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A08

INTERACTION IN CARBOCATIONS AND HÜCKEL'S 4*n* + 2 RULE

A11

D. Sunko

A14

Faculty of Natural Sciences and Mathematics, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

The molecular orbital model of hyperconjugation was utilized in rationalizating some long range interactions in carbocations *(1)*. Conveniently such interactions can be detected by measuring secondary kinetic deuterium isotope effects *(2)*. Hückel's 4*n* + 2 rule can be extended to interactions between the cationic center and *pseudo*-π orbitals of CH_3, CH_2 and CH groups, respectively *(3)*. Thus, in analogy to hyperconjugation one can envisage homohyperconjugation as the probable cause of normal γ-deuterium isotope effects *(4)*. Results are presented of studies of these effects in the adamantane and norbornane system. The stability of the 1-adamantyl cation can be ascribed to a favorable 4*n* + 2, configuration of σ-electrons comprising the β,γ-carbon carbon and/or γ-carbon hydrogen bonds. It is however not possible to distinguish between these alternatives since both could explain the observed γ-isotope effects. In contrast, the four CH_2 groups flanking C_7 in the 7-norbornyl cation form an antiaromatic 4*n* *pseudo*-π system which could explain the exceptional instability of this cation. Interactions of the empty *p*-orbital with the subjacent $4B_2$ *pseudo*-π orbitals give rise to small normal γ-deuterium isotope effects of homohyperconjugative origin. In this system, due to symmetry constrains hyperconjugative interaction with the ribbon orbitals of the σ-framework is not possible.

DESCRIPTORS

Carbocations
interactions in, Hückel's 4*n*+2 rule for,

Molecular orbital
HMO, 4*n*+2 rule and interactions in carbocations,

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Abstractor: N. Trinajstić

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A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat.Chem.Acta*	SHORT TITLE	A45	40	REFERENCES	
				1	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		3	FIGURES	
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A07	*CCA – 1239*	OTHER IDENTIFIC.				

A08

A THEORETICAL INFORMATION APPROACH TO RING AND TOTAL AROMATICITY IN GROUND AND EXCITED STATES

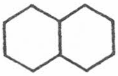
A11

F. Fratev, D. Bonchev, and V. Enchev*

A14

Institute of Organic Chemistry, BAN, Sofia 1113, and *Higher School of Chemical Technology, Burgas 8010, Bulgaria

By applying the Shannon equation *(1)* to the electron density matrix of a molecule, an information index is defined and used as the quantitative estimate of the ring *(2)* and total aromaticity of molecules in the ground and excited states. The approach is applicable within each LCAO-method. The index reproduces well the classification of molecules into aromatic, nonaromatic and antiaromatic, and correlates well with the results of other authors obtained by completely different approaches *(3-6)*. Below is given a comparison with topological resonance energy per electron, TRE(PE), index *(5)* for several conjugated molecules.

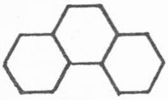
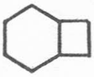
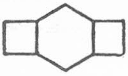
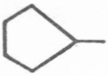
Molecule[a]	Information aromaticity index	TRE(PE)	Status[b]
	1.000	0.046	A
	0.625	0.039	A

DESCRIPTORS

Information theory
in molecular properties prediction,

Mathematics
topological resonance energy calculation for conjugated molecules,

Resonance
topological energy, electron index for conjugated molecules,

	0.544	0.034	A
	0.557	0.039	A
	0.070	− 0.307	AA
	0.232	− 0.049	AA
	0.152	− 0.079	AA
	0.294	0.003	NA
	0.238	0.016	NA

[a] Graphs of studied molecules; [b] A= aromatic, NA = non-aromatic; AA = anti-aromatic.

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.

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A03	*Croat. Chem. Acta*	SHORT TITLE	A45	7	REFERENCES
				3	TABLES
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A08

DO THE C–H BONDS CONTRIBUTE TO THE STABILIZATION ENERGY OF BENZENE?

