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Article

Density, Degeneracy, Delocalization-Based Index of Aromaticity (D_3BIA)

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A aromaticidade tem sido exaustivamente discutida e continua sendo um tema misterioso. Nesse trabalho é proposto um novo índice de aromaticidade chamado índice baseado na densidade-degenerescência-deslocalização ou, simplesmente, D_3BIA, numa tentativa de lançar nova introspecção sobre esse tema. Esse índice é baseado na teoria de átomos em moléculas (AIM) e, de certa forma, é suportado pela teoria dos spins acoplandos (SC). A aromaticidade diminui com o número de heteroátomos na molécula aromática, pois a degenerescência diminui, e diminui com o aumento do tamanho do anel do composto aromático porque desfavorece a sobreposição dos estados monoeletrônicos. A relação entre planaridade do anel, sua densidade eletrônica e aromaticidade é também observada. A interação atrativa da ressonância de 6 elétrons π no diânion ciclobutadieno compensa sua interação repulsiva carbono-carbono enquanto no seu parente dicatiônico a ressonância de 2 elétrons π é insuficiente para contrabalancear sua interação repulsiva e adota uma estrutura não-plana.

Aromaticity has been exhaustedly discussed for several years and it remains as a misterious issue. In this work it is proposed a new index of aromaticity named density, degeneracy and delocalization-based index of aromaticity or simply D_3BIA in an attempt to cast new insight and perspective over this theme. This index is based on AIM (atoms in molecules) theory and it is somewhat supported by SC (spin-coupled) theory. Aromaticity decreases as the number of heteroatoms in the aromatic molecule increases since degeneracy decreases and it decreases as the ring size of an aromatic compound increases because it disfavors overlap of single-electron states. The relation between planar structures, electron density and aromaticity is also observed. The attractive interaction of 6π-electron resonance in cyclobutadiene dianion compensate its carbon-to-carbon repulsive interaction while in its dicationic parent the 2π-electron resonance is insufficient to counterbalance its carbon-to-carbon repulsive interaction and it adopts a puckered structure.

Keywords: delocalization index; degeneracy; ring density; aromaticity

Introduction

In the nineteenth century benzene was the pivot of the aromatic empiricism.[1] After its early studies by Couper and Loschmidt,[2] Kekulé proposed the most important theory about benzene: the oscillation hypothesis.[3] Other theories at that time were Claus'centric hypothesis,[4] Bayer's reformulations of centric benzene,[5] Dewar's hypothesis[6] and Ingold's bridged formula.[7]

In the early twentieth century quantum theory study gave rise to a novel hypothesis for benzene. From a molecular orbital (MO) study of benzene and other unsaturated cyclic systems, Hückel[8] arrived at his famous rule for aromaticity. Two years later, Pauling and Wheland's[9] valence bond (VB) study of benzene (and naphtalene) gave the same result by following Hückel's premises and Slater method. Their simpler treatment was based on resonance[10] among independent Kekulé and Dewar canonical structures and became known as resonance hybrid hypothesis.[9] However, for cyclobutadiene both theories gave completely different results.[8,11] Hückel's MO study predicted the stability of other aromatic compounds and zero stability for conjugated cyclic systems such as cyclobutadiene.[8] The

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latter ones were ascribed by Breslow and Dewar to have anti-aromatic character.[12]

It was established that aromatic species have π electrons in delocalized bonds, uniform geometry and special stability with respect to an open chain referential. Conversely, anti-aromatic systems have π electrons in localized bonds and non-uniform geometries in alternate single and double bonds.[13] Several criteria to evaluate aromaticity were created so far: energetic criterion,[14] geometric criterion[15] and magnetic criterion.[16] However, Schleyer and Jiao[17] stated that magnetic susceptibility is the unique criterion applied to aromaticity. Schleyer *et al.*[18] also remarked that downfield proton chemical shifts are not a reliable aromaticity criterion and that aromaticity phenomenon can be statistically regarded as multi-dimensional.[19] Many different magnetic criteria have appeared so far, based on magnetic shielding or ring current.[20]

Within MO theory, the aromatic character of benzene is explained through delocalized orbitals. Nevertheless by using the spin coupled valence bond theory (SCVB), Gerratt *et al.*[21] established that all the six π electrons of benzene are localized and symmetrically distorted towards neighboring carbon atoms on each side and possess the same energy and shape. Other studied aromatic molecules have similar features.[22] Within the description SCVB, the stability of aromatic systems is ascribed to the modes of coupling the electron spins which resembles Pauling's resonance structures.[21,23] Hiberty *et al.*[24] demonstrated that delocalization of the π-electrons in benzene is energetically unfavorable and the σ-framework determines the structural symmetry of benzene. They[25] stated that π electronic system distorts benzene to D_{3h} symmetry while σ-framework keeps it in D_{6h}, although Havenith *et al.*[14f] have established the necessity of resonance to obtain a fully symmetric benzene molecule. Havenith[26a] demonstrated that resonance between Kekulé structures does not influence the magnetic and electric properties of benzene and that ring currents exist in its D_{3h} symmetry.[26] Within modern VB scope Cooper *et al.*[27] obtained the following order of degree of aromaticity: $C_6H_6 \sim B_6 > N_6 > Al_6 \sim Si_6H_6 > P_6$.

Atoms in molecules (AIM) theory has also been applied to study aromaticity.[30] Bader *et al.*[28] found out a greater π density delocalization in cyclic unsaturated hydrocarbons than that in acyclic ones. Solà *et al.*[29] related the delocalization index[30] (DI) to different aromatic criteria. They introduced a new local aromatic criterion: the paradelocalization index (PDI). Hernández-Trujillo and Matta[31] also proposed a geometric criterion that takes into account the DI as a measure of electron-sharing alternation.

From the AIM theory,[32] we propose a new criterion for aromaticity based on the electronic density in the ring, on the degree of delocalization uniformity and on the degree of degeneracy of atoms in the ring, named D_3BIA (density, degeneracy and delocalization-based index of aromaticity). This criterion casts new light on the way aromaticity has been reasoned.

Computational Methods

All calculations were performed using the GAUSSIAN 2003 package.[33] The geometries were optimized in DFT level employing Becke three-parameter interchange functional[34] (B3) in conjunction with Lee-Yang-Parr[35] correlation functional (LYP) and the split valence basis set[36] 6-311++G**.

The AIM 2000 software[37] was used for charge density calculations from the electronic densities (ρ) obtained at B3LYP/6-311++G** level.

Rationale

Rationale on D_3BIA index was influenced by modern (VB) studies on aromaticity and particularities of some aromatic compounds.[38] The similarities of results between AIM and SC encouraged us to use the former since it provides us important and complementary information. The coherence between AIM and SC can be noticed from AIM results of benzene. The DI between carbon atoms in benzene is 1.39. Since DI between carbon atoms in ethane is 1.0, it is established that 0.39 e. from π system is delocalized in each C-C bond of benzene ring. This means that 0.61 from each $2p_z$ electron is localized in each carbon atom in benzene. This result matches with the SC one in which a $2p_z$ electron of benzene is localized and symmetrically distorted towards neighboring carbon atoms on each side.[21] Moreover, Gerratt *et al.*[21] remarked that distortion effects of $C(2p_z)$ orbitals are not larger than those of C-C π bonds in conjugated systems. From AIM calculations, DI's for hexatriene are 1.74 (double bond) and 1.14 (single bond). This indicates another convergence of results between SC and AIM theories since the latter shows that delocalization index in double bonds in acyclic conjugated systems is greater than that in benzene.

