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Conference Paper

A Theoretical Information Approach to Ring and Total Aromaticity in Ground and Excited States*

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Applying the Shannon equation to the density matrix of a molecule, an information index is specified for the quantitative estimation of the ring and total aromaticity of molecules in ground and excited states. The approach is applicable within each LCAO-method. The information index reproduces well the classification of molecules as aromatic, nonaromatic, and antiaromatic. It also correlates with results of other authors obtained by radically different approaches. A tendency is found for the aromaticity of aromatic molecules to decrease and of antiaromatic molecules to increase when the molecule is excited to the S_1 -state.

INTRODUCTION

The phenomenon of aromaticity, is of particular interest in contemporary chemistry. Numerous attempts have been made to generalize the classical rule of Hückel to polycyclic condensed molecules¹⁻⁵. The conditions were specified for nonplanar conjugated systems to display aromaticity⁶. A quantitative estimate of the aromatic character of molecules has been introduced, on the basis of their resonance energy⁷⁻¹³, using their NMR-spectra^{14,15}, molecular geometry^{16,17}, the distribution of the π -electron charges on atoms¹⁸, the concept of conjugated π -electron circuits⁴, etc. The so-called ring aromaticity^{19,20}, i. e. the aromatic character of different benzene fragments in polycyclic aromatic molecules, is also an object of study along with the total aromaticity of molecules.

The experimental and theoretical studies^{18,21} show that electron delocalization, and aromaticity in particular, are related to two characteristic factors: a) a decrease in the alternation of the single and double bonds; b) a decrease in the differences between the π -electron charges on atoms which results in intensified ring currents throughout the different ring fragments. All this results in a more even electron distribution on atoms and bonds in the molecule M or molecular fragment M_i . Conversely, molecules with an electron density, that is strongly localized on atoms (or bonds) are as a rule very reactive, i. e. low aromatic. According to the Information Theory, however, the most general definition of the notion of information is based on the unevenness in the distribution of matter or energy in a given system²², i. e. information is a measure of the deviation of the system from the most probable uniform distribution²³.

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Hence, it is logical to suppose that the information content, calculated on the basis of a set of quantities characterizing the electron (or energy) distribution, could also be used to estimate the aromaticity of molecules (M) or their fragments (M_i).

THE METHOD

The electron distribution in molecules can be described by means of the reduced density matrix (i.e. the one-particle matrix) which in the LCAO — approximation is presented by the so-called charge — bond order matrix²⁴. Within some LCAO methods like EHT, PPP, CNDO, etc., it is possible to define an analogous matrix for the electron energy distribution over AO's or between them²⁵. These quantum-chemical matrices — $Q(Q_{11}, Q_{12}, \dots, Q_{\mu\nu}, \dots)$ give information on the character of the distribution of the matter (electrons) or energy in a molecule. If the elements $Q_{\mu\nu}$ are transformed:

$$\frac{Q_{\mu\nu}}{A} = P_i, \quad \text{where} \quad A = \sum_{\mu, \nu} Q_{\mu\nu} \quad (1)$$

then the quantities $\{P_i\}$ ($i \in < 1, k >$ and $\sum P_i = 1$) can be regarded as relative characteristics of the electron (or energy) distribution over and between AO's, which for each matrix (i.e. for each M or M_i in the electron state α) is normalized to a unity. Moreover, the distribution has, although indirectly, a probabilistic character²⁶ since the elements (i.e. the charges and bond orders) reflect the probability of the electron distribution over and between AO's²⁴. According to the Information Theory²⁷, a mean entropy $H(P)$ corresponds to each probability distribution $P(P_1, P_2, \dots, P_1, \dots, P_k)$:

$$H(P) = - \sum_{i=1}^k P_i \log_2 P_i \quad (2)$$

The only assumption in the present work is that equation (2) is valid also for the probability distribution defined by eqn. (1). This assumption is made following the principal idea of the work as given in the first chapter.

