{a,b} Z_{m,n} + \delta_{a+1,b} X_{m,n} - \delta_{a-1,b} X_{n,m} \quad (10)$$

Now we introduce the unitary matrix U with elements

$$U_{a,m; k,n} = \delta_{m,n} e^{-i a k / \sqrt{N}} \quad (11)$$

where N is the number of unit cells (the $N \rightarrow \infty$ limit being taken at a later stage). Now S is readily block-diagonalized

$$(U^\dagger S U)_{k,m; k',n} = \delta_{k, k'} \Delta^{(k)}_{m,n} \quad (12)$$

where the k th block is $\Delta^{(k)}$ and

$$\begin{aligned} \Delta^{(k)}_{m,n} &= Z_{m,n} + e^{-i k} X_{m,n} - e^{i k} X_{n,m} \\ , k &= 2 \pi a / N , \quad a = 1, 2, \dots, N \end{aligned} \quad (13)$$

Thence, we obtain the inverse of S as

$$S^{-1} = U \Delta^{-1} U^\dagger \quad (14)$$

with elements

$$(S^{-1})_{a,m; a+\delta,n} = \frac{1}{N} \sum_k e^{i \delta k} [(\Delta^{(k)})^{-1}]_{m,n} \quad (15)$$

Here we are guaranteed an inverse so long as the polymer graph supports Kekule structures, as is seen from (5). For the asymptotic $N \rightarrow \infty$ (high-polymer) limit, (15) yields

$$(S^{-1})_{a,m; a+\delta,n} = \frac{1}{2\pi} \int_{-\pi}^{+\pi} e^{i \delta k} [(\Delta^{(k)})^{-1}]_{m,n} dk \quad (16)$$

Here $\Delta^{(k)}$ is generally a complex matrix, with components Ω_1 and Ω_2 in the real and imaginary directions,

$$\begin{aligned}
 \Delta^{(k)} &= \Omega_1 + i \Omega_2 \\
 \Omega_1 &= Z + (\cos k) (X - X^\dagger) \\
 \Omega_2 &= -(\sin k) (X + X^\dagger)
 \end{aligned} \tag{17}$$

One way to avoid complex arithmetic is to collect together the $+k$ and $-k$ terms and (back) transform to a real result,

$$\begin{pmatrix} \Omega_1 + i \Omega_2 & 0 \\ 0 & \Omega_1 - i \Omega_2 \end{pmatrix} \rightarrow \begin{pmatrix} \Omega_1 & \Omega_2 \\ -\Omega_2 & \Omega_1 \end{pmatrix} \tag{18}$$

Alternatively inverses Ω_I^{-1} and

$$V = (\Omega_1 + \Omega_2 \Omega_1^{-1} \Omega_2)^{-1} \tag{19}$$

typically seem to exist, and one can manipulate (16) to the form

$$(S^{-1})_{a,m; a+\delta,n} = \frac{1}{2\pi} \int_{-\pi}^{+\pi} \{ \cos(k\delta) V_{m,n} + \sin(k\delta) [(\Omega_1^{-1} \Omega_2 V)^{-1}]_{m,n} \} dk \tag{20}$$

Clearly, Ω_1 is skew-symmetric, and Ω_2 is symmetric, so that anti-hermiticity of Δ is maintained. Combining the results of (6) and (20), one has

$$\frac{\#_{i(n)}}{K} = [\det (S^{-1})_{i(n); i(n)}]^{1/2} \tag{21}$$

where $i(n) = i_1, i_2, i_3, \dots, i_n$ is a cyclic sequence of n sites. Thence, we have achieved our desired result.

4. COMPUTATIONAL RESULTS

The method for obtaining S^{-1} is via numerical quadrature of (20). One simple common technique for this purpose is Simpson's rule if we are able to evaluate the integrand at a suitable set of points in the interval $[-\pi, +\pi]$. In (20), the integrand is a matrix function so that matrix operations have to be done at the desired quadrature points. The criterion used to stop the refinement of the numerical-integration procedure should clearly be based on a comparison between successive estimates obtained after increasing the number of quadrature points by a factor h say of $h = 10$. (Further the computations with two different densities of quadrature points can easily be extrapolated to yield an even better estimate^[11].) For our application here the criterion for convergence taken was $\epsilon = 1.0 \times 10^{-6}$, which generally may require about 10^5 quadrature points.