Pauling and Wheland[9] stated that benzene is represented by a linear combination of five independent canonical structures. This view is emphasized by SC theory,[21,23] in which a two-electrons spin coupling allows the description of the different possible resonance structures and generates the stability of aromatic systems.

From a more rigorous quantum mechanical standpoint,[39] benzene has no resonance[40] since there is no intersection of degenerate point group states. It means that benzene (D_{6h} symmetry) cannot be related to Kekulé (D_{3h} symmetry) or Dewar (D_{2h}) structures (see Electronic Supplementary Information). In this case, benzene stability is ascribed to maximum overlap among six degenerate single-electron states.[41]

Then, the existence of resonance in benzene depends on the rigor of the theory applied to it. By spin coupling π electrons, within same D_{6h} symmetry in SC, it is possible to associate the obtained stability with resonance of hybrid structures.[21] Otherwise, benzene molecule cannot be represented by "hybrids" of symmetries D_{3h} and D_{2h} since it is forbidden by point group symmetry rules.[42]

The index D_3BIA is based on the density in the ring, the degeneracy and the delocalization index of atoms in the ring. With respect to AIM theory, degeneracy is the similar energy of basins. Delocalization index (DI) is a measure of the number of electrons that are shared between two atoms or basins. All data are obtained from AIM theory.

Results and Discussion

All studied compounds are depicted in Scheme 1.

For an aromatic system, according to modern VB theory, the degeneracy of single-electron states plays an important role on aromaticity.[41] In AIM theory, the degeneracy can be reasoned in terms of energy of each atomic basin of atoms in the aromatic ring and also associated with its delocalization indexes of each atomic pair im the aromatic ring. The greater the uniformity of atomic energy and the DIs among atoms in the ring is, the greater is the degeneracy of atoms of the aromatic system.

The importance of the electron density in aromaticity arises from the following points: *(i)* the relative stability of three-membered rings is related to the electron density in the ring;[30] *(ii)* the overlap among (near) degenerate p_z single-electron states can be correlated to the electron density in the ring; *(iii)* the spin coupling to form Dewar structures can be correlated to the electron density in the ring.

The D_3BIA formula is:

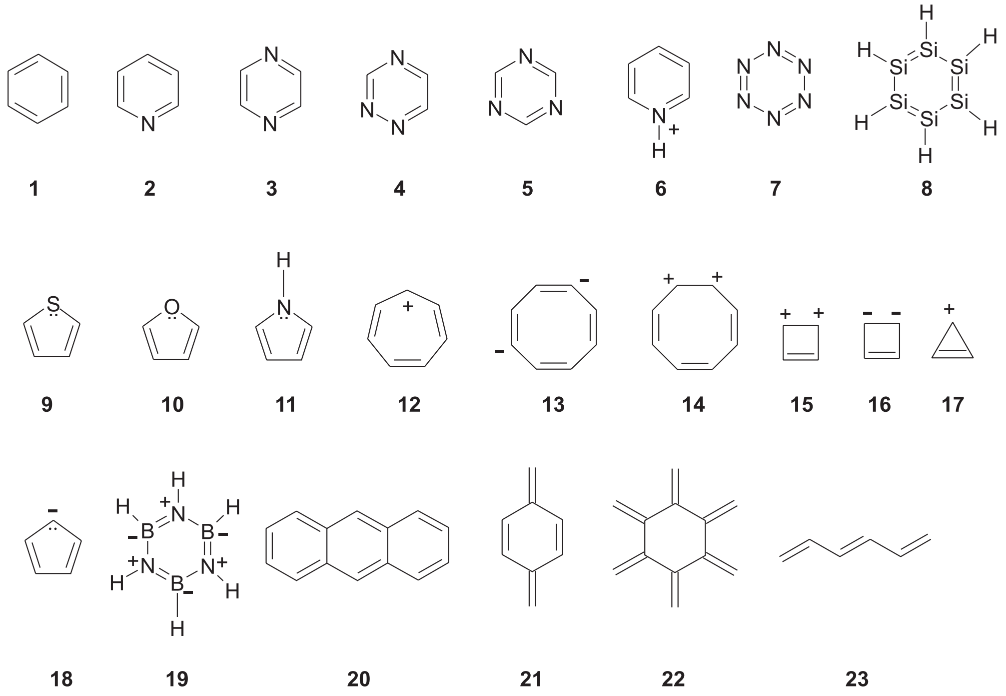
$$D_3\text{BIA} = [\text{RDF}][\text{DIU}]\delta \qquad (1)$$

The ring density factor (RDF) formula is:

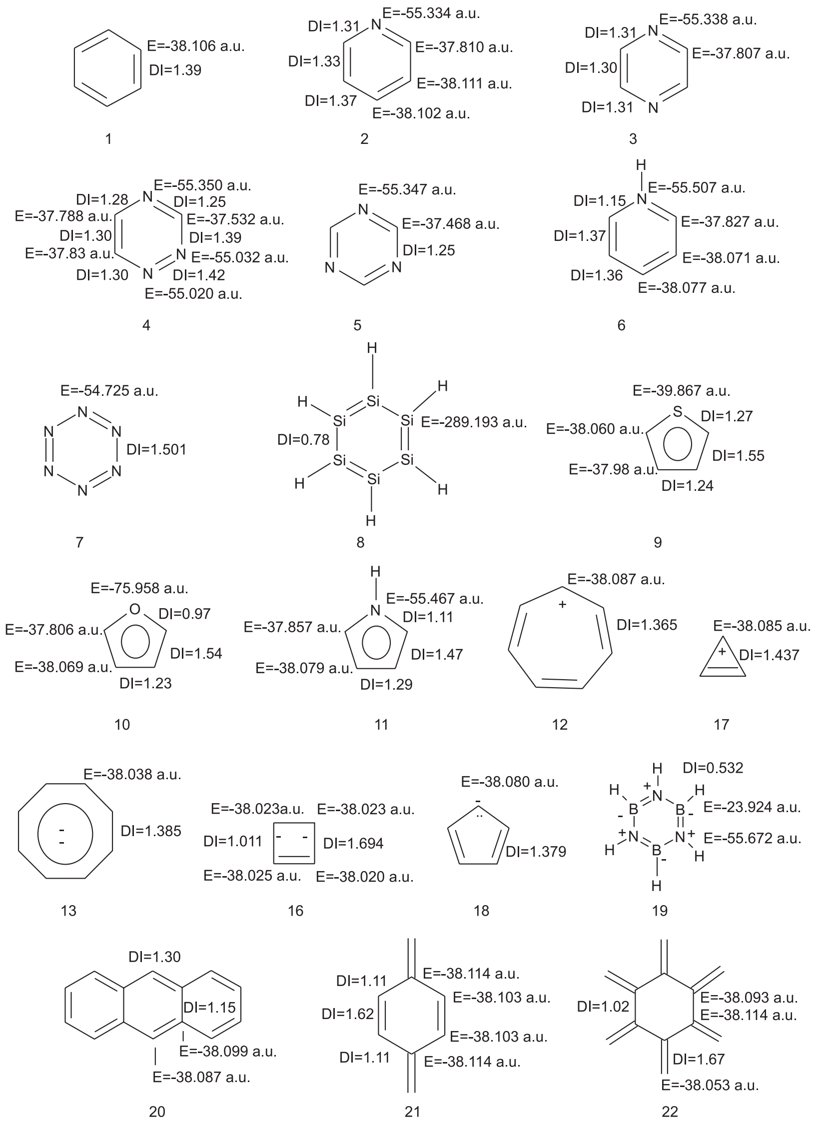
$$\text{RDF} = (1 + \lambda_2)\,\rho_{\text{RCP}} \qquad (2)$$

