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Review

Topological Ring-Currents in Condensed Benzenoid Hydrocarbons*

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Topological ring-currents are defined as being π-electron ring-current intensities in condensed, benzenoid hydrocarbons that (i) are calculated by the simplest Hückel-London-Pople-McWeeny method, (ii) are based on a molecular geometry of regular hexagons of carbon atoms, and (iii) are expressed as a ratio to the corresponding ring-current intensity calculated, by the same method, for benzene. Once a particular benzenoid hydrocarbon has been specified, such topological ring-currents are predetermined and do not further depend on any subjective (or other) parameters; they are, therefore, purely graph-theoretical indices, reliant solely on knowledge of a vertex-adjacency matrix for the graph representing the connectivity of the carbon atoms in the benzenoid molecule under study. For convenient reference, tables of all known topological ring-current intensities – some published, and others so-far unpublished – are presented for future evaluation and possible comparison with other graph-theoretical indices that characterise the individual rings of a condensed, benzenoid hydrocarbon.

HISTORICAL BACKGROUND

In the mid-1930s, two eminent scientists[1,2] simultaneously put forward the idea that the pronounced anisotropy that had long been experimentally observed in the diamagnetic susceptibilities of the condensed, benzenoid hydrocarbons may be attributed to the circulation of their π-electrons around the carbon-atom σ-bond frameworks of such molecules, to form what were termed[1,2] "inter-atomic currents", when these hydrocarbons are in the presence of an external magnetic-field. In practice, of course, the π-electrons do not move along the σ-bonds themselves, that is, in the molecular plane; rather, they should be considered to be above and below the plane. This model nevertheless purported to explain why the diamagnetic susceptibility in a direction at right angles to the molecular plane of a condensed, benzenoid hydrocarbon was invariably found experimentally to be markedly greater than that along two perpendicular axes lying in the plane of the molecule itself. The theories of Linus Pauling[1] and Dame Kathleen Lonsdale[2] were unashamedly non-quantum-mechanical, making appeal, as they did, to the classical treatment of induced currents due to Larmor precession which were then considered to obey Kirchhoff's First and Second Laws of electricity. In this way, these authors regarded the σ-bond framework of a conjugated hydrocarbon as effectively being a microscopic analogue of an ordinary macroscopic electrical network to which Kirchhoff's Laws could naturally be applied.[3] Almost immediately, these ideas were

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* Respectfully dedicated to Professor Roy McWeeny on the fiftieth anniversary of his seminal paper: Ring Currents and Proton Magnetic Resonance in Aromatic Molecules, *Molecular Physics* **1** *(*1958) 311–321.

put on a quantum-mechanical footing when London[4–7] made the seminal contribution of casting this model of inter-atomic currents in terms of Hückel's then recently proposed LCAO-MO method,[8–13] itself based on the Bloch molecular-orbital theory of metals, as applied by Peierls, four years earlier.[14] This was, in a sense, doubly appropriate, because – as Lonsdale herself had observed[2] – in addition to having proposed the MO method now known by his name,[8–13] Hückel was also one of several people who had earlier suggested[14] qualitatively that diamagnetic anisotropy in conjugated molecules might be due to the postulated mobility of their π-electrons.

The Second World War then intervened and little further was done concerning these matters until the late 1940s when the French school,[15,16] in particular, and others,[14] applied London's method to calculate the magnetic susceptibilities of a large number of conjugated molecules; (for reviews and further details, see Refs. 3, 14–18). With the advent of ^{1}H-NMR spectroscopy in the early 1950s there arose the observation of a so-called "downfield shift" in the ^{1}H-NMR signals of the peripheral attached protons in benzene and related molecules.[19] In order to explain this phenomenon, Pople[20] revived the idea of inter-atomic currents that had been introduced by Pauling[1] and Lonsdale[2] – and set in a quantum-mechanical context by London[4–7] – to account for diamagnetic anisotropies, and he used this same model to rationalise the observed ^{1}H-NMR downfield-shifts[19] by suggesting that they were due to secondary magnetic-fields – at the peripheral, attached protons in benzene – caused by the inter-atomic current. Despite the fact that London's quantum-mechanical method[4–7] had by then been on record for almost twenty years, Pople's initial treatment[20] of the effect of inter-atomic currents on ^{1}H-NMR chemical-shifts in benzene was avowedly classical in nature. Nor, contrary to popular belief, did Pople actually coin the term "ring current" in that celebrated 1956 paper:[20] Pople did, however, use this appellation in a second paper – applying his classical model of ^{1}H-NMR downfield-shifts to polycyclic conjugated molecules – that he co-authored later that same year.[21] Almost immediately, however, Pople[22] himself came forward with an extension of the London method[4–7] – likewise based on a Hückel molecular orbital[8–13] – to present a quantum-mechanical formulation that enabled calculation of individual ring-current intensities associated with each ring of a polycyclic molecule, rather than just its overall diamagnetic-susceptibility, which was all that could be obtained by an application of the Hückel-London formalism. The effects of such quantum-mechanically calculated ring-currents on ^{1}H-NMR chemical-shifts in conjugated hydrocarbons were, however, still to be estimated classically.[21] Just 136 pages after Pople's paper[22] in Volume **1** of *Molecular Physics*, McWeeny[23] offered an alternative extension of the Hückel-London approach.[4–7] By means of his novel device of introducing what is termed a "test dipole", McWeeny[23] provided an entirely quantum-mechanical method of calculating the ring-current contribution to the ^{1}H-NMR secondary magnetic-field at a peripheral attached proton in a conjugated molecule.

RING CURRENT INTENSITIES *VIA* THE McWEENY FORMALISM

What, however, McWeeny[23] did not ostensibly do (which, as already mentioned, Pople, in his own paper[22] in *Molecular Physics*, had in fact done) was to give an explicit expression for the ring-current intensity associated with each of the individual rings in a polycyclic, conjugated, molecule – though such was in fact implied in McWeeny's treatment,[23] as will be seen. As the present author has shown,[24,25] however, it is not difficult to re-cast the second version of McWeeny's equations – the ones that he obtained by effecting a clever unitary transformation[23,26,27] of the basis orbitals when the system is in the presence of an external magnetic-field – in a way that provides an explicit expression for individual ring-current intensities in each of the several rings of a conjugated molecule.[24,25] When the ring current in the *i*th ring, J_i, is expressed as a ratio to J_{benzene} – the ring-current intensity calculated, by the same method, to be associated with the unique ring in benzene – this expression is as follows:[18,24]

$$(J_i / J_{\text{benzene}}) = 9\{\sum_{(\mu)} [P_{(\mu)}\eta_{(\mu)} + \beta\bar{\pi}_{(\mu)(\mu)}(\eta_{(\mu)})^2]\, S_{(\mu)}\, C^{i}_{(\mu)} + \sum\sum_{(\mu<\nu)} \beta\bar{\pi}_{(\mu)(\nu)}\eta_{(\mu)}\eta_{(\nu)}[S_{(\mu)}C^{i}_{(\nu)} + C^{i}_{(\mu)}S_{(\nu)}]\} \qquad (1)$$