A11 *Á. Furka and F. Sebestyén*

A14 Department of Organic Chemistry, Eötvös Loránd University, Budapest, 1088 Hungary

DESCRIPTORS

Energy
stabilization, of benzene,

Heat of formation
of 1,3-butadiene,
of ethylene,
of *trans*-1,3,5-hexatriene,

Stabilization energy of benzene (SE) has long been defined as the difference between the heat of formation (ΔH_f) of benzene and that of a hypothetic reference compound: 1,3,5-cyclohexatriene. Since this compound does not exist, its ΔH_f, of course, cannot be determined experimentally. The reference ΔH_f has usually been calculated from empirically or theoretically derived bond energies. In this way, for example, Klages *(1)* and Dewar *(2)* suggested 35.9 and 20 kcal/mol for SE, respectively.

In order to avoid uncertainties connected with the non-existence of the reference compound, the authors of the present paper suggest the definition and calculation of SE to be based on experimentally determined ΔH_f-s of conjugated polyenes. From the ΔH_f-s of the neighbouring members of the homologous series of linear open chain conjugated polyenes, ΔH_f increments can be derived. A ΔH_f increment may be considered as a contribution of two =CH– groups to ΔH_f-s. Since benzene consists of six =CH– groups, a threefold value of the ΔH_f increment can well be accepted as reference ΔH_f for the calculation of SE.

This way 19.7 and 23.0 kcal/mole are derived for SE, when benzene is compared to *trans* and *cis* type polyenes, respectively. A comparison of the estimated C–C bond energy of benzene to that of olefins leads to the conclusion that C–C bonds are responsible for only about 2/3 of SE. It is suggested that the rest of SE is connected with the difference in strength of the aromatic and olefinic C—H bonds.

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A05	53 (1980)	VOL. NO. (YEAR)		4	FIGURES
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A07	*CCA – 1241*	OTHER IDENTIFIC.			

A08

WHY ARE THE PROPERTIES OF POLYCYCLIC HYDROCARBONS ADDITIVE OVER CONJUGATION CIRCUITS?

A11 *J. A. N. F. Gomes*

A14 Departamento de Quimica, Faculdade de Ciências, 4000 PORTO, Portugal

Properties as different as resonance energies and magnetic ring-currents are investigated and a non-empirical system of increments is proposed. It is shown that the π-electron properties of conjugated, polycyclic hydrocarbons are additive over all conjugation circuits that can be identified in the molecule. The contribution from each individual conjugation circuit is calculated non-empirically on a simple, free-electron model for the associated annulene.

Within a special form of the resonance theory, it is shown that all conjugation circuits should contribute with equal weight, and not only the 'independent circuits' as proposed earlier by Randić *(1,2)* or certain lower circuits as postulated by Herndon *(3)*. Contributions from higher circuits turn out quite naturally, however, to be small.

Results for a wide variety of polycyclic hydrocarbons, alternant and non-alternant, are presented. Both for resonance energies and for magnetically-induced ring currents, satisfactory agreement with conventional calculations has been obtained *(4)*.

DESCRIPTORS

Conjugation
of polycyclic hydrocarbons,

Hydrocarbons, properties
cyclic, alternant and non-alternant, conjugated circuits, MO calculation of,

Resonance
energy, of alternant and nonalternant hydrocarbons,

REFERENCES

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A03	*Croat.Chem.Acta*	SHORT TITLE	A45	10	REFERENCES	
				3	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		1	FIGURES	
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A08

GRAPH–THEORETICAL SEARCH FOR BENZENOID POLYMERS WITH ZERO ENERGY GAP

A11

A. Graovac, M. Randić, and N. Trinajstić*

A14

'Ruđer Bošković' Institute, P.O.Box 1016, 41001 Zagreb, Croatia, Yugoslavia, and *Energy and Mineral Resources Research Institute, Iowa State University, Ames, Iowa 50011, U.S.A.

Recently structural features which characterize the energy gap in polymeric conjugated hydrocarbons *(1)* within the framework of the simple Hückel MO theory have been specified using graph-theoretical methods *(2)*. It has been shown that molecules of interest as potential units in polymers with zero energy gap have to satisfy certain structural conditions which relate the number of selected 'excited' valence structures to thet of the Kekule structures for the system. As in the previous work units separated by essentially single bonds are considered.