Where λ_2 is the mean eigenvalue of the density Hessian matrix from the bond critical point (BCP) towards the ring critical point (RCP) and ρ_{RCP} is the density value of ring critical point. One can see that the more negative is λ_2 the steeper is the curvature of the surface of the density at this direction.

AIM provides a delocalization index for each bond between vicinal atoms.[30,37] The delocalization index uniformity (*DIU*) can be correlated to the efficiency of the single-electron states interaction (or overlap). The



Scheme 1.



Scheme 2.

maximum degree of delocalization uniformity parallels the maximum overlap among single-electron states, which can be verified in benzene (**1**) (Scheme 2).

The delocalization index of uniformity (DIU) formula is:

$$DIU = 100 - \left(\frac{100\sigma}{\overline{DI}}\right) \quad (3)$$

Where σ is mean deviation and $\overline{\text{DI}}$ is mean DI of the ring.

The uniformity of delocalization is also taken into account in the degree of degeneracy to fine tune this parameter because a molecule may have atoms nearly degenerate, but with completely different delocalization indexes (see *p*-xylylene (**21**) in Scheme 2). Then, uniformity of delocalization is used to adjust the degree of degeneracy.

The formula of the degree of degeneracy (δ) is the number of degenerate atoms divided by the number of atoms in the ring. The δ takes into account the following requisites: *(i)* if all atoms of the ring are degenerate and if all of these atomic pairs have same delocalization indexes, the molecule has the maximum degree of degeneracy (δ=1); *(ii)* if the atoms of the atomic ring are near-degenerate (within range of 0.3 a.u.) and have near delocalization indexes (within range of 0.05) they may be regarded degenerate; *(iii)* if all atoms of the ring are near-degenerate and have completely different delocalization indexes (ΔI > 0.3) the molecule has the minimum degree of degeneracy (δ=0), where ΔI is the difference between DI's.

From D_3BIA formula (equation 1) *p*-xylylene (**21**) does not have aromaticity since it has δ=0 (requisite III). Hexaradialene (**22**) has no aromaticity either. It has no planar structure and no π electrons between C-C bonds in the ring (Scheme 2), as can be seen by its DI values (similar to single bonds).

In Table 1 it is depicted either the values of the individual parameters and D_3BIA values. Energy and DI values are also depicted in Scheme 2.

By analyzing D_3BIA values of compounds **1** to **4** in Table 1 it is remarkable that the decrease of degeneracy of single-electron states and aromaticity of the respective compound are related to the number of heteroatoms in the aromatic molecule. The more heteroatoms in the ring then, the smaller are the degeneracy and the aromaticity. The heteroatoms break uniformity of the electron density in the ring as one can see Figure 1. It is known from literature that benzene has different aromaticity from the corresponding aromatic compounds containing nitrogen atoms, *e.g.*, pyridine.[43] One also can see that D_3BIA value of 1,3,5-triazine (**5**) is greater than that from 1,2,4-triazine (**4**) since the former is more symmetric than the latter. Moreover, the pyridinium (**6**) has smaller D_3BIA value than that from non-protonated species (**2**) because the former lost some of delocalization index uniformity (DIU) and degree of degeneracy (δ) (see Scheme 2).

From the analysis of D_3BIA values (Table 1) of compounds **1**, **12** and **13** one can also notice that ring size and aromaticity are inversely related, where other parameters are kept constant. Moreover, compound **8** has smaller D_3BIA than that from compound **1** where C-C bond length (1.394 Å) in compound **1** is smaller than Si-Si bond length (2.219 Å) in compound **8**. However, Si_6H_6 is not a minimum in the potential energy surface. This reverse relation is probably due to decrease of the density in the ring which disfavors overlap of single-electron states.[41] In Figure 1 it is possible to see how electronic interaction inside the ring is stronger in benzene than in compounds **8** and **13** since there is only one Laplacian line inside benzene ring unlike **8** and **13**.

Table 1. Charge density of the ring critical point (ρ_{RCP}), eingenvalue of density Hessian matrix from BCP towards RCP ring (λ_2), ring density factor (RDF), degree of delocalization index uniformity (DIU), degree of degeneracy (δ), D_3BIA

Entry	RCP × 10^3 (a.u.)	λ_2	RDF × 10^3 (a.u.^{2})	DIU	δ	D_3BIA × 10^3
1	21.5	-0.54	9.9	1.000	1.00	9.9
2	23.5	-0.57	10.1	0.980	0.83	8.2
3	26.1	-0.62	9.9	0.996	0.67	6.6
4	26.9	-0.69	8.3	0.936	0.33	2.6
5	29.0	-0.69	9.0	1.000	0.50	4.5
6	22.0	-0.57	9.5	0.913	0.50	4.3
7	25.0	-0.92	2.0	1.000	1.00	2.0
8	3.7	-0.07	3.4	1.000	1.00	3.4
9	39.0	-0.42	22.6	0.887	0.40	8.0
10	53.0	-0.49	27.0	0.776	0.40	8.4
11	51.0	-0.50	25.5	0.860	0.40	8.8
12	9.2	-0.57	4.0	1.000	1.00	4.0
13	3.8	-0.48	2.0	1.000	1.00	2.0
16	98.5	-0.44	55.2	0.747	0.50	20.6
17	62.0 [b]	-0.47	32.9	1.000	1.00	32.9 [c]
18	48.2	-0.48	25.1	1.000	1.00	25.1
19	19.7	-0.44	11.0	1.000	0.50	5.5
20 [a]	20.0	-0.52	9.6	0.938	0.67	6.0

[a] Data from central ring; [b] Densities of ring critical point in cyclopropane and in cyclopropenyl cation are 0.195 a.u. and 0.257 a.u., respectively, and difference between them represents the electron density in RCP from p electrons without influence of r electrons. However, it remains a partial r electron influence in the density of RCP since C-C bond lengths in cyclopropenyl cation are smaller than those in cyclopropane; [c] Imprecise value of D3BIA as there exists an influence of r electrons which cannot be excluded.

The difference among D_3BIA values of thiophene (**9**), furane (**10**) and pyrrole (**11**) is not so large (Table 1). One can also realize that the expected smaller aromaticity of anthracene (**20**) with respect to benzene (**1**) is supported by their D_3BIA values (Table 1).