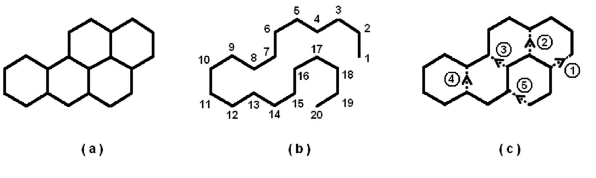


Figure 1. The construction of an open-chain spanning-tree which could be used for an application of the McWeeny method[23] to perform a topological ring-current calculation on the benzenoid hydrocarbon 3,4-benzopyrene; (a) the carbon-atom connectivity/molecular graph of 3,4-benzopyrene; (b) a continuous open-chain (a non-branched spanning-tree)[25] for 3,4-benzopyrene; (c) a suitable set of "circuit-completing bonds" ("chords"[28] of the spanning tree) associated with the open chain in (b).

The symbols in Eq. (1) are explained with reference to Figure 1, which is the starting point for a calculation, by McWeeny's method, of the topological ring-currents in the notorious carcinogen 3,4-benzopyrene. The following procedure is adopted:

(a) First, the carbon-carbon σ-bond connectivity-network of the molecule is schematically depicted in the form of a molecular graph, as in Figure 1(a).

(b) Second, a spanning tree[25] is selected (Figure 1(b)), in which certain carbon-carbon bonds of the molecule's σ-bond network (that is, edges of the molecular graph) have been deleted in such a way as to leave a continuous, open chain (without circuits, rings or branches) – a chain that does, however, still connect all the carbon atoms that were in the original conjugation-network of the molecule under study (here, 3,4-benzopyrene).

(c) Third, since an anti-clockwise circuit is conventionally taken to be positive, the next stage is to number the skeletal chain sequentially in an anti-clockwise manner. In practice, however, such a labelling scheme is merely a convenience, and the labelling could in fact have been capriciously effected quite arbitrarily.

(d) Finally, what McWeeny[23] called the "circuit-completing bonds" are re-inserted – these are schematically depicted as dotted lines Figure 1 (c); these are those carbon-carbon σ-bonds that have to be added to the open-chain spanning-tree of Figure 1(b) in order to reconstitute the carbon-carbon σ-bond-network of the original (in this case, 3,4-benzopyrene) molecule depicted in Figure 1(a). Graph-theoretically, they are the chords of the chosen spanning tree.[28] The direction of these circuit-completing bonds is (arbitrarily) defined, and is denoted by means of arrows, as in Figure 1(c): the convention has been followed that the "circuit-completing" bonds are defined from the carbon atom whose label in Figure 1(b) is higher, to the carbon atom whose label is lower. However, the opposite (or no) convention could equally well have been adopted. The choice of a spanning tree that constitutes a continuous, open, chain, without branches, was presupposed by McWeeny and, indeed, the unitary transformation of the molecule's basis-orbitals (when it is in the presence of an external magnetic field) that McWeeny proposed requires the choice of such a non-branched spanning-tree. By definition, a non-branched spanning-tree does always exist if the graph representing the carbon-atom framework of the molecule is semi-Hamiltonian.[25,29] All the benzenoid molecules considered in this paper are associated with semi-Hamiltonian molecular-graphs, but some molecular graphs – such as, for example, that of the ten-ring conjugated molecule decacyclene (not a condensed, benzenoid hydrocarbon: see Figure 3 of Ref. 25, and Figure 3 of Ref. 18) – are not semi-Hamiltonian. For such molecules it is therefore not possible to select a "continuous open-chain" on which McWeeny's[23] unitary transformation must necessarily be based. Accordingly, in such cases, a more-general unitary-transformation of the basis orbitals must be applied, and such was eventually provided by Gayoso and Boucekkine.[30] Even if the underlying molecular-graph itself is actually semi-Hamiltonian (as that of 3,4-benzopyrene is), it is still possible, if desired, to base the calculation on a spanning tree with branches (such as, for example, the one depicted in Figure 2) – but then the unitary transformation proposed by Gayoso and Bouceekine,[30] rather than the original one effected by McWeeny,[23] must be invoked (after which Eq. (1) then still applies).

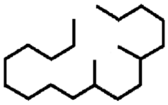


Figure 2. A branched spanning-tree of the 3,4-benzopyrene molecular-graph – depicted in Figure 1(a) – on which a topological ring-current calculation by the McWeeny method[23] could be based, after an application of the Gayoso-Boucekkine[30] unitary-transformation.

In Eq. (1) – which represents the most-general form arising out of the McWeeny method,[23] incorporating Veillard's adaptation[31] of it to accommodate, if necessary, different resonance integrals for different bonds – all the Greek subscripts refer to circuit-completing bonds, as described, as well as to the circuits that they complete; specifically, in that equation:

(i) $\beta\eta_{(\omega)}$ is the resonance integral for the ωth circuit-completing bond. β is the standard Hückel resonance-integral and the $\eta_{(\omega)}$-terms are dimensionless numbers (that arise in Veillard's generalisation[31] of McWeeny's original formalism[23]), all of which, in the case of the topological ring-currents being defined and discussed here, will invariably be assigned the standard value of unity. This assumption is tantamount to insisting that all carbon-carbon resonance-integrals are set equal to the value appropriate for a carbon-carbon bond in benzene.

(ii) $S_{(\omega)}$ is the signed (algebraical) area of the ω^{th} circuit (*i.e.*, the enclosed area formed when the ω^{th} circuit-completing bond, only, is inserted). These areas are to be counted positive if the arrow on the ω^{th} circuit-completing bond points in the anticlockwise sense around the circuit that it completes (the ω^{th} circuit), and are to be counted negative if that arrow points in the clockwise sense around the circuit that the ω^{th} circuit-completing bond completes. Thus, in Figure 1(c), $S_{(1)} = 4$ (measured in benzene ring-area units), $S_{(2)} = 3$, $S_{(3)} = 2$, $S_{(4)} = 1$ and $S_{(5)} = -1$.

(iii) $C^{i}_{(\omega)} = 0, +1$, or -1 according to the following rules:

$C^{i}_{(\omega)} = 1$ if (a) the ω^{th} circuit-completing bond contains the ring i and
if (b) the ω^{th} circuit-completing bond is

defined in the positive (anticlockwise) sense around the circuit that it completes (the ω^{th} circuit);

$C^{i}_{(\omega)} = -1$ if (a), above, applies and if (b) the ω^{th} circuit-completing bond is defined in the negative (clockwise) sense around the circuit that it completes (the ω^{th} circuit);

$C^{i}_{(\omega)} = 0$ if the ω^{th} circuit does not contain the ring i.