Application has been made to a variety of conjugated polymers, using parameter values from Randić *et al*^[12]




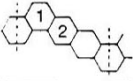

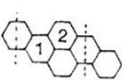






$R_1 = 0.869 \text{ eV}$	$Q_1 = -0.781 \text{ eV}$
$R_2 = 0.247 \text{ eV}$	$Q_2 = -0.222 \text{ eV}$
$R_3 = 0.100 \text{ eV}$	$Q_3 = -0.090 \text{ eV}$

though for the benzenoid polymers only conjugated circuit contributions up through 10-sites have been retained (the contributions from $4n$ -circuits being exactly 0 by theorem^[13]).

i). Benzenoid Polymers

TABLE I lists the benzenoid polymers studied. All of them have been investigated using the transfer-matrix technique^[6], though focus previously was on an associated long-range spin-pairing order and its relation to Hückel band gaps. Here we report new results concerning local

TABLE 1 Conjugated-circuit counts and resonance energy for benzenoid polymers

No.	Polymers	6-circuits	10-circuits	RE expressions	RE/e
I		$s_1=0.00000$	$t_1=0.00000$		0.0000
II		$s_1=0.00000$	$t_1=0.00000$ $t_2=0.00000$		0.0000
III		$s_1=0.00000$ $s_2=0.00000$	$t_1=0.00000$ $t_2=0.00000$ $t_3=0.00000$		0.0000
IV		$s_1=0.21822$ $s_2=0.17267$	$t_1=0.21822$ $t_2=0.17267$ $t_3=0.04555$	$(4s_1+4s_2)R_1$ $+(2t_1+4t_2$ $+2t_3)R_2$	0.1037
V		$s_1=0.25000$ $s_2=0.12500$	$t_1=0.12500$ $t_2=0.00000$	$(4s_1+4s_2)R_1$ $+(8t_1+2t_2)R_2$	0.1107
VI		$s_1=0.21289$ $s_2=0.14843$	$t_1=0.16341$ $t_2=0.14843$ $t_3=0.06446$ $t_4=0.00000$	$(4s_1+4s_2)R_1$ $+(4t_1+4t_2$ $+2t_3+2t_4)R_2$	0.1104
VII		$s_1=0.37500$ $s_2=0.12500$	$t_1=0.12500$	$(4s_1+2s_2)R_1$ $+2t_1R_2$	0.1174
VIII		$s_1=0.25000$ $s_2=0.11111$	$t_1=0.16667$ $t_2=0.05556$	$(4s_1+2s_2)R_1$ $+(2t_1+8t_2)R_2$	0.1253
IX		$s_1=0.27639$	$t_1=0.17028$	$(4s_1+4s_2)R_1$	0.1411
X		$s_1=0.50000$		$2s_1R_1$	0.1448
XI		$s_1=0.35355$ $s_2=0.14645$	$t_1=0.14645$ $t_2=0.03033$ $t_3=0.00000$	$(4s_1+4s_2)R_1$ $+(8t_1+2t_2$ $+2t_3)R_2$	0.1458
XII		$s_1=0.34929$ $s_2=0.10757$	$t_1=0.10757$ $t_2=0.08627$ $t_3=0.00000$	$(4s_1+4s_2)R_1$ $+(4t_1+8t_2$ $+4t_3)R_2$	0.1553

contributions to the resonance energies. In our TABLE 1 the first column assigns an identification number. The second column gives the polymer π -network, with the dotted lines dividing unit cells. The third and fourth columns of TABLE 1 give the fractions of Kekulé structures containing conjugated 6- and 10-circuits around given cycle fragments. The fifth column lists the formulae for resonance energies per unit cell for each polymer. In the last column, the conjugated-circuit resonance energies per π -electron are given, and are found to agree with previous transfer-matrix results [6]. (Some authors [14] do not count species VII and X with "bridge" bonds as benzenoids, though Clar [1] seems to include them. Certainly VII and X must be more benzene-like in ordinary chemical senses than the so-called "benzenoid" species I, II, and III. Indeed we will see that X is naturally viewed to be the first fully benzenoid member of a sequence of benzenoid polymers.)