In Scheme 2 one can see that from all ionic aromatic species, cyclobutadiene dianion (**16**) is the unique with non-uniform delocalization indexes involving its C-C bonds and non-degeneracy among all carbon atoms. One can also see in Scheme 2 that delocalization indexes involving carbon and nitrogen atoms are quite similar in pyridine and pyrazine unlike 1,3,4-triazine where they are completely different. Furthermore, the carbon atoms in the ring of *p*-xylylene (**21**) are near-degenerate but they have different delocalization indexes which shows the importance of uniformity of the delocalization index, of all atomic pairs belonging to the aromatic ring, in aromaticity (Scheme 2).

Optimization calculations were performed for the dicationic species **14** and **15**, but they gave no planar structures as it is supported experimentally[38] and computationally.[44] On the other hand, their dianion parents, cyclooctetraene dianion (**13**) and cyclobutadiene dianion (**16**), respectively, have planar structures.[45]

The high D_3BIA value of **16** might explain its planar structure since its 6π-electron resonance compensates its carbon-to-carbon repulsive interaction in which each carbon atom has a charge of -0.5 a.u. Its parent dication (**15**) probably has a puckered structure because the 2π-electron resonance does not compensate its carbon-to-carbon repulsive interaction (with 0.5 a.u. positively charged carbons). Accordingly, the puckered structure of cyclooctatetraenyl dication (**14**) is probably due to its overall 2.0 a.u. charge and ineffective 6π-electron resonance in an eight-membered ring while its dianion parent (**13**) has planar structure because of its 10π-electron resonance.

From all studied ionic aromatic species the cyclopentadiene anion (**18**) is the most aromatic system since the D_3BIA value of **17** (Table 1) is overestimated because it is not possible to eliminate thoroughly the influence of its C-C ρ electrons.

Borazine[46] (**19**) D_3BIA value higher than those from triazines, N_6H_6 and Si_6H_6 but smaller value than those from other six-membered and five-membered aromatic compounds as one might expect.

Other examples of application of D_3BIA can be found in the Electronic Supplementary Information section.

Another important analysis from AIM theory is the Laplacian of the charge density. It is defined as the sum of the three principal curvatures of the function at each point of the space. The density is locally concentrated in those regions where $L(r)>0$, since $\nabla^2 \rho<0$ when $\rho(r)$ is a local maximum. Likewise, the density is locally depleted in those regions where $L(r)<0$, since $\nabla^2 \rho<0$ when $\rho(r)$ is a local minimum.[30]

In Figure 1, one can see that the inner part of benzene ring is surrounded by only one $L(r)<0$ Laplacian line (first green line within the ring) while compounds **8** and **13** have another inner concentric $L(r)<0$ Laplacian lines within their rings. This means that the electronic interaction inside the ring is stronger in benzene than in compounds **8** and **13**. As for 1,3,4-tryazine (**4**) one can realize that the $L(r)<0$ Laplacian lines inside its ring are not concentric. This demonstrates how heteroatoms impair a uniform electronic interaction.

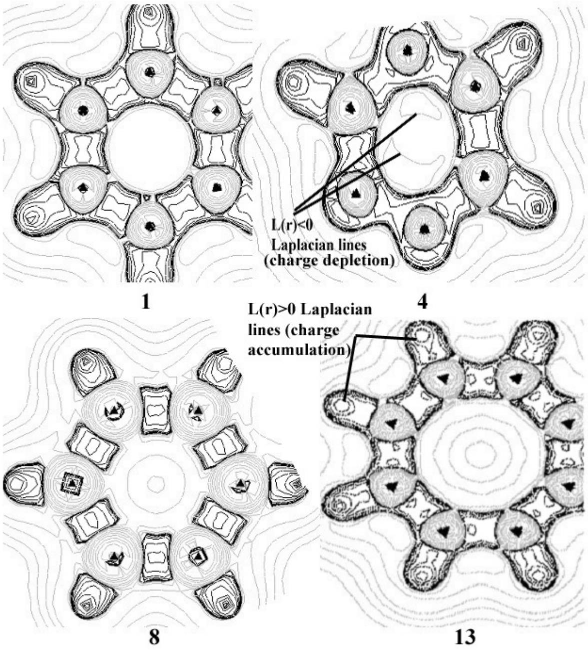


Figure 1. Contour maps of the negative of the Laplacian distribution of the electronic charge density for compounds **1**, **4**, **8**, **13** within the ring plane. The green curves are related to charge depletion, while the black lines are charge concentration.

Conclusions

We have proposed an index for quantifying aromaticity (D_3BIA). This index shows that aromaticity decreases as the number of heteroatoms in the aromatic molecule increases, since the degeneracy of single-electron states decreases. The ring size of an aromatic compound and aromaticity are inversely related, because the decrease of the charge density in the ring which disfavors the overlap of single-electron states.

The attractive interaction of 6ρ-electron resonance in cyclobutadiene dianion compensate its carbon-to-carbon repulsive interaction, while in its dicationic parent the 2π-electron resonance is insufficient to counterbalance its carbon-to-carbon repulsive interaction and it adopts a puckered structure. Accordingly, the puckered structure of cyclooctatetraenyl dication is probably due to its overall 2.0 a.u. charge and ineffective 6π-electron resonance in an eight-membered ring while its dianion parent has planar structure because of its 10π-electron resonance.

Cyclopentadiene anion is the most aromatic molecule of all studied ionic aromatic species.

Acknowledgments

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Supplementary Information

Examples of application of D_3BIA and other data are available free of charge at http://jbcs.sbq.org.br/, as PDF file.

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Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian. Inc. Pittsburgh P. A. **2003**.

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Density, Degeneracy, Delocalization-Based Index of Aromaticity (D_3BIA)

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Benzene and resonance

Resonance is related to degeneracy or near-degeneracy effects. Degeneracy may be due to the existence of symmetry groups that commute with hamiltonian.[1] The eigenfunctions of the exact hamiltonian must transform as irreducible representations of the commuting symmetry groups. When a given group has degenerate representations, some or all eigenstates of the hamiltonian of the system will reflect its degeneracy.

The real Hilbert space is always partitioned into a direct sum of subspaces, each representing a different energy eigenvalue of the spectrum of the hamiltonian operator. The direct product decomposition is the mathematical tool to analyze the symmetry of the allowed individual states. It is related to the "ascent in symmetry" method[2] for decomposition of tensor spaces in independent parts and justified by the Littlewood-Richardson rules[3]. These rules define the only allowed decompositions of a tensor space (e.g. point group space), providing us with the possible symmetries of the resonance hybrids, which reproduce the total symmetry of the system. Only invariant subgroups of some larger group can accommodate coherent states.

The possible forms of decomposing D_{6h} point group in direct products[4] are:

$$D_{6h} = D_6 \otimes Ci,\ D_6 \otimes C_s,\ C_{6v} \otimes C_s$$

The ground state of benzene is not degenerate, and there is no theoretical or experimental evidence of a near-degenerate electronic state with same geometry as the ground state. If there is no intersection of degenerate point group states one cannot follow the symmetry descent path in this case. The only alternative would be that of an accidental symmetry, but this is not possible since there is not direct product decomposition[5] from D_{3h} (Kekulé structure) and D_{2h} (Dewar structure).