The uniform distribution $P_1 = P_2 = \dots = P_k = P$, has a maximum entropy:

$$H_{\max}(P) = \log_2 k \quad (3)$$

The information content of the system $I(\alpha)$ is:

$$I(\alpha) = H_{\max}(P) - H(P) \quad (4)$$

Replacing eqns. (3) and (2) in eqn. (4), and taking into account eqn. (1) we obtain:

$$I(\alpha) = \log_2 \left(\frac{k}{A} \right) + \frac{1}{A} \sum_{\mu\nu} Q_{\mu\nu}(\alpha) \log_2 Q_{\mu\nu}(\alpha) \quad (5)$$

Here $I(\alpha)$ is the information content of the molecule (or fragment), defined as a measure of the unevenness in the distribution of electrons (the entries of the charge — bond order matrix $P_{\mu\nu}$) or energy ($E_{\mu\nu}$ — matrix²⁵). $P_{\mu\nu}$ — matrices can be calculated within each LCAO-MO-CI method for an arbitrary electron state α , while $E_{\mu\nu}$ ^{25,28} — only under the restrictions of ZDO and EHT — approximations²⁴.

Conversely, we shall define the evenness of distribution by means of a reciprocal index $\tilde{I}(\alpha)$ called the *information index of aromaticity* (delocalization) of molecule M or fragment M_i in the ground ($\alpha = S_0$) or the excited ($\alpha = S_1$) states:

$$\tilde{I}(\alpha) = I^B(0)/I^M(\text{or } M_i)(\alpha) \quad (6)$$

Here $I^B(0)$ is the reference information content of benzene in the ground state ($\alpha = S_0$, $Q_{\mu\nu} = P_{\mu\nu}$ or $E_{\mu\nu}$). $I^{M_i}(\alpha)$ is also calculated by eqn. (5) but the summation is over $(\mu, \nu) \in M_i$ only. $I^M(\alpha)$ is measured in bits, while $\tilde{I}(\alpha)$ is a dimensionless parameter: since $I^M(\alpha) \geq I^B(0)$, then $0 < \tilde{I}(\alpha) \leq 1$.

RESULTS AND DISCUSSION

In this first communication, the calculation of $I(\alpha)$ by eqn. (5) is made under the following conditions: 1) $Q_{\mu\nu} \equiv P_{\mu\nu}$ only; 2) $P_{\mu\nu}$ -matrix is calculated in a π -electron approximation using the SCF-CI-PPP method including all monoexcited configurations²⁴; 3) $\alpha = S_0, S_1$; 4) The summation over (μ, ν) in eqn. (5) comprises only chemically bonded atoms, as well as the entries $P_{\mu\nu}$, for which $\mu \geq \nu$.