The search for benzenoid systems which can satisfy the requirement is now elaborated. A necessary condition that a system may have zero energy gap is that the repeating benzenoid unit has a non-prime number (K) of Kekulé valence structures. Then K could be factored: $K_1 \cdot K_2 \ldots K_m$. (Generally, there are more factorizations of K and the procedure needs to be carried out over all of them.) Fragments F_i that have the number of Kekulé structures given by K_i are recognized, and we try to superimpose all of them over the skeleton of monomer unit. (The procedure needs to be carried out for all possible fragmentations corresponding to a given factorization.) If it is possible to cover the monomer unit with all the fragments leaving at least two positions available for linking the units in polymer form, then the energy gap of such a polymer is zero.

DESCRIPTORS

Mathematics
grapg theory, in search for benzenoid polymers,

Molecular orbital
Hückel theory,

Polymers
conjugated, graph theoretical search for benzenoid systems,

In a number of examples it is illustrated how the actual search is performed. A list of benzenoid systems of interest as units in a polymer with the zero energy gap is given. The search is quite efficient and speedy as it requires the enumeration of Kekulé valence and related structures of monomer unit under consideration only.

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A08

EFFECT OF CYCLES ON TOPOLOGICAL RESONANCE ENERGY

A11

I. Gutman

A14

Faculty of Science, P.O.Box 60, 34000 Kragujevac, Yugoslavia

Topological resonance energy, TRE, a new concept in theoretical organic chemistry introduced by the Zagreb group *(1)*, is defined as follows *(2)*,

$$TRE = \sum_{j=1}^{N} (g_j x_j - h_j x_j^R) \qquad (1)$$

which for $g_j = h_j$ reduces *(1,3)* to

$$TRE = \sum_{j=1}^{N} g_j (x_j - x_j^R) \qquad (2)$$

where x_j and x_j^R ($j = 1, 2, ..., N$) are the zeros of the characteristic (Hückel) and acyclic (reference, matching) polynomial, respectively, of a conjugated molecule, whilst g_j (and h_j) is (are) the pertinent occupation number(s).

The author has analysed some general mathematical properties of TRE. Three basic properties of TRE are established:

1. TRE represents the joint effect of all cycles on total π-electron energy (E) of conjugated system.

DESCRIPTORS

Mathematics
graph theory, topological resonance energy, effect of cycles on,

Resonance
topological energy, effect of cycles on

2. The effect of a particular cycle on TRE is equal to the effect of the same cycle on E.

3. An approximate formula enables one to express TRE as a linear combination of contributions of single cycles,

$$\mathrm{TRE} \simeq \sum_{C} I(G,C) \tag{3}$$

where

$$I(G,C) = -2(-1)^{|C|/2} \langle (G-C) \rangle \tag{4}$$

Symbol C stands for cycle. The validity of formula (3) was tested on a number of conjugated systems, to the alternant and non-alternant, monocyclic and polycyclic. The relation between the approximation (3) and the exact TRE is not linear. The correlation is good for systems having positive and small negative values of TRE, but considerably hihg violations occur in the case of anti-aromatic molecules, especially [4N]-annulenes.

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A08

ON TOPOLOGICAL RESONANCE ENERGY OF COUMARIN AND ITS DERIVATIVES

A11

P. Ilić, A. Jurić, and N. Trinajstić

A14

'Ruđer Bošković' Institute, P.O.Box 1016, 41001 Zagreb, Croatia, Yugoslavia

DESCRIPTORS

Coumarin
topological resonance energy of,

Resonance
topological energy, of coumarins,

Topological resonance energies (TREs) of coumarin and the following derivatives: 3-hydroxycoumarin, 4-hydroxycoumarin, 3,4-dihydroxycoumarin, 4,5,7-trihydroxycoumarin, 3-carboxy-4-hydroxycoumarin, 3-bromo-4-hydroxycoumarin, and 6-bromo-4-hydroxycoumarin, are reported.

The following TRE formula is used for the numerical work *(1-4)*

$$\mathrm{TRE} = \sum_{j=1}^{N} g_j (x_j - x_j^{ac}) \qquad (1)$$

where x_j and x_j^{ac} represent the Hückel spectrum of a given structure and the spectrum of the corresponding acyclic polynomial *(1,2)*, respectively, while g_j $(j = 1, 2, ..., N)$ are the orbital accupancy numbers.