Also in Eq. (1), $P_{(\mu)}$ is the standard Coulson bond-order[11] of the μ^{th} circuit-completing bond; $\bar{\pi}_{(\mu)(\mu)}$ is the imaginary self-polarisability[23] of that bond and $\bar{\pi}_{(\mu)(\nu)}$ ($\mu \neq \nu$) is the imaginary mutual bond-bond polarisability of two distinct circuit-completing bonds.[23] Coulson and Longuet-Higgins[32] had previously defined the real mutual bond-bond polarisability of two bonds, μ and ν, as

$$\pi_{(\mu)(\nu)} = \frac{\partial P_{(\mu)}}{\partial \beta_{(\nu)}} \tag{2}$$

Here, $P_{(\mu)}$ is (as above) the ordinary Coulson bond-order[11] of bond μ, and $\beta_{(\nu)}$ is the resonance integral for bond ν. By analogy with this, the imaginary mutual bond-bond polarisability, $\bar{\pi}_{(\mu)(\nu)}$ – required for the complex perturbations that arise when the molecule is in the presence of an external magnetic-field – is[23] the imaginary part of the change in the bond order $P_{(\mu)}$ per unit change in the imaginary part of the resonance integral $\beta_{(\nu)}$. Once given a ground-state electronic-configuration for the molecule, deduced from the Aufbau Principle[11] – which itself may be considered to be a purely graph-theoretical algorithm[33,34] – $P_{(\mu)}$, $\bar{\pi}_{(\mu)(\mu)}$ and $\bar{\pi}_{(\mu)(\nu)}$ may all be evaluated solely from the eigenvalues and eigenvectors of the ordinary, standard Hückel Hamiltonian-matrix[23,25] that is appropriate when the molecule is in the absence of an external magnetic-field. Such a Hückel Hamiltonian also depends only on molecular topology[11,35–37] – that is, the carbon-carbon σ-bond connectivity of the conjugated system in question. It has been pointed out[18,25] that the expression for $\bar{\pi}_{(\mu)(\nu)}$ given originally by McWeeny[23] as being applicable to the alternant hydrocarbons contains a misprint; all the relevant equations for defining $\bar{\pi}_{(\mu)(\nu)}$, applicable to both alternant and non-alternant systems, are, however, conveniently combined into the Appendix of Ref. 25.

In order to obtain the summation over rings[18,23–25] – and hence to bring out the fundamentals of the "ring-current" idea – McWeeny,[23] making what the author considers to be one of the most exquisite applications of Hückel Theory, performed an ingenious unitary-transformation on the original basis-orbitals in such a way that all the perturbation brought about by the external magnetic-field was concentrated into just one bond in each ring of the conjugated system under study – the very bonds that we have here called the "circuit-completing bonds". As has previously been pointed out,[18,23] this latter observation alone emphasises the fact that, in the Hückel[8–13]-London[4–7]-Pople[22]-McWeeny[23] model – hereafter given the acronym HLPM – the applied, external magnetic-field manifests itself through ring fluxes and that without the rings and other "closed circuits" (see, for example, Figure 1(c)) – which, by virtue of the $S_{(\omega)}$-terms in Eq. (1), give rise to these magnetic fluxes when the external magnetic-field is perpendicular to the molecular plane of the conjugated system in question – such a field can have no effect whatsoever in exciting "ring currents".[18]

Despite being superficially very different, the methods of Pople[22] and of McWeeny[23] are entirely equivalent, numerically, when calculations of ring-current intensities that are effected by use of these methods are based on the same Hückel molecular-orbitals and identical assumptions are made about the molecular geometry of the conjugated molecules under study. It may also be observed that yet another extension of the London formalism for calculating magnetic susceptibilities – this one due to Coulson[38,39] – is also entirely equivalent, numerically, to those of Pople[22] and of McWeeny,[23] even though the somewhat arcane expressions embodied in it are couched in terms of the Coulson contour-integral formalism,[40] and thus do not immediately appear to be related in any obvious way to those arising in the other two[22,23] approaches.

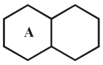
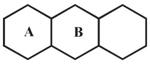
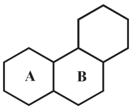
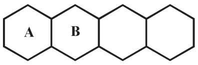
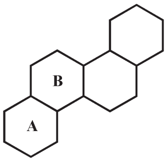
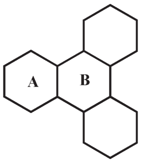
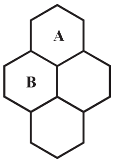
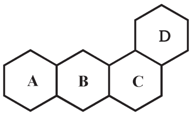
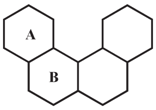
THE CONCEPT OF TOPOLOGICAL RING-CURRENTS

Most calculations performed by use of the HLPM model in the fifty years since the final part of it was formulated have made the simplest assumptions about Hückel theory and molecular geometry: standard Coulomb and resonance integrals have been adopted for all carbon atoms and carbon-carbon bonds (respectively) and all hexagons of carbon atoms are taken to have the area of a standard benzene-ring, and to have sides equal in length to the unique carbon-carbon bond-length in benzene. Now, the present author argued[25] many years ago that although much Graph Theory – for example, the idea of a spanning tree, referred to earlier – is inherent in the ring-current concept, the ring-current index itself, depending, as it does (by virtue of the $S_{(\omega)}$-terms in Eq. (1)), on molecular geometry, is manifestly not a completely topological quantity – even when a purely topological wave-function (that is, the simple Hückel one[8–13,25,41]) has been used to calculate it. Nevertheless, notwithstanding this observation, the present author (alone,[25] and with Coulson,[41] and with Gomes[18]) has previously drawn attention to the fact that

(a) when the HLPM method is used, and

(b) when only benzenoid hydrocarbons[42] are considered, and

TABLE I. Topological Ring-Currents in Benzenoid Hydrocarbons comprising 1–4 Rings

Molecule	Topological Ring-Current Intensity in Rings				Reference Source
	A	B	C	D	
One Ring					
	1.000	–	–	–	By Definition
Two Rings					
	1.093	–	–	–	Refs. 5, 15, 23 & 70
Three Rings					
	1.085	1.280	–	–	Refs. 70 & 62
	1.133	0.975	–	–	Ref. 70
Four Rings					
	1.068	1.305	–	–	Refs. 62 & 71
	1.152	1.067	–	–	Refs. 72* & 62
	1.111	0.747	–	–	Ref. 70
	1.327	0.964	–	–	Refs. 70, 62 & 63 Note that Ref. 70 reports 1.329 (not 1.327) for Ring A
	1.119	1.271	0.891	1.122	Ref. 73
	*1.150*	*1.073*	–	–	Refs. 62 & 64 **Non-Planar** **Molecule**† (Hα4 Protons)[69]