However, in SCVB study of benzene, Gerratt *et al.*[6] stated that spin coupling two electrons (within same D_{6h} symmetry) allows the description of the different possible resonance structures and generates the stability of aromatic systems.

Then, the existence of resonance in benzene depends on the rigor of the theory applied to it. By spin coupling ð electrons, within same D_{6h} symmetry in SCVB, it is possible to associate the obtained stability with resonance of hybrid structures[6]. Otherwise, benzene molecule cannot be represented by "hybrids" of symmetries D_{3h} and D_{2h} since it is forbidden by point group symmetry rules[5].

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Table 1. Density of ring critical point [$\rho_{(RCP)}$], density of bond critical point [$\rho_{(BCP)}$], eingenvalue of density Hessian matrix from BCP towards RCP (λ_2), mean delocalization index ($\overline{DI}$), density value of the first inner isodensity contour line [ρ-FICL], ring density factor (RDF), delocalization index uniformity (DIU), degree of degeneracy and delocalization (*δ*) and D_3BIA of cyclopropane **1**, cyclotrisilane **2** and oxirane **3**[a]

Entry	$\rho_{(RCP)}$	$\rho_{(BCP)}$	λ_2	$\overline{DI}$	ρ FICL	RDF	DIU	*δ*	D_3BIA
1	0.195	0.237	-0.304	0.99	0.2	0.134	100	1	13.4
2	0.062	0.088	-0.060	0.79	0.08	0.046	100	1	4.6
3	0.210	0.249	-0.291	0.95	0.2	0.141	98.6	0.67	9.3

a. Firme, C.L.; Antunes, O.A.C.; Esteves, P.M. "differences of the electronic nature between cyclopropane and cyclotrisilane", to be submitted.

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Other examples of D$_3$BIA application

Computed energy values of compounds **1** to **22**

Entry	H (Hartree)	S(cal mol^{-1} K^{-1})	G(Hartree)
1	-232.205849	64.137	-232.236323
2	-248.209492	68.707	-248.242137
3	-264.305792	68.377	-264.338281
4	-280.326802	68.421	-280.359311
5	-280.369164	68.201	-280.401568
6	-248.611219	69.098	-248.644049
7	-328.335146	63.925	-328.365519
8	-1740.563821	106.940	-1740.614631
9	-553.001853	67.902	-553.034115
10	-230.018224	65.11	-230.044494
11	-210.143473	65.924	-210.174796
12	-270.615437	74.696	-270.650927
13	-309.440110	83.234	-309.479658
14	-308.751424	76.907	-308.787965
15	-153.834554	62.849	-153.864416
16	-154.505413	62.541	-154.535129
17	-115.711986	58.324	-115.739698
18	-193.497856	66.211	-193.529315
19	-242.649258	72.150	-242.683538
20	-539.456780	95.232	-539.502027
21	-309.560749	80.578	-309.599034
22	-464.294248	103.558	-464.343452
23	-233.341880	79.454	-233.379631

Z matrices of optimized structures

Structure ***1***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
C,1,B5,2,A4,3,D3,0
H,1,B6,6,A5,5,D4,0
H,2,B7,1,A6,6,D5,0
H,3,B8,2,A7,1,D6,0
H,4,B9,3,A8,2,D7,0
H,5,B10,4,A9,3,D8,0
H,6,B11,1,A10,2,D9,0
Variables:
B1=1.39440453
B2=1.39440453
B3=1.39440453
B4=1.39440453
B5=1.39440453
B6=1.08414438
B7=1.08414438
B8=1.08414438
B9=1.08414438
B10=1.08414438
B11=1.08414438
A1=120.
A2=120.
A3=120.
A4=120.
A5=120.
A6=120.
A7=120.
A8=120.
A9=120.
A10=120.
D1=0.
D2=0.
D3=0.
D4=180.
D5=180.
D6=180.
D7=180.
D8=180.
D9=180.

Structure ***2***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
N,1,B5,2,A4,3,D3,0
H,3,B6,2,A5,1,D4,0
H,1,B7,6,A6,5,D5,0
H,2,B8,1,A7,6,D6,0
H,4,B9,3,A8,2,D7,0
H,5,B10,4,A9,3,D8,0
Variables:
B1=1.39765067
B2=1.39572729
B3=1.39569785
B4=1.39761187
B5=1.34053352
B6=1.08632025
B7=1.08804934
B8=1.08557689
B9=1.08557602
B10=1.08805026
A1=118.44942731

A2=118.55732361
A3=118.45459639
A4=123.64708704
A5=120.72340293
A6=115.96448905
A7=120.23365301
A8=121.3227876
A9=120.39469107
D1=-0.00085748
D2=-0.00027783
D3=0.00084097
D4=179.99973377
D5=-179.99860638
D6=179.99938554
D7=179.99866508
D8=179.99786837

Structure **3**

C
C,1,B1
N,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
N,5,B5,4,A4,3,D3,0
H,1,B6,6,A5,5,D4,0
H,2,B7,1,A6,6,D5,0
H,4,B8,3,A7,2,D6,0
H,5,B9,4,A8,3,D7,0
Variables:
B1=1.3944643
B2=1.33517205
B3=1.33516227
B4=1.39447345
B5=1.33516151
B6=1.08581257
B7=1.08581242
B8=1.08581332
B9=1.08581322
A1=121.95775055
A2=116.08438257
A3=121.95783498
A4=121.95778353
A5=117.14731371
A6=120.89500816
A7=117.14769003
A8=120.89436211
D1=0.
D2=0.
D3=0.
D4=179.99961332
D5=179.99960988
D6=-179.99992285
D7=-179.99961172

Structure **4**

C
C,1,B1
N,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
N,1,B4,2,A3,3,D2,0
H,1,B5,5,A4,4,D3,0
H,2,B6,1,A5,5,D4,0
H,4,B7,3,A6,2,D5,0
N,5,B8,1,A7,2,D6,0
Variables:
B1=1.39694097
B2=1.32613093
B3=1.33897954
B4=1.33095238
B5=1.08461118
B6=1.08650035
B7=1.08496975
B8=1.33096423
A1=120.53452404
A2=114.56815535
A3=121.52415286
A4=116.19633291
A5=121.6757319
A6=117.49143894
A7=118.33975949
D1=0.0008028
D2=-0.00007078
D3=179.99969931
D4=-179.99967331
D5=-179.99729214
D6=-0.00006306

Structure **5**

C
N,1,B1
C,2,B2,1,A1
C,1,B3,2,A2,3,D1,0
N,4,B4,1,A3,2,D2,0
H,3,B5,2,A4,1,D3,0
H,1,B6,2,A5,3,D4,0
H,4,B7,1,A6,2,D5,0
N,4,B8,1,A7,2,D6,0
Variables:
B1=1.33431752
B2=1.33409095
B3=2.24199906
B4=1.33408459
B5=1.08627642
B6=1.08622505
B7=1.08628641
B8=1.33447517
A1=114.3206068
A2=92.83816582
A3=32.84183836
A4=117.19154735
A5=117.16232203
A6=150.03164766
A7=92.85549533
D1=-0.00014012
D2=-179.99931832
D3=-179.99970637
D4=-179.99953958
D5=-179.99881671
D6=-0.00016944