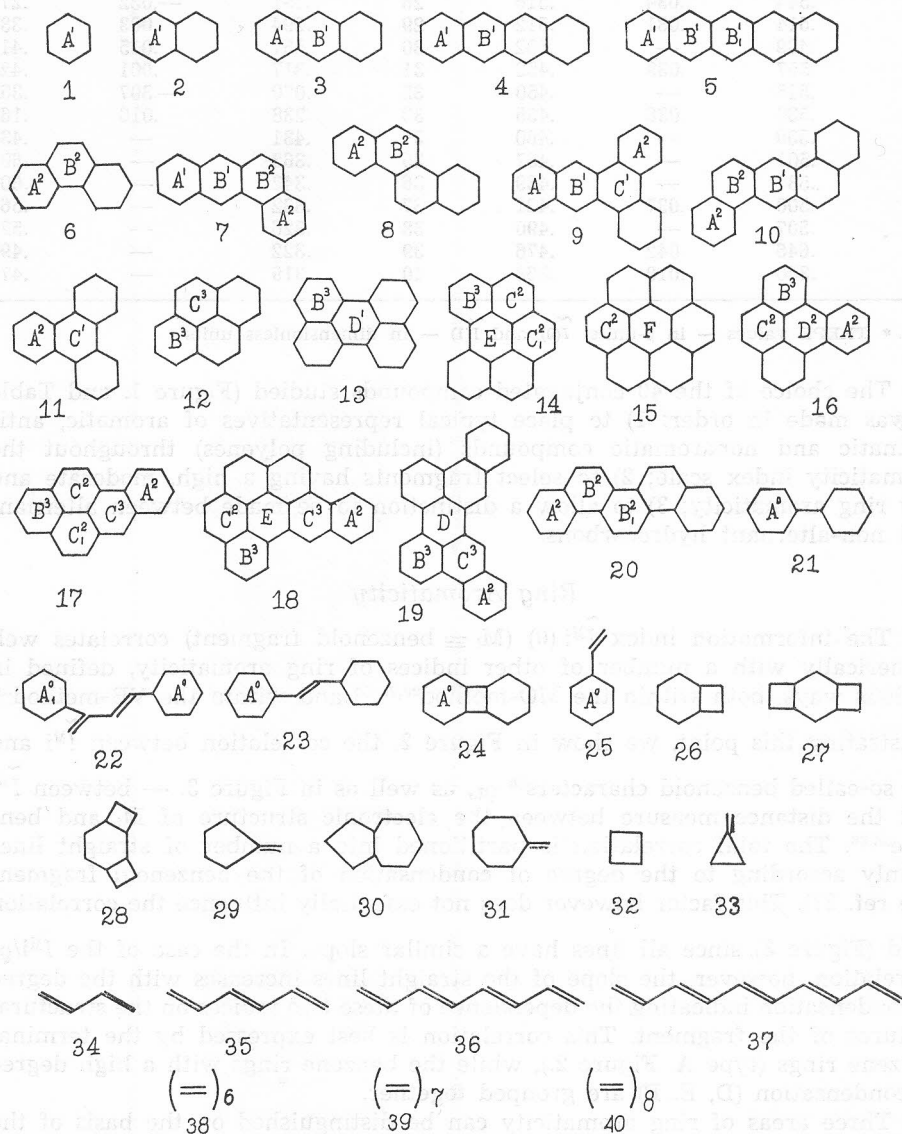


Figure 1. The compounds under study.

TABLE I

The Information Index of Aromaticity \tilde{I} in the S_0 and S_1 State and the Topological Resonance Energy of One Electron (TREPE) of the Compounds From Figure 1*

No.	$\tilde{I}(0)$	TREPE	$\tilde{I}(1)$	No.	$\tilde{I}(0)$	TREPE	$\tilde{I}(1)$
1	1.000	.046	.355	26	.232	-.049	.360
2	.625	.039	.408	27	.152	-.079	.285
3	.544	.034	.516	28	.191	-.032	.272
4	.514	.031	.512	29	.294	.003	.333
5	.499	—	.502	30	.557	.015	.419
6	.557	.039	.452	31	.317	.001	.421
7	.515	—	.450	32	.070	-.307	.355
8	.530	.038	.455	33	.238	.016	.168
9	.509	—	.460	34	.431	—	.432
10	.501	—	.457	35	.362	—	.601
11	.537	—	.469	36	.342	—	.600
12	.500	.037	.421	37	.332	—	.561
13	.507	—	.490	38	.326	—	.524
21	.646	.042	.476	39	.322	—	.495
24	.360	.010	.368	40	.319	—	.471

* TREPE values — in β -units; $\tilde{I}(0)$ and $\tilde{I}(1)$ — in dimensionless units

The choice of the 40 conjugated compounds studied (Figure 1. and Table I) was made in order: 1) to place typical representatives of aromatic, anti-aromatic and nonaromatic compounds (including polyenes) throughout the aromaticity index scale; 2) to select fragments having a high, moderate and low ring aromaticity; 3) to allow a distinction to be made between alternant and non-alternant hydrocarbons.

Ring Aromaticity

The information index $\tilde{I}^{M_i}(0)$ ($M_i \equiv$ benzenoid fragment) correlates well numerically with a number of other indices of ring aromaticity, defined in various ways, both within the MO-method^{20,29-33} and within the VB-method³⁴.