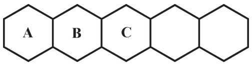
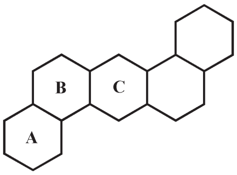
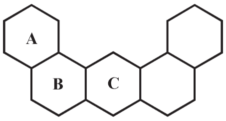
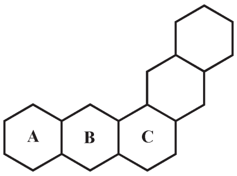
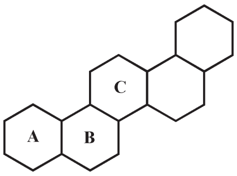
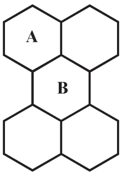
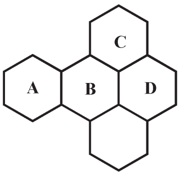
(c) when all Hückel Coulomb integrals are assigned the value (α) appropriate for a carbon atom in benzene, and all resonance integrals are likewise set equal to the standard value (β) for a carbon-carbon bond in benzene, and

(d) when a molecular geometry comprising regular hexagons of benzene dimensions is assumed, and, finally,

(e) when the resulting calculated ring-current intensities are expressed as a ratio to the ring-current intensity evaluated, by the same method, for benzene,

then, once the carbon-carbon connectivity of a benzenoid molecule has been specified, the (topological) ring-current intensities so-calculated are predetermined and do not further depend on any subjective (or other) pa-

TABLE II. Topological Ring-Currents in Five-Ring Benzenoid Hydrocarbons (continued in Tables III & IV)

Molecule	Topological Ring-Current Intensity in Rings				Reference Source
	A	B	C	D	
Five Rings					
	1.06*	1.30*	1.35*	–	Ref. 65*
	1.138	0.943	1.289	–	Refs. 73 & 65*
	1.14*	0.944	1.29*	–	Ref. 65*
	1.11*	1.23*	0.784	–	Ref. 65*
	1.16*	1.06*	1.15*	–	Ref. 65*
	0.970	0.239	–	–	Disagreement between Ref. 70 and Ref. 65 is adjudicated in Refs. 62 & 63. This favoured the values quoted in Ref. 65, which are the ones given here
	1.10*	0.719	1.29*	0.987	Ref. 65*

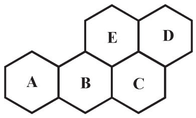
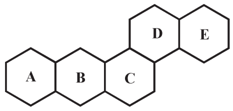
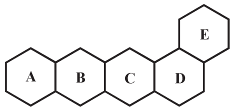
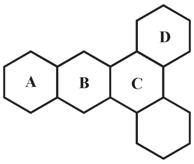
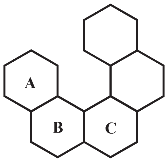
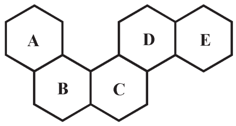
(Five-Ring Benzenoid Hydrocarbons are continued in Table III.)

rameters. In that sense, the ring-current intensity that characterises each of the diverse rings in benzenoid molecules is a purely graph-theoretical index that depends solely on the knowledge of a vertex-adjacency matrix[43] for the graph representing the connectivity of the carbon atoms in the particular benzenoid molecule under study. Because of this, Gomes and the present author have ventured to speculate[18] that "... despite technically being semi-empirical, such calculations may be regarded as possibly having an unexpected degree of respectability." Ring-current intensities calculated and presented in this way will be referred to as topological ring-currents. All the ring-current intensities that are reported in this paper come into this category.

TABLES OF TOPOLOGICAL RING-CURENTS

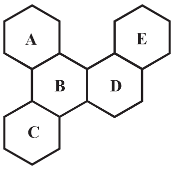
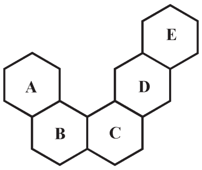
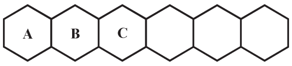
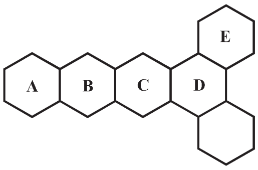
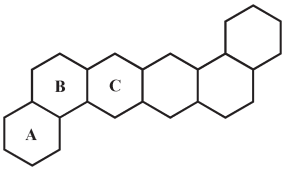
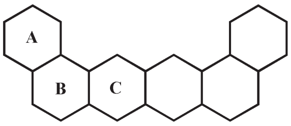
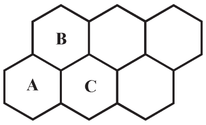
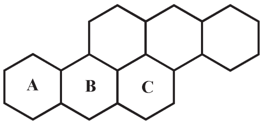
The author has recently compiled, initially for private use, an extensive table of such topological ring-currents. Even though they are from a wide variety of sources, all have been consistently calculated by the HLPM method, based on the assumptions about Coulomb and resonance integrals and molecular geometry stated earlier, and are each expressed as a ratio to the corresponding ring-current intensity calculated, by the same method, for benzene – just as has been described. This wide-ranging numerical tabulation was devised with the intention of being able to compare[44] topological ring-current intensities, so calculated, with the "π-electron-partition" index for each symmetrically non-equivalent ring of a polycyclic con-

TABLE III. Topological Ring-Currents in Five-Ring Benzenoid Hydrocarbons (continued from Table II and further continued in Table IV)

Molecule	Topological Ring-Current Intensity in Rings					Reference Source
	A	B	C	D	E	
Five Rings (Continued)						
	1.205	1.290	0.848	1.302	1.077	Refs. 73, 65* & 74 There are slight discrepancies in the third decimal-place between Refs. 73 & 74 Values from Ref. 74 are given here
	1.12*	1.30*	0.993	1.08*	1.15*	Ref. 65*
	1.09*	1.32*	1.35*	0.847	1.11*	Ref. 65*
	1.12*	1.21*	0.648	1.08*	–	Ref. 65*
	*1.153*	*1.055*	*1.160*	–	–	R. B. Mallion, unpublished & Ref. 65* **Non-planar**† **Molecule** (Hα5 Protons)[69]
	*1.15**	*1.06**	*1.16**	*1.05**	*1.15**	Ref. 65* **Non-planar**† **Molecule** (Hα4 Protons)[69]

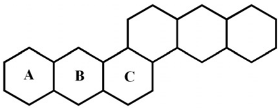
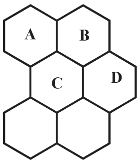
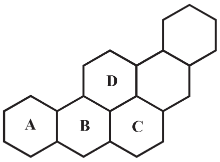
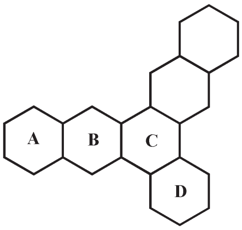
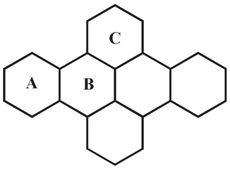
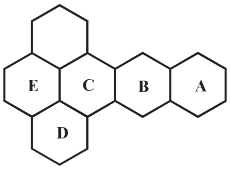
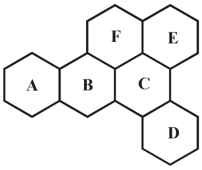
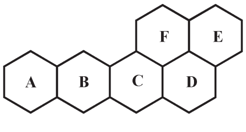
(Five-Ring Benzenoid Hydrocarbons are continued in Table IV.)