The heteroatomic parameters are taken from the work by Hess and Schaad *(5)*. In order to compare aromatic stability of coumarin and related compounds the normalized form of TRE, TRE per electron, TRE(PE), is used *(4)*

$$\mathrm{TRE\ (PE)} = \mathrm{TRE}/N \qquad (2)$$

where N is the total number of π electrons in the system.

Theoretical predictions that these all coumarins should exhibit aromatic properties are sustained by the ample experimental evidence *(6)*. In addition, coumarin and isocoumarin are predicted to be much more stable than the corresponding quinonoid isomer.

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A08

ON THE TOPOLOGICAL RESONANCE ENERGY OF PORPHINS AND RELATED STRUCTURES

A11

P. Ilić and N. Trinajstić

A14

'Ruđer Bošković' Institute, P.O.Box 1016, 41001 Zagreb, Croatia, Yugoslavia

Porphinoid, both existing and hypothetic systems, are represented by graphs at the nearest-neighbour level of approximation. By covering a graph by a dimer *(1)*, one gets the characteristic polynomial in the form *(2,3)*

$$P(G;x) = \sum_{i}^{i_{\max}} \sum_{j(i)} \sum_{d=0}^{m_{i,j(i)}} (-1)^{i+d}\ 2^{i}\ D(G-R_{i,j(i)};\ d)\ x^{N-2d-n_{i,j(i)}} \qquad (1)$$

d the number of dimers; dimer is defined as such: ○—○

D the number of arguments of *d* dimers on a graph G,

N the number of vertices of a graph G,

R ring that are to be excised from a graph G,

m the maximal d number in a subgraph G–R,

n the number of vertices in a subgraph G–R,

i, j(i) index for counting of disjoint elements; $i = 1, 2, ..., r$,

$i = 2d + n_{i,\ j(i)}$

r the number of principal rings in a G.

DESCRIPTORS

Mathematics
graph theory, topological resonance energy of porphins and related structures,

Resonance
topological energies of porphins and related structures,

Linearly realated structures have interesting combinatorial properties; since they are obtained by covering a graph G with monovalent, dimer subgraphs, we imputed them a name 'acyclic'. Thus, the acyclic polynomial of a complete graph, G, reads,

$$P^{ac}(G;x) = \sum_{d} (-1)^{d} D(G;d)\, x^{N-2d} \tag{2}$$

This polynomial was given a meaning of reference polynomial. Associating to the zeros of both polynomials, *i.e.* characteristic and acyclic, respectively, the common quantity β, ($\sim 2.3 \times 10^{5}$ J/mol) *(4)*, one can speak about the energy of a conjugated molecule and its reference structure. A simple linear relation,

$$\begin{aligned} \Delta &= a_1 x_1 + a_2 x_2 + \dots + a_k x_k - b_1 y_1 - b_2 y_2 - \dots - b_m x_m = \\ &= (a_1 x_1 - b_1 y_1) + (a_2 x_2 - b_2 y_2) + \dots + (a_k x_k - b_m y_m) \end{aligned} \tag{3}$$

where,

x_k, y_m are the zeros of the characteristic and the acyclic polynomial, respectively, and

a_k, b_m are the corresponding 'orbital' occupancy numbers,

quantifies the π-electron energy difference between conjugated cyclic system and its reference structure. This difference was named the topological resonance energy, TRE, and has been shown *(2-4)*, to correlate with the general properties of conjugated hydrocarbons. In this work has been found that aromatic stabilization of porphins is mainly due to the high topological resonance energy value of pyrrole-type rings, while aromatic stabilization of phthalocyanins is due mainly to high resonance stabilization of i-indole-type rings.

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A03	*Croat.Chem.Acta*	SHORT TITLE	A45	13	REFERENCES	
				1	TABLES	
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A08

π CHARGE DISTRIBUTION FROM MOLECULAR TOPOLOGY AND π ORBITAL ELECTRONEGATIVITY

A11

M. Marsili and J. Gasteiger

A14

Organisch Chemisches Institut der Technischen Universität, München, D-8046 Garching, West Germany

The automatic and computer-aided prediction of reactivity by means of a few basic atomic parameters is achieved. Considering that only the topology of a molecule is required for the computation it is evident that PEOE (partial equalization of orbital electronegativity) and SD-POE (sigma dependent POE) models proposed by the authors together establish a valid alternative to the presently available, time consuming quantum mechanical procedures.