Illustrating this point, we show in Figure 2. the correlation between \tilde{I}^{M_i} and the so-called benzenoid characters²⁰ Q_L , as well as in Figure 3. — between \tilde{I}^{M_i} and the distance measure between the electronic structure of M_i and benzene^{35,36}. The total correlation is partitioned into a number of straight lines mainly according to the degree of condensation of the benzenoid fragment (see ref. 37). This factor however does not essentially influence the correlation \tilde{I}^{M_i}/d (Figure 3) since all lines have a similar slope. In the case of the \tilde{I}^{M_i}/Q_L correlation, however, the slope of the straight lines increases with the degree of condensation indicating the dependence of these two indices on the structural features of the fragment. This correlation is best expressed by the terminal benzene rings (type A, Figure 2.), while the benzene rings with a high degree of condensation (D, E, F) are grouped together.

Three areas of ring aromaticity can be distinguished on the basis of the information index: high — $\tilde{I}^{M_i} \in (1 - 0.666)$; moderate — $\tilde{I}^{M_i} \in (0.666 - 0.333)$;

and low ring aromaticity — $\tilde{I}^M_i \in (0.333 - 0)$. The first area comprises the benzenoid fragments of polyphenyls, biphenylpolyenes and A-type of fragments in polyphenylenes (biphenylene, triphenylene), i. e. all fragments with full aromatic sextets according to Clar³⁸.

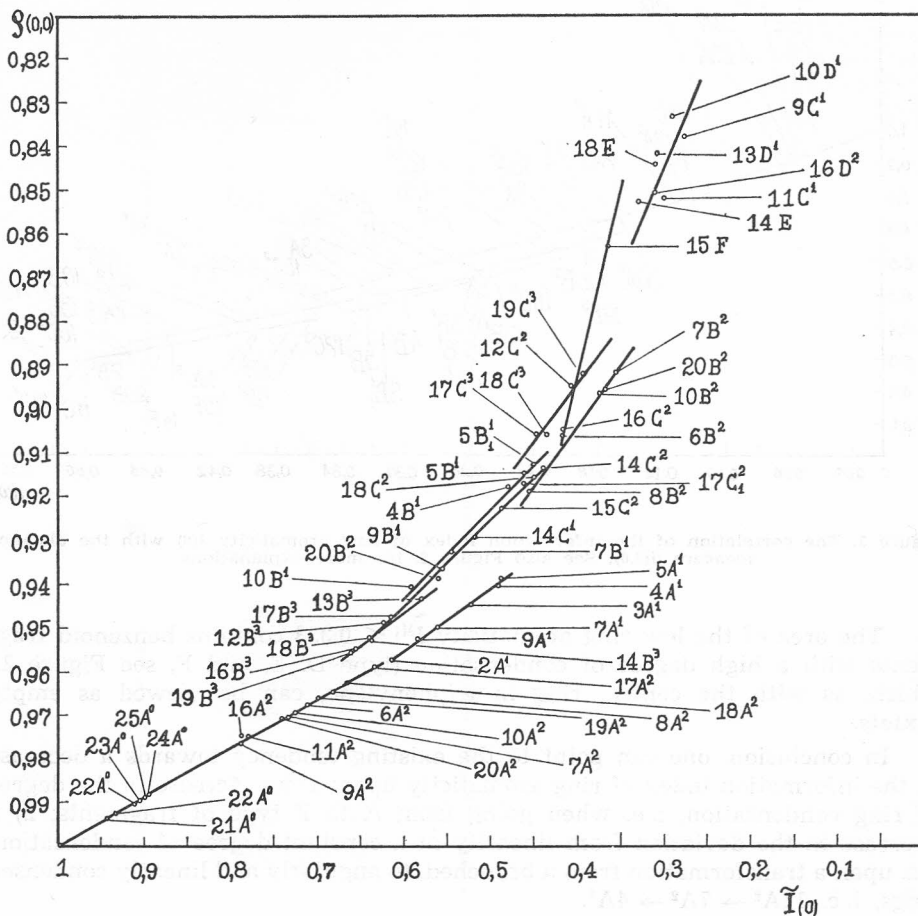


Figure 2. The correlation between the information index for ring aromaticity $I(0)$ and the benzenoid character order $\rho(0,0)$. A, B, C, D, E, and F — a benzene ring condensed on 1, 2, 3, 4, 5, and 6 sites, respectively (see also Figure 1); the number standing in front of the capital letter is that from Figure 1; the right superscript signifies the cases of benzene (0); linear (1), angular (2), and more complex (3) condensation of the benzene fragment, respectively.