TABLE IV. Topological Ring-Currents in Five-Ring Benzenoid Hydrocarbons (continued from Tables II & III) and Six-Ring Benzenoid Hydrocarbons (continued in Tables V–VII)

Molecule	Topological Ring-Current Intensity in Rings					Reference Source
	A	B	C	D	E	
Five Rings (Continued)						
	_1.13*_	_0.853_	_1.14*_	_1.09*_	_1.10*_	Ref. 65* **Non-planar Molecule†** (Hα4 Protons)[69]
	_1.14*_	_1.08*_	_1.00*_	_1.30*_	_1.12*_	Ref. 65* **Non-planar Molecule†** (Hα4 Protons)[69]
Six Rings						
	1.048	1.291	1.352	–	–	Refs. 75, 62 & 71
	1.094	1.311	1.194	0.603	1.061	Ref. 75
	1.121	0.877	1.299	–	–	Ref. 75
	1.119	0.876	1.298	–	–	Ref. 75
	1.337	0.854	1.297	–	–	Ref. 75
	1.197	1.310	0.979	–	–	Ref. 75

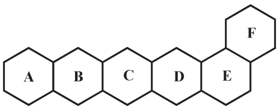
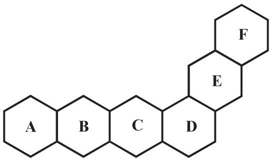
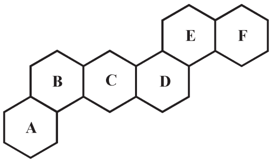
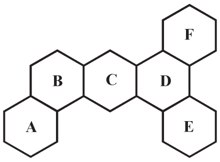
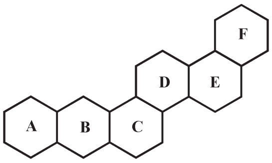
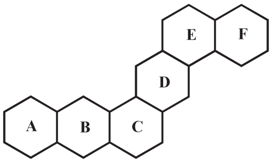
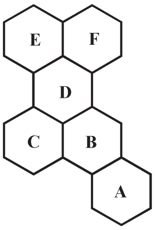
(Six-Ring Benzenoid Hydrocarbons are continued in Table V.)

TABLE V. Topological Ring-Currents in Six-Ring Benzenoid Hydrocarbons (continued from Table IV and further continued in Tables VI & VII)

Molecule	Topological Ring-Current Intensity in Rings						Reference Source
	A	B	C	D	E	F	
Six Rings (Continued)							
	1.121	1.305	1.011	–	–	–	Ref. 75
	1.292	1.075	0.684	1.380	–	–	Ref. 75
	1.191	1.214	0.725	1.181	–	–	Ref. 75
	1.104	1.170	0.548	1.044	–	–	Ref. 75
	1.109	0.745	1.270	–	–	–	Ref. 75
	1.111	1.194	0.614	1.260	0.989	–	Ref. 75
	1.196	1.226	0.606	1.058	1.264	1.089	Ref. 75
	1.143	1.372	1.205	0.790	1.268	1.089	Ref. 75

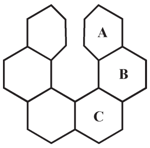
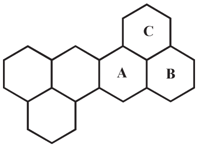
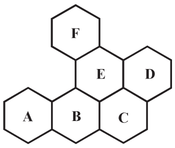
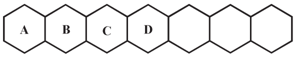
(Six-Ring Benzenoid Hydrocarbons are continued in Table VI.)

TABLE VI. Topological Ring-Currents in Six-Ring Benzenoid Hydrocarbons (continued from Tables IV & V and further continued in Table VII)

Molecule	Topological Ring-Current Intensity in Rings						Reference Source
	A	B	C	D	E	F	
Six Rings (Continued)							
	1.072	1.321	1.356	1.244	0.825	1.101	Ref. 75
	1.091	1.311	1.216	0.732	1.209	1.108	Ref. 75
	1.138	0.936	1.312	1.046	1.080	1.153	Ref. 75
	1.140	0.962	1.247	0.698	1.094	1.096	Ref. 75
	1.125	1.299	0.973	1.154	1.044	1.153	Ref. 75
	1.121	1.257	0.839	1.262	0.951	1.138	Ref. 75
	1.077	0.875	1.041	0.236	0.974	0.973	Ref. 75

(Six-Ring Benzenoid Hydrocarbons are continued in Table VII.)

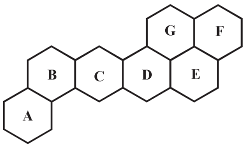
TABLE VII. Topological Ring-Currents in Six-Ring Benzenoid Hydrocarbons (continued from Tables IV–VI) and in Seven-Ring Benzenoid Hydrocarbons (continued in Tables VIII & IX)

Molecule	Topological Ring-Current Intensity in Rings						Reference Source
	A	B	C	D	E	F	
Six Rings (Continued)							
	*1.155*	*1.068*	*1.150*	–	–	–	R. B. Mallion, unpublished **Non-Planar Molecule**† (Hα6 Protons)[69]
	0.365	0.865	0.922	–	–	–	(Partly) Ref. 75 & Ref. 25
	*1.195*	*1.326*	*0.888*	*1.297*	*0.843*	*1.127*	R. B. Mallion, unpublished **Non-Planar Molecule**† (Hα4 Protons)[69]
Seven Rings							
	1.045	1.285	1.348	1.361	–	–	Refs. 62 & 71

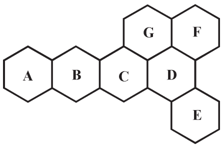
(Seven-Ring Benzenoid Hydrocarbons are continued in Table VIII.)