Structure **6**

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
N,1,B5,2,A4,3,D3,0
H,3,B6,2,A5,1,D4,0
H,1,B7,6,A6,5,D5,0
H,2,B8,1,A7,6,D6,0
H,4,B9,3,A8,2,D7,0
H,5,B10,4,A9,3,D8,0
H,6,B11,1,A10,2,D9,0
Variables:
B1=1.38495874
B2=1.39961462
B3=1.39960315
B4=1.38485835
B5=1.35312794
B6=1.08539941
B7=1.08346699
B8=1.08389172
B9=1.08389127
B10=1.0834634
B11=1.0174324
A1=119.09207833
A2=120.02583016
A3=119.10219566
A4=119.25212563

A5=119.99099241
A6=116.83818764
A7=119.41328103
A8=121.49457477
A9=123.91934849
A10=118.35573423
D1=-0.00090959
D2=0.00062294
D3=0.00051687
D4=-179.99924284
D5=-179.99982947
D6=-179.99978996
D7=-179.99931003
D8=179.99956296
D9=179.99938435

*Structure **7***

N
N,1,B1
N,2,B2,1,A1
N,1,B3,3,A2,2,D1,0
N,1,B4,4,A3,3,D2,0
N,2,B5,1,A4,5,D3,0
Variables:
B1=2.64387171
B2=1.32191784
B3=1.32191784
B4=1.32191784
B5=1.32191784
A1=59.99934566
A2=29.99979642
A3=119.9986908
A4=59.99934514
D1=180.
D2=0.
D3=0.

*Structure **8***

Si
H,1,B1
Si,1,B2,2,A1
H,3,B3,1,A2,2,D1,0
Si,3,B4,1,A3,2,D2,0
H,5,B5,3,A4,1,D3,0
Si,5,B6,3,A5,1,D4,0
H,7,B7,5,A6,3,D5,0
Si,7,B8,5,A7,3,D6,0
H,9,B9,7,A8,5,D7,0
Si,9,B10,7,A9,5,D8,0
H,11,B11,9,A10,7,D9,0
Variables:
B1=1.48250009
B2=2.21926329
B3=1.48249901
B4=2.21924638
B5=1.48249901
B6=2.21926329
B7=1.48250009
B8=2.21926329
B9=1.48249902
B10=2.21924638
B11=1.48249902
A1=120.00043164
A2=120.00654187
A3=120.00043159
A4=119.9930266
A5=120.00043158
A6=120.00043167
A7=119.99913684
A8=120.00654189
A9=120.00043157
A10=119.99302648
D1=0.
D2=180.
D3=180.
D4=0.
D5=180.
D6=0.
D7=180.
D8=0.
D9=180.

*Structure **9***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
S,1,B4,2,A3,3,D2,0
H,1,B5,2,A4,3,D3,0
H,2,B6,1,A5,5,D4,0
H,3,B7,2,A6,1,D5,0
H,4,B8,3,A7,2,D6,0
Variables:
B1=1.36602858
B2=1.42752012
B3=1.36607262
B4=1.73300885
B5=1.07910408
B6=1.08209208
B7=1.08208892
B8=1.0791118
A1=112.71240688
A2=112.71233472
A3=111.54582158
A4=128.47885155
A5=123.27047263
A6=124.01571123
A7=128.48698442
D1=0.01504194
D2=-0.01394321
D3=179.9935755
D4=179.99606713
D5=-179.99303583
D6=179.99482022

*Structure **10***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
O,4,B4,3,A3,2,D2,0
H,1,B5,2,A4,3,D3,0
H,2,B6,1,A5,5,D4,0
H,3,B7,2,A6,1,D5,0
H,4,B8,3,A7,2,D6,0
Variables:
B1=1.35823665
B2=1.43538838
B3=1.35828896
B4=1.36309213
B5=1.0766432
B6=1.07833604
B7=1.07833992
B8=1.0766494
A1=106.13630242
A2=106.13732933
A3=110.40067299
A4=133.70318445
A5=126.43720024
A6=127.42939036
A7=133.69973475
D1=0.01483043
D2=0.00869411
D3=179.99375372
D4=179.98073612
D5=-179.98738933
D6=179.99555833

*Structure **11***

C
C,1,B1

C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
N,1,B4,2,A3,3,D2,0
H,5,B5,1,A4,2,D3,0
H,1,B6,5,A5,4,D4,0
H,2,B7,1,A6,5,D5,0
H,3,B8,2,A7,1,D6,0
H,4,B9,3,A8,2,D7,0
Variables:
B1=1.37685212
B2=1.4249325
B3=1.37690055
B4=1.37501039
B5=1.00606914
B6=1.07782742
B7=1.0788239
B8=1.07882856
B9=1.07783011
A1=107.43848758
A2=107.43918282
A3=107.65260156
A4=125.09167455
A5=121.27400334
A6=125.72591563
A7=126.83823262
A8=131.06976646
D1=0.01231332
D2=-0.00700582
D3=179.99477434
D4=179.9960186
D5=179.99842797
D6=-179.9961642
D7=179.99489475

Structure ***12***

C
C,1,B1
C,2,B2,1,A1
C,1,B3,2,A2,3,D1,0
C,3,B4,2,A3,1,D2,0
C,4,B5,1,A4,2,D3,0
C,5,B6,3,A5,2,D4,0
H,1,B7,2,A6,3,D5,0
H,2,B8,1,A7,4,D6,0
H,3,B9,2,A8,1,D7,0
H,4,B10,1,A9,2,D8,0
H,5,B11,3,A10,2,D9,0
H,6,B12,4,A11,1,D10,0
H,7,B13,5,A12,3,D11,0
Variables:
B1=1.39590979
B2=1.39595673
B3=1.39595673
B4=1.39593647
B5=1.39593647
B6=1.39597973
B7=1.08564984
B8=1.08564984
B9=1.08565496
B10=1.08565496
B11=1.08565253
B12=1.08565253
B13=1.08564337
A1=128.57422566
A2=128.57422566
A3=128.56663523
A4=128.56663523
A5=128.57662225
A6=115.71234436
A7=115.71234436
A8=115.71246798
A9=115.71246798
A10=115.71515045
A11=115.71515045
A12=115.71748367
D1=0.
D2=-0.00848507
D3=0.00848507
D4=0.00237422
D5=-179.99537418
D6=179.99537418
D7=179.9975722
D8=-179.9975722
D9=-179.98409157
D10=179.98409157
D11=-179.99713128