To prove the reliability of the σ charges calculated by the PEOE model, the authors compared them with experimental quantities known to be intrinsically related to atomic charges. This test is of great importance for defining the quality of predicted σ charges which are necessary to enter the π-level calculation. Atomic potential models have been quite successful in correlating core electron binding energy shifts as obtained through ESCA measurements. Authors therefore correlated the carbon charges of a large and representative number of organic molecules with their C-1s-ESCA shifts as shown in Fig 1.

The result is exellent as evident from the correlation coefficient of 0.987. In comparison, for the same compounds, the *ab initio* charges calculated on a STO-3G basis set show a much poorer agreement.

DESCRIPTORS

Electronegativity
orbital, π charge distribution from,

Mathematics
topology molecular, π charge distribution from,

Reactivity
prediction of, basic atomic parameters in relation to,

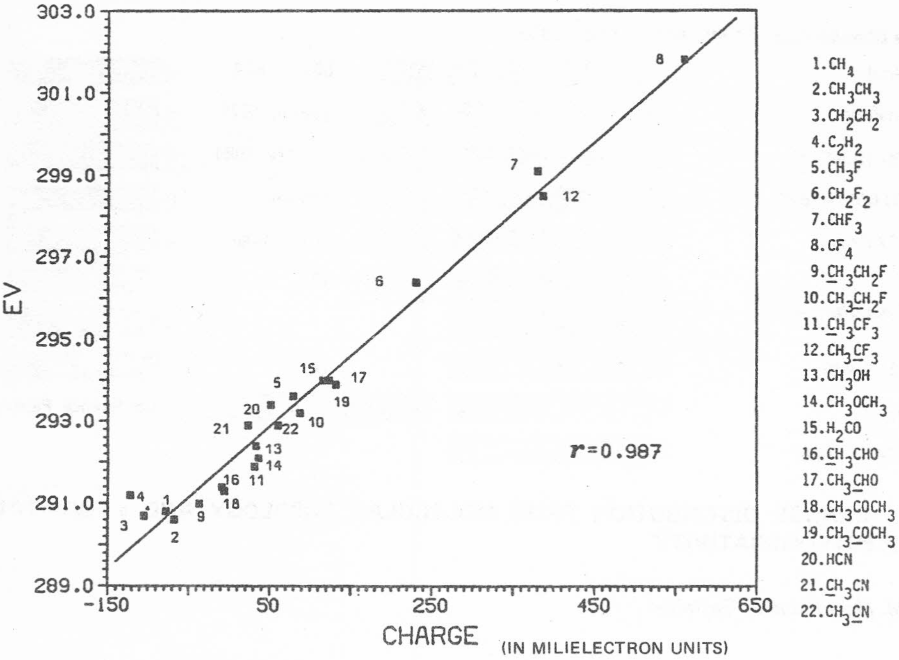

Fig. 1

Furthermore, this approach gives a new insight into the interaction between σ and π electrons which seems worthy of further investigation. In addition, the authors have revived the concept of orbital electronegativity *(1-3)*, especially in the case of the π electrons for which no calculation based on POE (pi orbital electronegativity) has, up to now, ever been performed.

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Abstractor: N. Trinajstić

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Croatica Chemica Acta 53 (4) 615 – 623 (1980)

	Serial	LITERATURE TYPE	A20	615 – 623	PAGES
	Analytic	BIBLIOGR. LEVEL	A21	Sep. 3, 1979	RECEIPT DATE
	547.89	UDC	A22	January 1981	PUBLICAT. DATE
A01	YU 0011–1643	ISSN	A23	English	TEXT LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY LANG
A03	*Croat. Chem. Acta*	SHORT TITLE	A45	23	REFERENCES
				–	TABLES
A05	53 (1980)	VOL. NO. (YEAR)		19	FIGURES
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper	
A07	*CCA – 1247*	OTHER IDENTIFIC.			