TABLE VIII. Topological Ring-Currents in Seven-Ring Benzenoid Hydrocarbons (continued from Table VII and further continued in Table IX)

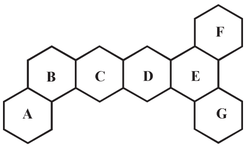
Seven Rings (Continued)



Topological Ring-Current Intensity in Rings							Reference Source
A	B	C	D	E	F	G	
1.139	0.932	1.366	1.263	0.824	1.288	1.092	Refs. 76 & 74



Topological Ring-Current Intensity in Rings							Reference Source
A	B	C	D	E	F	G	
1.141	1.355	1.136	0.559	1.038	1.234	1.096	Ref. 76



Topological Ring-Current Intensity in Rings							Reference Source
A	B	C	D	E	F	G	
1.122	0.886	1.294	1.232	0.628	1.071	1.070	Ref. 76

(Seven-Ring Benzenoid Hydrocarbons are continued in Table IX.)

jugated system, just proposed by Balaban *et al.*,[45–51] and with the "*ef*-values" recently defined by Gutman[52] – though it has to be said that sample preliminary confrontations between topological ring-current intensities and these quantities have not been encouraging.[44,53] These data would, however, also be available for comparison with any other (possibly future) theoretical π-electron indices that are attributable to the individual rings of a condensed, benzenoid hydrocarbon.[42] This compilation, which is presented in Tables I–XIII, comprises 330 individual topological ring-current intensities, for each of the many symmetrically non-equivalent rings in 79 different condensed, benzenoid hydrocarbons. Nearly 100 of these topological ring-currents, in more than 20 different molecules, are new and unpublished, and are taken from the author's personal files.[54] The rest are from literature sources (all of which are stated). The list includes certain molecules that are so severely overcrowded that they are non-planar.[55–61] Strictly, the unmodified HLPM method should not be applied to these molecules;[62–64] such has, however, occasionally been done, in the past,[65–67] and – because the ring current is here effectively being regarded as a purely mathematical, topological index, and not as an assumed "physical" quantity *per se* – this will again be done (though with reservations) in the ring-current lists presented in Tables I–XIII. The following points should be noted, concerning this compilation:

1. Because topological ring-currents – such as those featuring in Tables I–XIII – are, by definition, calculated ring-currents whose intensities are expressed as a ratio to the ring-current intensity evaluated, by the same (HLPM) method, for benzene, the topological ring-current intensities themselves (being, thereby, pure numbers) are dimensionless.
2. All the topological ring-currents listed here are quoted to three decimal places, apart from those from Refs. 65 and 68 – which, exceptionally, present their calculations to three significant figures (Ref. 65) or to two decimal places (Ref. 68). Accordingly, all topological ring-current intensities from Ref. 68 and those in Ref. 65 that are greater than the benzene value – both denoted by the symbol "*" attached to the figures reporting them and to the corresponding reference numbers, in Tables I–XIII – are available only to two decimal places. Where there are alternative sources that give topological ring-currents to three places of decimals, these latter have been used in preference, when selecting data to be compiled into this list.
3. Molecules in the list that, in the right-hand column of the Tables, are signalled by means of the superscript symbol "†" and the label "**Non-Planar Molecule**" are benzenoid hydrocarbons that suffer more severe steric overcrowding amongst the peripheral, attached hydrogen-atoms than is provided by what Martin[69] calls "Hα3" protons, and so these benzenoid hydrocarbons are non-planar.[57] As already noted, it is not legitimate to perform HLPM ring-current calculations on such conjugated systems and to attribute to the results any physical significance,[62–64] because "ring-current" in the HLPM model is precisely defined as an exact quantity only for planar molecules; (please see Refs. 62–64 for detailed discussion on this aspect). The topological ring-currents reported in Tables I–XIII for such molecules are thus, in effect, those for a hypothetical molecule having the same carbon–carbon connectivity as the actual molecule under consideration, but envisaged as if it were planar. The numerical values of such topological ring-currents are printed in *italics* when they are documented in Tables I–XIII.
4. The right-hand column of Tables I–XIII cites the publication(s) from which the quoted topological ring-current data are taken. Previously unpublished calculations – comprising approximately 100 ring-current intensities in some 20 different molecules – are from the author's personal files.[54]

The transcriptions of original data into these Tables have all been diligently checked and cross-checked directly with the primary sources – including (in the case of previously unpublished topological ring-currents computed by the present author) the earliest relevant manuscript that was available in the author's own archives. The compilation just described is presented at various points, dispersed throughout the paper.

INITIAL DISCUSSION AND INTENDED FUTURE USE OF THE TABLES

As stated, the main purpose of this paper is to collate in one place all the known topological ring-currents for the condensed, benzenoid hydrocarbons, and thereby to facilitate their comparison with other indices – extant[44–53] or in the future – that characterise the individual, symmetrically non-equivalent rings in such molecules.[44–53] Only very general, qualitative trends in the topological ring-currents themselves are, accordingly, given here. Such trends (albeit based on more-limited data) have, in any case, already been given very detailed consideration in Refs. 78 and 18, and elsewhere.

It may first be mentioned that nine of the molecules considered in the Tables were included by Berthier, Pullman and Pullman[15] in their early list of overall diamagnetic susceptibilities calculated by the London method,[4–6] published in Chapter IX of Pullman and Pullman's seminal book *Les Théories Electroniques de la Chimie Organique*.[15] For the condensed benzenoid hydrocarbons in Tables I–XIII, these London susceptibilities – expressed as a ratio to the diamagnetic susceptibility, likewise calculated by the London method,[4–6] for benzene – may be obtained by simply summing the topological ring-current intensities reported in the Tables over all rings within a given molecule; (this process is valid because all ring-areas in these molecules are taken to be the same as the area of a standard benzene-hexagon). The ring-current intensities in the Tables are consistent (to three significant figures) with the London values[15] of overall susceptibilities in the case of seven molecules, and they disagree in the case of two molecules. Those consistent are: naphthalene (the 2nd structure of Table I), anthracene (3rd structure, Table I), phenanthrene (4th structure, Table I), triphenylene (7th structure, Table I), pyrene (8th structure, Table I), pentacene (1st structure, Table II), and perylene (6th structure, Table II); those inconsistent are: chrysene (6th structure, Table I) and coronene (6th structure, Table IX).