The angularly condensed benzenoid fragments of type A² (i. e. compounds 6, 7, 11, etc. in Figure 2.) have a higher information index of ring aromaticity than the linearly condensed terminal fragments (i. e. fragments A¹ in compounds 3, 4, 5, etc.). \tilde{I}^M_i of angularly condensed fragments lies within the first area, while that of linearly condensed fragments lies in the second area of the aromaticity scale. A moderate ring aromaticity is also displayed by benzenoid fragments condensed with 2 and 3 other rings i. e. types B and C).

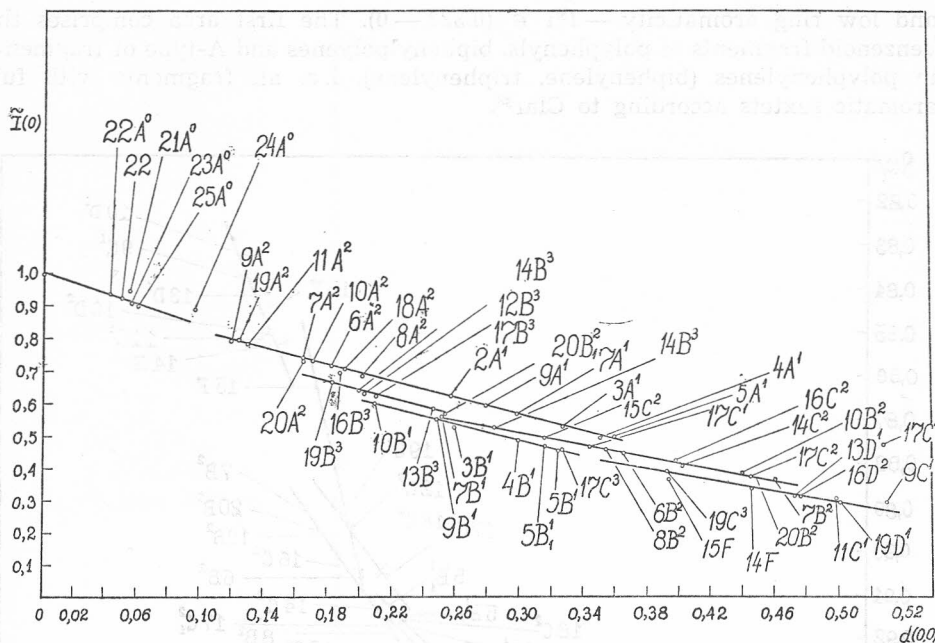


Figure 3. The correlation of the information index of ring aromaticity $\tilde{I}(0)$ with the distance measure $d(0,0)$. See also Figure 2. for more explanations.

The area of the low ring aromaticity $\tilde{I}^M_i < 0.333$ contains benzenoid fragments with a high degree of condensation (type D, E, and F, see Figure 2.) which, as with the central ring in triphenylene, can be viewed as empty sextets.

In conclusion, one can point to the existing tendency towards a decrease in the information index of ring aromaticity upon: 1) an increase in the degree of ring condensation, i. e. when going from A to F type of fragments; 2) a decrease in the deviation from linearity at a constant degree of condensation, i. e. upon a transformation from a branched, to angularly and linearly condensed rings, i. e. $11A^2 \rightarrow 7A^2 \rightarrow 4A^1$.