A08

A REMARKABLY STABLE AND SIMPLE MONOCYCLIC THIEPIN. SYNTHESIS AND PROPERTIES OF 2,7-DI-*tert*-BUTYL-4-ETHOXYCARBONYL-5-METHYLTHIEPIN

A11

I. Murata, K. Nishino, S. Yano, Y. Kohashi, and K. Yamamoto

A14

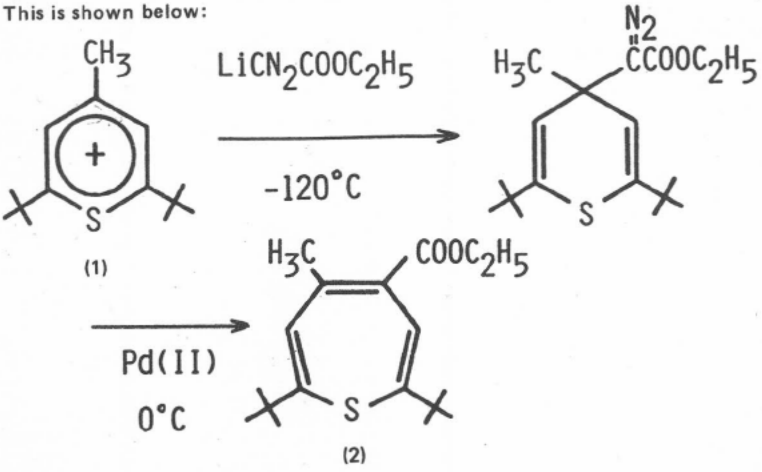
Department of Chemistry, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan

DESCRIPTORS

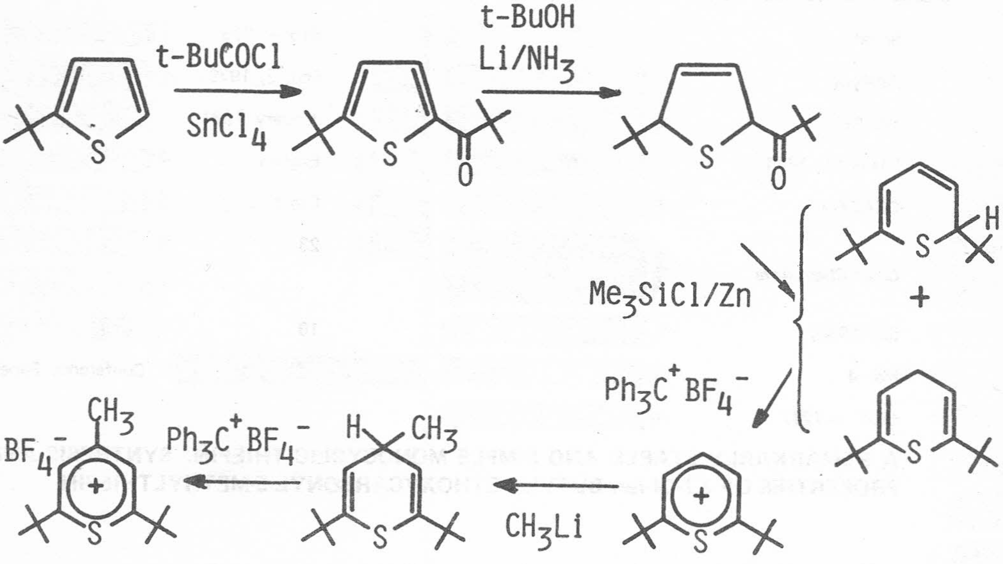
A simple monocyclic 8π electron thiepin, 2,7-di-*tert*-butyl-4-ethoxycarbonyl-5-methylthiepin (2) stabilized by two bulky *tert*-butyl groups at 2- and 7-positions, was synthesized from 2,6-di-*tert*-butyl-4-methylthiopyrylium tetrafluoroborate (1). This is shown below:

Aromaticity
of 8π electron monocyclic thiepin,

Heterocyclic compounds
preparation of thiepin derivative,



The compound 1 is prepared in the following way:



(1)

Inspite of its monocyclic thiepin structure, the compound 2 showed remarkable thermal stability and half-life of 7.1 h at 130 °C. Judging from the ^{1}H-NMR spectrum, the thiepin 2 is considered to be an atropic molecule.