It was qualitatively noted very early on[65,72,73,75,76] that the more condensed a given ring is in a condensed, benzenoid hydrocarbon, the smaller the ring current it appears to bear. Motivated by this observation, the present author and Haigh[77,78] have rationalised why molecules related to perylene (the 6th structure of Table II) manifest a very small topological ring-current in their central ring (labelled ring B in the structure of perylene depicted in the penultimate row of Table II) of only about one quarter of the benzene value. This low ring-current was shown[77,78] to arise because such rings display what has been called "bond-fixation"[79,80] when that central ring (B) is considered formally to be created by joining two entities (in this case, both are naphthalene units) each of which is possessed of at least one Kekulé structure; as a result, the unshared bonds in that central ring (B) never appear other than as single bonds in any Kekulé structure that can be written for the perylene molecule as a whole. Similar considerations apply to the following benzenoid hydrocarbons, all related to perylene: the 7th structure (ring D) in Table VI, the 4th and 5th structures (rings D) of Table IX, the 2nd structure (ring B) of Table X, the 6th structure (ring E) of Table XI, the 1st structure (ring E), the 2nd structure (ring C) and the 5th structure (rings B and D) of Table XII; ring G of the 1st structure of Table XIII is also a ring of this type but it bears a considerably higher ring-current (0.706). By contrast, the central ring (C) in peropyrene (the 2nd structure in Table IX) – which, formally, is similarly condensed with four surrounding rings and is thus ostensibly analogous to the corresponding ring (B) in perylene – has associated with it a topological ring-current of intensity about 50 % greater than the benzene value (that is, about six times[76] the value in the corresponding central ring (B) of perylene (the 6th structure of Table II)). Haigh and the present author[77,78] have rationalised this observation by noting that this central ring (C) in peropyrene may formally be considered to be created by joining two entities neither of which is possessed of a Kekulé structure. Each of the unshared bonds in that central ring (C) of peropyrene is single in some Kekulé structures that can be written for the peropyrene molecule as a whole, and is double in others. As a result of this, the central ring of peropyrene (C) may be considered to participate fully[77,78] in the conjugation between the upper and lower halves of the molecule, and this, it was claimed,[77,78] rationalises the observation of a large topological ring-current in that ring. Similarly large topological ring-currents also arise in the corresponding rings (rings E) in the 4th and 5th structures in Table XI, both closely related to peropyrene. Haigh and the present author[25,75,77,78] have also drawn attention to what Clar[79,80] refers to as "bond fixation" in the central rings (A) of zethrene (the 2nd structure in Table VII), which bears a small topological ring-current of only about one-third of the benzene value. Similar situations arise in rings A of the following structures related to zethrene: the 3rd structure of Table IX, the 4th and 5th structures of Table X, the 1st and 2nd structures of Table XI, the 3rd structure of Table XII, and in rings C and D of the 1st structure of Table XIII. It is worth noting that, with one minimal exception – ring E of the 2nd structure in Table XI, whose ring current is a mere 0.2 % more than the benzene value – all the rings in the listed molecules related to zethrene have topological ring-current intensities smaller than the benzene value. It is, for example, remarkable that each and every one of the rings in the thirteen-ring benzenoid hydrocarbon illustrated as the 1st structure in Table XIII has associated with it a topological ring-current smaller than that in benzene. This all contrasts strongly with the patterns observed[68] in molecules (the 2nd and 3rd structures in Table XIII) derived from coronene (the 6th structure in Table IX): the central ring (D) in the nineteen-ring benzenoid hydrocarbon dodecabenzocoronene (the final structure in Table XIII) is still[18] the ring in this series of molecules that is associated with the largest topological ring-current so far reported.

Finally, it may be noted in conclusion that the semi-quantitative trends described above are in complete accord with the general qualitative claims made in Clar's classic little book,[80] all based on his "aromatic-sextet" arguments; (see also Ref. 42, Chapter 7, pp. 93–116). The following quotations from that source make this point. Concerning perylene (the 6th structure in Table II), Clar writes (page 59 of Ref. 80): "Perylene can be considered to be built up from two naphthalene complexes connected by two single bonds ... and the [^{1}H-NMR] spectra do not support the assumption of a ring current in the central ring." About the central ring (C) of peropyrene (the 2nd structure of Table IX), Clar observes (page 89 of Ref. 80) that ^{1}H-NMR data indicate a "... large ring current [which is] a direct proof for the inherent sextet in the centre". Calling again on ^{1}H-NMR evidence regarding zethrene (the 2nd structure of Table

TABLE IX. Topological Ring-Currents in Seven-Ring Benzenoid Hydrocarbons (continued from Tables VII & VIII)

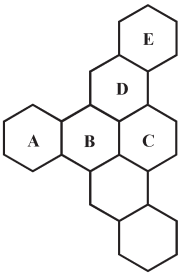
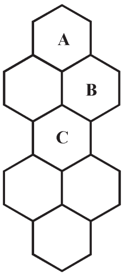
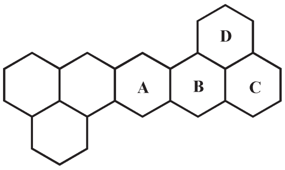
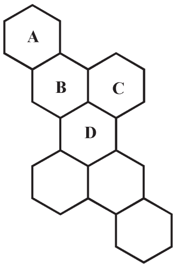
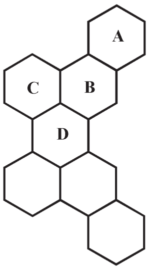
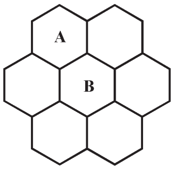
Molecule	Topological Ring-Current Intensity in Rings					Reference Source
	A	B	C	D	E	
Seven Rings (Continued)						
	1.022	0.508	1.183	1.161	1.184	Ref. 76
	1.332	1.031	1.446	–	–	Refs. 76, 77 & 78
	0.577	0.410	0.820	0.905	–	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.078	0.877	1.041	0.232	–	R. B. Mallion, unpublished
	1.077	0.876	1.043	0.233	–	R. B. Mallion, unpublished
	1.460	1.038	–	–	–	Refs. 68* & 70

TABLE X. Topological Ring-Currents in Eight-Ring Benzenoid Hydrocarbons

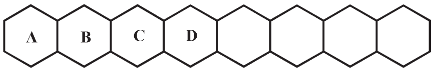
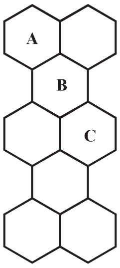
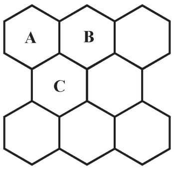
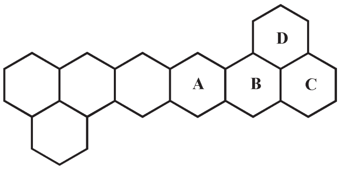
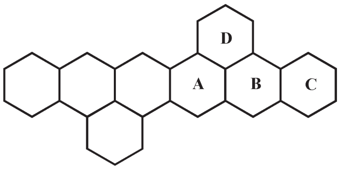
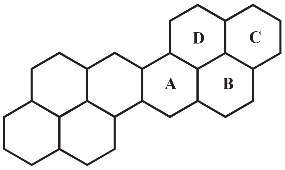
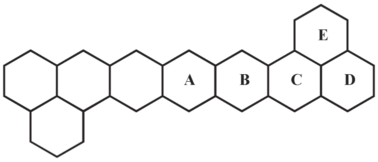
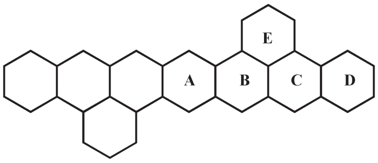
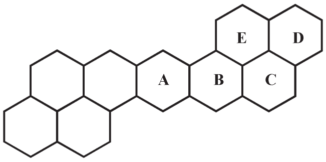
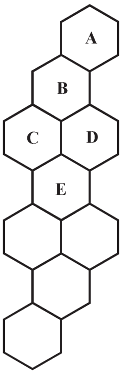
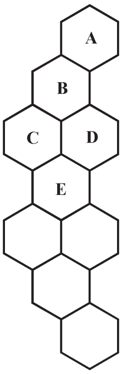
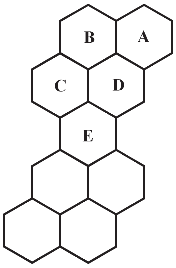
Molecule	Topological Ring-Current Intensity in Rings				Reference Source
	A	B	C	D	
Eight Rings					
	1.040	1.279	1.342	1.358	Refs. 62 & 71
	0.947	0.321	0.908	–	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	0.967	1.000	0.442	–	(Partly) Ref. 77, and the rest: R. B. Mallion, unpublished
	0.662	0.424	0.796	0.895	R. B. Mallion, unpublished
	0.363	0.784	1.018	1.013	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.355	0.885	1.313	1.094	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished

TABLE XI. Topological Ring-Currents in Nine-Ring Benzenoid Hydrocarbons (continued in Table XII)

Molecule	Topological Ring-Current Intensity in Rings					Reference Source
	A	B	C	D	E	
Nine Rings						
	0.776	0.704	0.434	0.785	0.890	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	0.574	0.405	0.739	0.985	1.002	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.447	1.252	0.813	1.279	1.100	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.195	1.270	0.926	1.131	1.377	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.193	1.244	0.867	1.173	1.345	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	1.194	0.948	1.207	0.874	0.311	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished

(Nine-Ring Benzenoid Hydrocarbons are continued in Table XII.)

TABLE XII. Topological Ring-Currents in Nine-Ring Benzenoid Hydrocarbons (continued from Table XI) and in Ten-Ring and Eleven-Ring Benzenoid Hydrocarbons

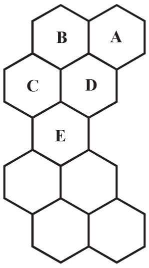
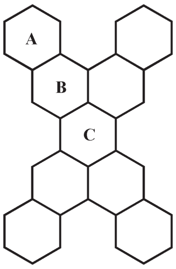
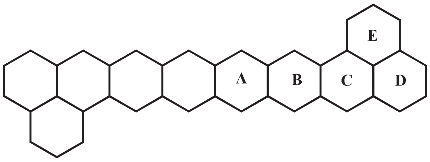
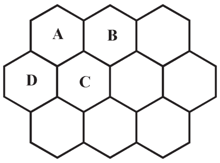
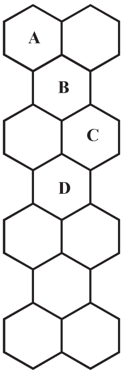
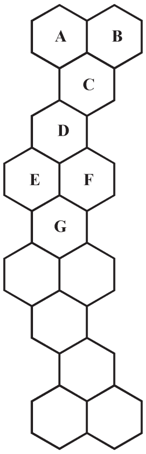
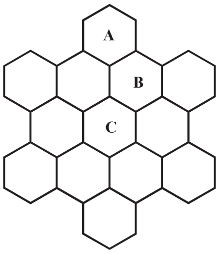
Molecule	Topological Ring-Current Intensity in Rings					Reference Source
	A	B	C	D	E	
Nine Rings (Continued)						
	1.194	0.944	1.197	0.880	0.311	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished
	*1.101*	*0.996*	*0.214*	–	–	R. B. Mallion, unpublished **Non-Planar**† **Molecule** (Ha4 Protons)[69]
Ten Rings						
	0.832	0.726	0.438	0.779	0.888	R. B. Mallion, unpublished
	1.339	1.786	1.307	1.665	–	R. B. Mallion, unpublished
Eleven Rings						
	0.938	0.354	0.905	0.447	–	(Partly) Refs. 77 & 78, and the rest: R. B. Mallion, unpublished

TABLE XIII. Topological Ring-Currents in Thirteen-Ring and Nineteen-Ring Benzenoid Hydrocarbons

Thirteen Rings

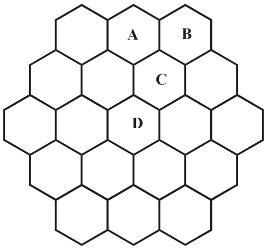


Topological Ring-Current Intensity in Rings							Reference Source
A	B	C	D	E	F	G	
0.895	0.824	0.462	0.640	0.846	0.968	0.706	Ref. 77



Topological Ring-Current Intensity in Rings			Reference Source
A	B	C	
1.34*	0.85*	1.81*	Ref. 68*

Nineteen Rings



Topological Ring-Current Intensity in Rings				
A	B	C	D	Reference Source
2.15*	1.49*	1.80*	2.44*	Ref. 68*

VII), Clar writes (on page 104 of Ref. 80): "The fixed double bonds in the zethrene series can be proved by the ^{1}H-NMR evidence..." and "...the fixed double bonds... belong to empty rings." The author was privileged to have had direct correspondence on some of these matters with the late Professor Clar in the early 1970s, immediately before and after his retirement. When the topological ring-current intensities for the 5th and 6th structures of Table X were reported to him in a letter from the author, Professor Clar wrote back:[81] "I was interested to learn that your calculation leads to the same results as the strict application of the aromatic sextet".

The data in Tables I–XIII are thus presented for further evaluation.

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SAŽETAK

Topološke struje prstenova u kondenziranim benzenoidnim ugljikovodicima

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Topološka struja prstena definirana je kao relativni intenzitet π-elektronske struje u prstenu kondenziranog benzenoidnog ugljikovodika, izračunat (i) najjednostavnijom Hückel-London-Pople-McWeeny metodom, (ii) iz molekulske geometrije s pravilnim heksagonima ugljikovih atoma, i (iii) izražen omjerom prema intenzitetu struje, izračunatom istom metodom, za molekulu benzena. Za zadani benzenoidni ugljikovodik tako definirana topološka struja neovisna je o subjektivnim (i drugim) parametrima i predstavlja čisti graf-teorijski indeks, potpuno određen samo matricom susjedstva grafa koji prikazuje povezanost ugljikovih atoma u benzenoidnoj molekuli. U radu su tabelirane sve poznate vrijednosti topoloških struja – dosad objavljene i neke nove – u svrhu buduće ocjene i usporedbe s drugim graf-teorijskim indeksima koji pojedinačno karakteriziraju prstenove kondenziranog benzenoidnog ugljikovodika.