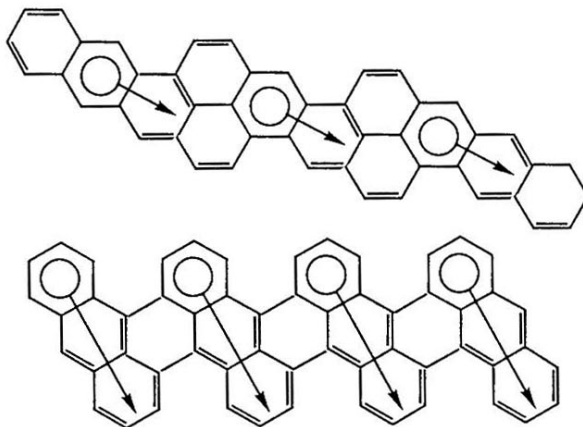


FIGURE 4 Clar's formulae for two benzenoid polymers

The results of column 3 in our TABLE 1 may be used to define a local hexagon resonance energy, or equivalently a local aromaticity index, $2R_{1fC}$ for each particular 6-cycle fragment C . The hexagons with larger values of localized resonance energy should correspond to circles drawn in Clar's preferred aromatic-sextet structures, such as illustrated in FIGURE 3, and in accord with a study ^[15] earlier made for finite benzenoid hydrocarbons. There are three cases of zero-weight contributions for 6- or 10-cycle fragments, which then are anticipated to be "nonaromatic". The first case is as in V and XI, and gives 0 regardless of chain length N . The second and third cases only approach a zero-weight asymptotically: the second case as for VI and XII approaching 0 exponentially fast with chain length N ; and the third case as for I, II, and III only approaching 0 as an inverse power of N . The tendency towards stability can be understood as in previous discussions to correlate with resonance energy.

ii). Fully Benzenoid Polymers

Notably the most stable (i.e. highest resonance energy per site) of all the polymers is the last (XII) which is *fully benzenoid* (meaning ^[1] there a Clar structure for which every π -center belongs to one aromatic sextet ring). See FIGURE 5, where besides the fully benzenoid nature of XII we also note the fully benzenoid character of the fifth member of the "polypolyphenanthrene" polymer class, the first and second members of which are species IX and XII. Indeed every third member of this family of polymers may be seen to be fully benzenoid (as also is supported by computations made elsewhere ^[16]). Another family of which every third member is fully benzenoid is that with first and second members being polymers X and VII of TABLE 1, and with fourth (fully benzenoid) member indicated in FIGURE 6. The first member of this sequence (X)

exhibits no possibility of mobility of its Clar sextets so although it is very stable (as judged by its RE/e) it is less so than the nonfully benzenoid species XI. Such does not occur for the higher fully benzenoid species in this sequence. Yet further fully benzenoid polymers can be obtained from any one of those already identified by erasing (in a translationally symmetric fashion) boundary (or "free") bonds not contained in one of Clar's aromatic sextets. Thence a wide range of fully benzenoid polymers are possible, and seem to be of special stability from the current evidence.

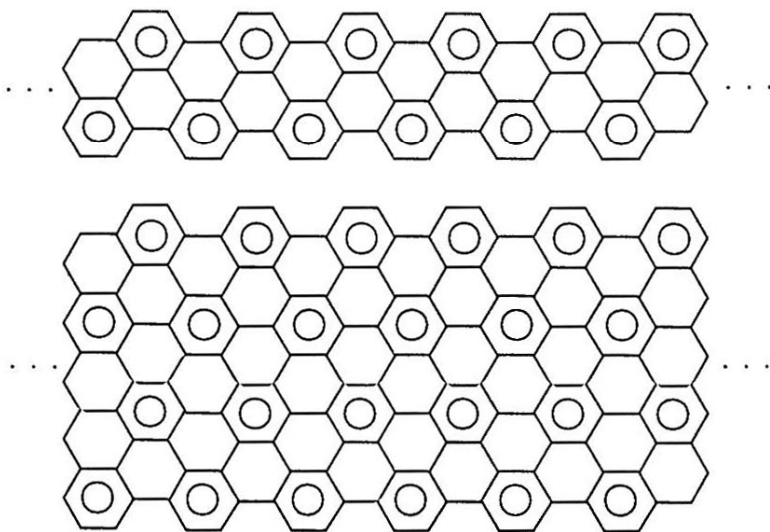


FIGURE 5 The preferred Clar structure identifying the two associated polymers as fully benzenoid.