Total Aromaticity in the Ground State

The information index of total aromaticity, obtained for the ground state of some molecules, $\tilde{I}^M(0) \equiv \tilde{I}(0)$, is shown in Table I. The selection of test compounds allows the grouping of $\tilde{I}(0)$ values into three classes:

aromatic: $\tilde{I} \approx 1-0.45$ (compounds 1-13, 21, 30)

nonaromatic: $\tilde{I} \approx 0.45-0.30$ (compounds 20, 24, 31 and 34-40)

antiaromatic: $\tilde{I} \approx 0.30-0$ (compounds 26-28, 32, 33)

It is important to notice that this classification of the compounds under study coincides in principle with their classification made on the basis of other criteria of quite a different nature like resonance energy (REPE)⁷⁻⁹, topological resonance energy (TREPE)¹⁰, conjugated π -electron circuits⁴, etc.

As an illustration, a comparison between $\tilde{I}(0)$ and TREPE is made in Table I. A negligible difference between the two indices appears solely at biphenylene (No 24, Figure 1.) and methylenecyclopropene (No 33) which belong to the nonaromatic and antiaromatic part of our scale, respectively, while being low aromatic it on the TREPE scale. The information estimate for antiaromaticity of No 33, however, is confirmed by the data for resonance energy by Hess and Schaad⁸ (REPE = 0.005 β), and similarly that for biphenylene — by the Randić aromaticity index⁴ ($\sim 15\%$ aromaticity). Some discrepancy also occurs in the relative ordering of the aromatic compounds in the two scales, but such a situation appears even when comparing two aromaticity indices having a very similar nature, like resonance energy and topological resonance energy^{8,10}.

The specification of the non-aromatic part of the information scale within the range 0.30—0.45 was also confirmed by the values obtained for seven all-trans polyenes (C_4 to C_{16}), No 34—40 in Figure 1: $\tilde{I}(0) = 0.32$ — 0.43, since by definition the non-aromatic compounds should be similar to acyclic polyenes⁷.

The analysis of the data from Table I enables the examination of the influence of some essential structural factors on $\tilde{I}(0)$. It is found, in accordance with other aromaticity scales^{8,10}, that $\tilde{I}(0)$ decreases with the increase in the number of benzenoid fragments (R), the decrease being less and less at every new fragment:

R	1	2	3	4	5
$\tilde{I}(0)$	1	0.60—0.65	0.54—0.56	0.50—0.54	0.50—0.51

This tendency is well manifested by polyacenes (Table I, Figure 1.) where the $\tilde{I}(0)$ index predicts a minimum difference in the aromatic character of higher members and a boundary value for infinite polyacenes ≈ 0.45 .

In the case of isomeric hydrocarbons having the same number of benzene rings, $\tilde{I}(0)$ increases with the change of condensation from a linear to an angular, biangular and branched one. For instance, for compounds Nos. 4, 7, 8, and 11, $\tilde{I}(0) = 0.514, 0.516, 0.530,$ and $0.537,$ respectively.

The mixing of $(4n + 2)$ with $4n-$ ring systems (Nos. 24, 26—28) results in a decrease in $\tilde{I}(0)$ values which gradually change their position from the middle of the nonaromatic region for biphenylene (No 24) to the highly antiaromatic region, going from No 26 to No 27 to No 28. The predicted higher antiaromaticity of No 27 in comparison with No 28 can be explained both by the influence of the cyclobutadiene rings being stronger through the *para*-, than through *meta*- position, and by the abovementioned tendency of aromaticity to strengthen on going from a linear to an angular condensation.

It is easily seen from Table I and eqn. (6) that the isomeric alternant hydrocarbons have a higher information index $\tilde{I}(0)$ than the corresponding non-alternant compounds (compare for instance 33, 34; 29, 35; 31, 36). This result is natural taking into account the complete evenness in the distribution of π -electron charges in the alternant compounds. Nevertheless, azulene (No 30) has an information index of aromaticity substantially higher than that of decapentaene in accordance with the well known aromatic properties of azulene.

Aromaticity in Excited State

The values of the information aromaticity index $\tilde{I}(1)$ for S_1 (fluorescent) excited state of the molecules studied were also calculated and are presented in Table I.