Structure ***13***

C
C,1,B1
C,1,B2,2,A1
C,2,B3,1,A2,3,D1,0
C,3,B4,1,A3,2,D2,0
C,5,B5,3,A4,1,D3,0
C,1,B6,2,A5,4,D4,0
C,7,B7,1,A6,2,D5,0
H,3,B8,1,A7,7,D6,0
H,5,B9,3,A8,1,D7,0
H,6,B10,5,A9,3,D8,0
H,4,B11,2,A10,1,D9,0
H,2,B12,1,A11,7,D10,0
H,1,B13,7,A12,8,D11,0
H,7,B14,1,A13,2,D12,0
H,8,B15,7,A14,1,D13,0
Variables:
B1=1.41956141
B2=3.41492222
B3=1.4120985
B4=1.41956141
B5=1.41209256
B6=1.41209256
B7=1.41956719
B8=1.09643308
B9=1.09643724
B10=1.09642834
B11=1.09648239
B12=1.09643308
B13=1.09643724
B14=1.09642834
B15=1.09648239
A1=89.99561258
A2=134.95702066
A3=90.00438718
A4=134.94481209
A5=134.94481208
A6=134.95700515
A7=157.55612631
A8=112.44156911
A9=112.60550474
A10=112.58452586
A11=112.41415679
A12=112.58583929
A13=112.60550474
A14=112.43914583
D1=-3.31967647
D2=-0.0076983
D3=3.32540648
D4=0.0025292
D5=-4.68978141
D6=5.96629019
D7=-178.79424031
D8=177.53378832
D9=-177.42326969
D10=-177.76916772
D11=177.43207854
D12=177.53378849
D13=-177.89162544

Structure ***14***

C
C,1,B1
C,1,B2,2,A1
C,2,B3,1,A2,3,D1,0

```
C,3,B4,1,A3,2,D2,0
C,5,B5,3,A4,1,D3,0
C,1,B6,2,A5,4,D4,0
C,7,B7,1,A6,2,D5,0
H,3,B8,1,A7,2,D6,0
H,5,B9,3,A8,1,D7,0
H,6,B10,5,A9,3,D8,0
H,2,B11,1,A10,7,D9,0
H,1,B12,2,A11,4,D10,0
H,8,B13,7,A12,1,D11,0
H,7,B14,1,A13,2,D12,0
H,4,B15,2,A14,1,D13,0
Variables:
B1=1.40088145
B2=3.79828706
B3=1.4924877
B4=1.40100457
B5=1.40112486
B6=1.40113204
B7=1.49233166
B8=1.08787294
B9=1.08430162
B10=1.08789305
B11=1.08785833
B12=1.08430633
B13=1.11345695
B14=1.0879014
B15=1.11340704
A1=73.22138143
A2=107.69742063
A3=106.76748429
A4=111.04401286
A5=111.04106818
A6=107.69753733
A7=127.87685331
A8=124.48298948
A9=125.24818968
A10=125.2563634
A11=124.47739963
A12=100.10319651
A13=125.23411849
A14=100.13882568
D1=9.55889677
D2=0.03567646
D3=-0.0260735
D4=9.54882201
D5=9.563192
D6=-176.40327871
D7=179.97662243
D8=176.54911144
D9=-176.55451486
D10=-170.45795261
D11=83.53719679
D12=-176.54100554
D13=83.57656755
```

*Structure **15***

```
C
C,1,B1
C,2,B2,1,A1
C,1,B3,2,A2,3,D1,0
H,4,B4,1,A3,2,D2,0
H,1,B5,4,A4,3,D3,0
H,3,B6,2,A5,1,D4,0
H,2,B7,1,A6,4,D5,0
Variables:
B1=1.42481184
B2=1.42487598
B3=1.4248786
B4=1.09788682
B5=1.09787609
B6=1.09787775
B7=1.09787671
A1=85.72387085
A2=85.72256906
A3=137.01596685
A4=137.02404
A5=137.02785756
A6=137.02698387
D1=30.54577791
D2=144.30018206
D3=144.24195093
D4=144.32832334
D5=-144.27358739
```

*Structure **16***

```
C
C,1,B1
C,2,B2,1,A1
C,1,B3,2,A2,3,D1,0
H,2,B4,1,A3,4,D2,0
H,3,B5,2,A4,1,D3,0
H,1,B6,4,A5,3,D4,0
H,4,B7,1,A6,2,D5,0
Variables:
B1=1.55338928
B2=1.36197633
B3=1.36197572
B4=1.08401868
B5=1.08401898
B6=1.08401955
B7=1.08401927
A1=89.96761182
A2=89.96764846
A3=135.40165693
A4=134.54735483
A5=134.54738473
A6=134.54739759
D1=-2.90867294
D2=-179.79098806
D3=179.48765503
D4=179.48927423
D5=179.4890158
```

*Structure **17***

```
C
C,1,B1
C,1,B2,2,A1
H,3,B3,1,A2,2,D1,0
H,1,B4,3,A3,2,D2,0
H,2,B5,1,A4,3,D3,0
Variables:
B1=1.36255632
B2=1.36255684
B3=1.08210653
B4=1.08211651
B5=1.08211651
A1=60.00001271
A2=150.00001273
A3=150.00124631
A4=149.99874094
D1=180.
D2=180.
D3=180.
```

*Structure **18***

```
C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
H,1,B5,2,A4,3,D3,0
H,2,B6,1,A5,5,D4,0
H,3,B7,2,A6,1,D5,0
H,4,B8,3,A7,2,D6,0
H,5,B9,4,A8,3,D7,0
Variables:
B1=1.41525085
B2=1.41502073
```

B3=1.4152511
B4=1.41525367
B5=1.0857133
B6=1.0857105
B7=1.08572847
B8=1.08571325
B9=1.08574101
A1=108.00057818
A2=107.99857183
A3=108.00837583
A4=126.00818589
A5=126.00566775
A6=125.98546177
A7=125.99542121
A8=126.00145392
D1=0.01984693
D2=-0.01237432
D3=-179.9750034
D4=179.99871732
D5=-179.98475189
D6=-179.93642063
D7=-179.91465701

Structure ***19***

N
N,1,B1
N,2,B2,1,A1
B,3,B3,2,A2,1,D1,0
B,1,B4,2,A3,4,D2,0
B,2,B5,1,A4,5,D3,0
H,5,B6,1,A5,6,D4,0
H,3,B7,2,A6,1,D5,0
H,4,B8,3,A7,2,D6,0
H,2,B9,1,A8,5,D7,0
H,6,B10,2,A9,1,D8,0
H,1,B11,5,A10,3,D9,0
Variables:
B1=2.44117417
B2=2.4412199
B3=1.4309723
B4=1.430987
B5=1.43097199
B6=1.19194899
B7=1.00883313
B8=1.19195049
B9=1.00883872
B10=1.19194913
B11=1.00883931
A1=60.00055053
A2=31.4636619
A3=91.46411968
A4=31.46461701
A5=121.4641091
A6=150.00235262
A7=121.46659511
A8=149.99908185
A9=121.46633735
A10=118.54039403
D1=-179.99472661
D2=-0.00238167
D3=179.99652677
D4=-179.9983263
D5=179.99778921
D6=179.99927961
D7=-179.99922231
D8=-179.99911442
D9=-179.99900556