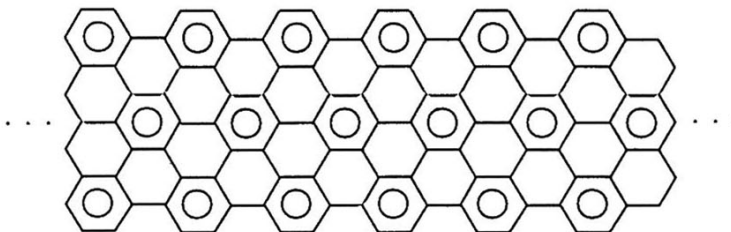


FIGURE 6 Another fully benzenoid polymer.

iii). Polyphenylenes

Polyphenylenes contain classical antiaromatic cyclobutadiene rings and aromatic benzene rings alternating with one another and have attracted both synthetic organic chemists^[17] and theoretical chemists^[18,19]. Some syntheses of (shorter) [N]phenylenes have been achieved. A recent theoretical study has appeared discussing resonance energy and frontier orbital separation^[19]. In order to determine their aromatic stabilities, we calculate the conjugated n -circuits ($n = 4, 6, 8, 10, 12, 14$) for linear and zigzag phenylene polymers using our present computational technique. Here in TABLE 2 we note that there are several relations between the various n -circuit counts which hold for infinite length chains. Both for linear and zigzag [N]phenylenes, such relations are only approached asymptotically as N increases (see FIGURE 7). In agreement with Ref. 19, the linear structure is predicted to be more stable than the zigzag, and the linear phenylene is expected to be an unusual quasi-one-dimensional organic conductor with a novel electronic structure.

iv). Azulenoid Polymers

Another kind of interesting class of polymers is that of the "azulenic" polymers as indicated in TABLE 3. The computational results are listed in

TABLE 2. Conjugated-circuit counts and π -resonance energy for linear and zigzag phenylene polymers

	linear	zigzag
4-cycle 6-cycle 8-cycle 10-cycle 12-cycle 14-cycle	$c = 0.14645$ $s = 0.35355$ $o = 0.14645$ $t = 0.06066$ $d = 0.14645$ $f = 0.06066$	$c = 0.27639$ $s = 0.27639$ $o = 0.17082$ $t = 0.10557$ $d = 0.10557$ $f = 0.06525$
Relations	$\#_4 = \#_{12}$ $\#_4 = 2 \#_8$ $\#_{10} = 2 \#_{14}$ $\#_4/\#_{10} = 1 + \sqrt{2}$ $\#_6/\#_4 = 1 + \sqrt{2}$	$\#_4 = \#_6$ $\#_{10} = \#_{12}$ $\#_4/\#_{10} = (3 + \sqrt{5})/2$ $\#_8/\#_6 = \sqrt{5} - 1$ $\#_{14}/\#_{12} = \sqrt{5} - 1$
RE/cell expressions	$4cQ_1 + 8oQ_2 + 4dQ_3$ $+ 4sR_1 + 4tR_2 + 8fR_3$	$4cQ_1 + 8oQ_2 + 4dQ_3$ $+ 4sR_1 + 4tR_2 + 8fR_3$
RE/e (eV)	0.0473	-0.0073

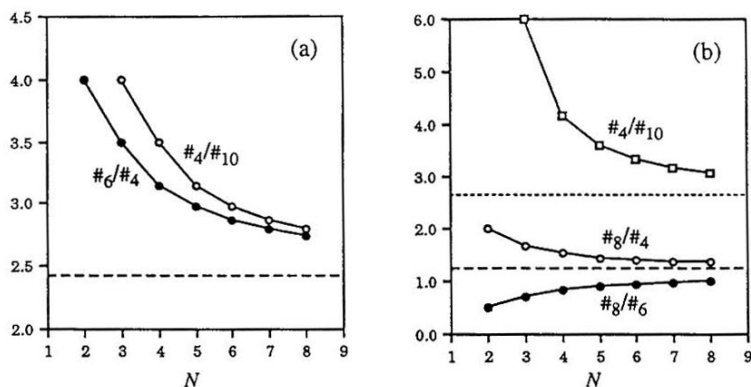
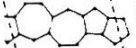
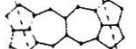
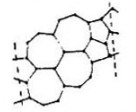
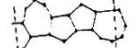
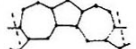
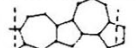
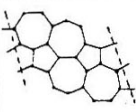
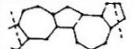
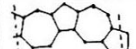
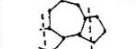
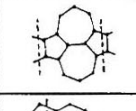



FIGURE 7 The ratios of various conjugated n -circuits in $[N]$ phenylenes: (a). linear; (b). zigzag.