It is worthwhile noticing that the index of benzene molecule decreases sharply on excitation ($1 \rightarrow 0.355$) and falls in the nonaromatic area near to its border with the antiaromatic area. This result is supported by the experimental geometry of benzene in the S_1 — state³⁹: $R_{C-C} = 1.434 \text{ \AA}$ instead of 1.397 \AA for the S_0 — state. This considerable stretching of the six C—C bonds reduces the overlap between the π -orbitals and results in a decrease in conjugation and aromaticity. The aromaticity index of Julg¹⁸ cannot be used to predict the lowering in the aromatic properties of benzene in the S_1 — state, indicating the same aromaticity for the S_0 , S_1 , and T_1 — state.

A lowering in the aromatic character on such excitation is predicted by $\tilde{I}(1)$ for nearly all aromatic compounds under examination, some of which fall into the nonaromatic area. Very surprisingly, the benzene and cyclobutadiene molecules, located in the S_0 — state at the two ends of \tilde{I} — scale, were found to have in the S_1 — state the same aromaticity index $\tilde{I}(1) = 0.355$. The tendency towards a similar aromatic character, which we have found for the aromatic and antiaromatic compounds on excitation to S_1 — state does not however seem so strange in the light of the results of Baird⁴⁰ for the T_1 ($\pi\pi^*$) state. Generalizing the Dewar resonance energy notion and utilizing the NNDO method, Baird has shown that aromaticity reverses in $3_{\pi\pi^*}$ state ($4n$ -rings display »aromatic« character whereas $(4n + 2)$ -systems display »antiaromaticity«). Related to this, it is likely that the aromaticity of the S_1 — state is intermediate between the aromaticities of the S_0 — and T_1 — states.

CONCLUSION

1. A new approach towards the aromaticity problem has been proposed which combines Information Theory with quantum chemistry introducing an information aromaticity index \tilde{I} . Differing from other indices, \tilde{I} is not deduced from any specific chemical or physical notions or models but automatically follows from the application of the Shannon equation to the entries of the charge- band order matrix. The information index has the same analytical form for total and for ring aromaticity and is applicable, in principle, to any LCAO method and any electronic state.

2. The information index on ring aromaticity correlates well numerically with a number of other indices of ring aromaticity, defined by various ways within MO and VB methods, as well as with the ideas of Clar for »empty« and »full« benzenoid fragments.

3. The information index of total aromaticity $\tilde{I}(0)$ enables the correct grouping of conjugated compounds into three classes: aromatic, nonaromatic, and antiaromatic. The first class of compounds is characterized by a low information content, or respectively, by an uniformity in the distribution of electron density over atoms and bonds. The influence of some essential structural factors on $\tilde{I}(0)$ has been studied, as well as the mutual influence of $(4n + 2)$ and $4n$ -rings.

4. It has been shown that the information index $\tilde{I}(0)$ of the non-aromatic non-alternant hydrocarbons is smaller than that of the corresponding alternant hydrocarbons, due to the uniform distribution of the π -electron charges in the latter hydrocarbons.

5. A tendency towards a similar aromatic character of the aromatic and antiaromatic compounds is established, resulting from the excitation from the ground to S_1 (fluorescent) state.

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SAŽETAK

Teorijsko-informatički pristup aromatičnosti prstena i ukupnoj aromatičnosti za temeljno i pobuđena stanja

F. Fratev, D. Bonchev i V. Enchev

Primjenom Shannonove jednadžbe na matricu elektronske gustoće molekule dobiven je informacijski indeks kojim se kvantitativno ocjenjuje aromatičnost prstena i ukupna aromatičnost molekula u temeljnom i pobuđenim stanjima. Pristup je primjenljiv za bilo koji LKAO-postupak. Informacijski indeks dobro reproducira podjelu molekula na aromatične, nearomatične i antiaromatične, i korelira s rezultatima drugih autora dobivenima potpuno drugačijim pristupima. Pri pobuđivanju molekule u S_1 -stanje zapaženo je da se aromatičnost aromatičnih molekula smanjuje a antiaromatičnih povećava.

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