Structure ***20***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
C,5,B5,4,A4,3,D3,0
C,3,B6,2,A5,1,D4,0
C,4,B7,3,A6,2,D5,0
C,8,B8,4,A7,3,D6,0
C,7,B9,3,A8,2,D7,0
C,10,B10,7,A9,3,D8,0
H,11,B11,10,A10,7,D9,0
C,11,B12,10,A11,7,D10,0
C,13,B13,11,A12,10,D11,0
C,14,B14,13,A13,11,D12,0
H,7,B15,3,A14,2,D13,0
H,1,B16,2,A15,3,D14,0
H,2,B17,1,A16,6,D15,0
H,5,B18,4,A17,3,D16,0
H,6,B19,5,A18,4,D17,0
H,8,B20,4,A19,3,D18,0
H,13,B21,11,A20,10,D19,0
H,14,B22,13,A21,11,D20,0
H,15,B23,14,A22,13,D21,0
Variables:
B1=1.36737552
B2=1.42927781
B3=1.44300659
B4=1.42919493
B5=1.36739747
B6=1.39872912
B7=1.39879051
B8=1.39872936
B9=1.39879098
B10=1.42919493
B11=1.08509336
B12=1.36739715
B13=1.42498276
B14=1.36737597
B15=1.08592918
B16=1.08420018
B17=1.08509634
B18=1.08509332
B19=1.08419031
B20=1.08592922
B21=1.08419022
B22=1.08420038
B23=1.08509646
A1=120.97349279
A2=118.57836209
A3=118.5888481
A4=120.97445592
A5=122.31290441
A6=119.10186462
A7=121.78943839
A8=121.78942638
A9=122.3092082
A10=118.56306847
A11=120.97443491
A12=120.43828126
A13=120.44660697
A14=119.10990854
A15=120.15616499
A16=120.46836662
A17=118.56291589
A18=120.1605731
A19=119.10138437
A20=120.16088871
A21=119.39771674
A22=120.4681715
D1=0.00536913
D2=-0.00454473
D3=0.0014198
D4=-179.99546081
D5=179.99862929
D6=0.
D7=179.99939625
D8=-179.9971509
D9=0.0012206
D10=179.99854933
D11=0.00413195
D12=-0.0027334

D13=-0.00235251
D14=179.99794777
D15=179.9973736
D16=-179.99789539
D17=179.99904075
D18=179.99877477
D19=-179.9971076
D20=-179.99972008
D21=-179.99894747

*Structure **21***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
C,1,B5,2,A4,3,D3,0
H,1,B6,2,A5,3,D4,0
H,2,B7,1,A6,6,D5,0
H,4,B8,3,A7,2,D6,0
H,5,B9,4,A8,3,D7,0
C,6,B10,1,A9,2,D8,0
H,11,B11,6,A10,1,D9,0
C,3,B12,2,A11,1,D10,0
H,13,B13,3,A12,2,D11,0
H,6,B14,1,A13,2,D12,0
H,3,B15,2,A14,1,D13,0
Variables:
B1=1.3469848
B2=1.45995185
B3=1.45994897
B4=1.34698645
B5=1.45995229
B6=1.08525062
B7=1.08525006
B8=1.08525056
B9=1.08525003
B10=1.35236259
B11=1.08374069
B12=1.35243419
B13=1.08374137
B14=2.1286993
B15=2.12876647
A1=121.94526317
A2=116.10923931
A3=121.94558559
A4=121.94512202
A5=120.30210049
A6=120.30168631
A7=117.75312282
A8=120.30136729
A9=121.94457217
A10=121.41739227
A11=121.94547563
A12=121.41805668
A13=147.69596096
A14=96.19498587
D1=-0.00158728
D2=0.00162492
D3=-0.00012555
D4=-179.99988566
D5=179.99942591
D6=-179.99840636
D7=-179.99982191
D8=-179.99888948
D9=0.00735204
D10=179.99820887
D11=-179.99025621
D12=179.99388427
D13=179.99925271

*Structure **22***

C
C,1,B1
C,2,B2,1,A1
C,3,B3,2,A2,1,D1,0
C,4,B4,3,A3,2,D2,0
C,1,B5,2,A4,3,D3,0
C,4,B6,3,A5,2,D4,0
H,7,B7,4,A6,3,D5,0
C,5,B8,4,A7,3,D6,0
H,9,B9,5,A8,4,D7,0
C,6,B10,1,A9,2,D8,0
H,11,B11,6,A10,1,D9,0
C,1,B12,2,A11,3,D10,0
H,13,B13,1,A12,2,D11,0
C,2,B14,1,A13,6,D12,0
C,3,B15,2,A14,1,D13,0
H,16,B16,3,A15,2,D14,0
H,3,B17,2,A16,1,D15,0
H,4,B18,3,A17,2,D16,0
H,5,B19,4,A18,3,D17,0
H,6,B20,1,A19,2,D18,0
H,1,B21,2,A20,3,D19,0
H,2,B22,1,A21,6,D20,0
H,2,B23,1,A22,6,D21,0
Variables:
B1=1.4908711
B2=1.49129294
B3=1.49100042
B4=1.49088033
B5=1.49096015
B6=1.34190586
B7=1.0827899
B8=1.33981052
B9=1.08313491
B10=1.33983748
B11=1.08342415
B12=1.34194677
B13=1.08277619
B14=1.33980549
B15=1.33986488
B16=1.08342612
B17=2.11181456
B18=2.11992518
B19=2.12071623
B20=2.11185213
B21=2.11994511
B22=2.11200849
B23=2.12069119
A1=114.80647967
A2=114.7841145
A3=114.97868068
A4=114.98047619
A5=122.57972911
A6=121.51274857
A7=123.70323842
A8=120.94389872
A9=123.79879544
A10=121.8259057
A11=122.43439061
A12=121.51022799
A13=123.70426236
A14=121.37472542
A15=121.83511502
A16=95.27732156
A17=96.83048624
A18=97.96385056
A19=149.89075453
A20=148.14262593
A21=149.79041254
A22=97.96373225
D1=-50.65383833
D2=23.87059589
D3=25.42255306
D4=-156.18876333
D5=-176.01720629
D6=-152.23338459
D7=178.83883109
D8=-153.81202523
D9=0.46050997

```
D10=-154.51979919
D11=3.92967224
D12=-152.23716343
D13=127.08376849
D14=-177.06483508
D15=127.66751525
D16=-154.46048011
D17=-152.0093962
D18=-152.80755224
D19=-157.71753492
D20=-151.21128088
D21=-152.01672643
```

Structure ***23***

```
C
H,1,B1
H,1,B2,2,A1
C,1,B3,3,A2,2,D1,0
H,4,B4,1,A3,3,D2,0
C,4,B5,1,A4,3,D3,0
H,6,B6,4,A5,1,D4,0
C,6,B7,4,A6,1,D5,0
H,8,B8,6,A7,4,D6,0
C,8,B9,6,A8,4,D7,0
H,10,B10,8,A9,6,D8,0
C,10,B11,8,A10,6,D9,0
H,12,B12,10,A11,8,D10,0
H,12,B13,10,A12,8,D11,0
Variables:
B1=1.08548362
B2=1.08312735
B3=1.34100541
B4=1.08831554
B5=1.44874714
B6=1.08891622
B7=1.34967469
B8=1.08891457
B9=1.44875221
B10=1.08831681
B11=1.34100412
B12=1.08548233
B13=1.08312884
A1=116.92879402
A2=121.60942933
A3=119.09982547
A4=124.49676363
A5=116.75511595
A6=124.30368758
A7=118.94216795
A8=124.30144385
A9=116.40186531
A10=124.49872358
A11=121.46312562
A12=121.60834053
D1=180.
D2=0.
D3=180.
D4=0.
D5=180.
D6=0.
D7=180.
D8=0.
D9=180.
D10=0.
D11=180.
```