TABLE 3 Conjugated-circuit counts and resonance energy for azulenic polymers

Polymers	8-cycle	10-cycle	12-cycle	RE expressions	RE/e
	$o_1=0.27639$	$t_1=0.00000$	$d_1=0.27639$	$o_1Q_2+2t_1R_2+d_1Q_3$	-0.0108
	$o_1=0.00000$	$t_1=0.00000$	$o_1=0.00000$	$o_1Q_2+4t_1R_2+d_1Q_3$	0.0000
	$o_1=0.15084$ $o_2=0.10928$	$t_1=0.15084$ $t_2=0.10928$ $t_3=0.07917$	$d_1=0.15084$ $d_2=0.10928$ $d_3=0.07917$	$(3o_1+2o_2)Q_2$ $+(2t_1+4t_2+t_3)R_2$ $+(3d_1+2d_2+2d_3)Q_3$ $+2f_1R_3$	0.0019
	$f_1 = 0.07917$		(14-cycle)		
	$o_1=0.13816$	$t_1=0.13816$	$d_1=0.13816$	$o_1Q_2+2t_1R_2+d_1Q_3$	0.0031
		$t_1=0.17237$ $t_2=0.07101$		$(2t_1+2t_2)R_2$	0.0150
		$t_1=0.17674$ $t_2=0.07320$		$(2t_1+2t_2)R_2$	0.0154
	$o_1=0.15084$ $o_2=0.10928$	$t_1=0.15084$ $t_2=0.10928$	$d_1=0.15084$ $d_2=0.10928$	$(o_1+2o_2)Q_2$ $+(6t_1+4t_2)R_2$ $+(d_1+2d_2)Q_3$ $+2f_1R_3$	0.0167
	$f_1 = 0.07917$		(14-cycle)		
		$t_1=0.13816$		$4t_1R_3$	0.0170
		$t_1=0.00000$ $t_2=0.27639$		$(2t_1+2t_2)R_2$	0.0170
		$t_1=0.13819$		$2t_1R_2$	0.0170
	$o_1=0.00000$	$t_1=0.21132$	$d_1=0.28868$	$o_1Q_2+4t_1R_2$ $+d_1Q_3+f_1R_3$	0.0180
	$f_1 = 0.15470$		(14-cycle)		
	$o_1=0.00000$	$t_1=0.15084$ $t_2=0.10928$	$d_1=0.15084$	$o_1Q_2+d_1Q_3$ $+(2t_1+4t_2)R_2$ $+2f_1R_3$	0.0224
	$f_1 = 0.07917$		(14-cycle)		

order of increasing resonance stabilities. As has been known for finite molecules, both fused pairs of pentagons and fused pairs of heptagons have a destabilizing effect, presumably because these fused pairs of rings lead to cycles of size $4n$ ($n = 2$ and 3) around the peripheries of these pairs. Generally it seems that fusing of a pentagon and heptagon together (with the consequent periphery of size $4n+2 = 10$) gives a stabilizing effect. The last two polymers in our TABLE 3 have much higher stabilities, even though both fused pentagon pairs and fused heptagon pairs occur. Evidently the Kekulé structures as arise on these polymer structures only infrequently lead to conjugation around such unfavorable pairs, thence these two polymers are expected to be somewhat novel organic polymers.

5. CONCLUSION

In conclusion, an efficient automated computational scheme for the conjugated-circuit treatment of resonance in regular (high) polymers has been described here, and has now been applied to a range of polymer structures to yield numerical results, both old (thereby checking the programming) and new. Some (anticipated) results concerning local aromatic character have been verified, and a couple novel polymer structures have been identified.

Acknowledgement is made for support of this research to the Welch Foundation of Houston, Texas and to the donors of The Petroleum Research Fund, administered by the American Chemical Society.

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