Abstractor: N. Trinajstić

published in
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	Serial	LITERATURE TYPE	A20	625 – 636	PAGES	
	Analytic	BIBLIOGR. LEVEL	A21	Sept. 9, 1979	RECEIPT	DATE
	547.6	UDC	A22	January 1981	PUBLICAT.	
A01	YU 0011–1643	ISSN	A23	English	TEXT	LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat.Chem.Acta*	SHORT TITLE	A45	39	REFERENCES	
				–	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		3	FIGURES	
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper		
A07	*CCA – 1248*	OTHER IDENTIFIC.				

A08

THE STRUCTURE OF POLYFULVENES

A11

M. Neuenschwander, P. Kronig, S. Schönholzer, M. Slongo. B. Ubersax, and C. Rentsch

A14

Institut für Organische Chemie der Univerität Bern, CH–3012 Bern, Switzerland

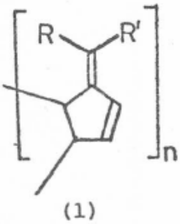
DESCRIPTORS

It is well known that pentafulvenes are very sensitive towards traces of acid, but the structure of the polymers has never been determined so far *(1,2)*. The authors found that the cationic polymerisation of 6,6-disubstituted pentafulvenes yields highly unsaturated, reactive macromolecules (1) of high molecular weight. The mechanistic pathways leading to the polymers are discussed, and the spectroscopic evidence for structure (1) is presented.

Diels-Alder reaction
in thermal oligomerization of pentafulvene,

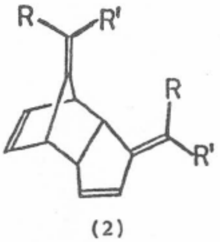
Fulvene
polymerization of,

Polymerization
cationic, of fulvene derivatives,



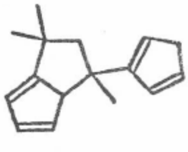
(1)

R, R'= Alkyl, Aryl



(2)

R, R' = H, CH_3



(3)

In contrast to indications of the literature *(3)* the main process in thermal oligomerisation of simple pentafulvenes is a Diels--Alder-reaction, giving products of the type (2).

Anionic polymerization of pentafulvenes may be initiated by traces of sodium cyclopentadienide and phenylsodium, respectively. The reaction product consists of a mixture of oligomers of the series $(\text{fulvene})_n$. This surprising result is explained by structure elucidation of the fulvene dimers, which gives formula (3). The mechanistic aspects of the reaction are discussed.

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Abstractor: N. Trinajstić

published in
Croatica Chemica Acta 53 (4) 637 – 642 (1980)

	Serial	LITERATURE TYPE	A20	637 – 642	PAGES	
	Analytic	BIBLIOGR. LEVEL	A21	Sept. 3, 1979	RECEIPT	DATE
	547.53	UDC	A22	January 1981	PUBLICAT.	
A01	YU 0011–1643	ISSN	A23	English	TEXT	LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat.ChemActa*	SHORT TITLE	A45	4	REFERENCES	
				1	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		4	FIGURES	
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper		
A07	*CCA – 1249*	OTHER IDENTIFIC.				

A08

CONSTRUCTION OF A [15] ANNULENONE – [15] ANNULENYL ION CYCLE

A11 *H. Ogawa, N. Kariya, T. Imoto, H. Kato, and Y. Taniguchi*

A14 Faculty of Pharmaceutical Sciencies, Kyushu University, Fukuoka 812, and Department of Chemistry, Kurume National Technical College, Komorino Kurume 830, Japan

Previously, the authors have reported *(1)* the synthesis of furanoid [15] annulenones (A and D) and their protonated species (B and C). With the benefits of FT nmr spectroscopy, some of experiments have now been reinvestigated.

The annulenone A may undergo dynamic conformational changes to provide an interesting cycle, which can be driven by protonation-deprotonation sequence. Annulenyl ion B formed by protonation step 1 triggers the movement of the inside OH group to the outside positions of the ring as depicted in step 2. The resulting isomeric annulenyl ion C is then deprotonated to provide a less stable annulenone D. The geometrical properties of annulenone D would result in its isomerization to regenerate annulenone A in step 4.

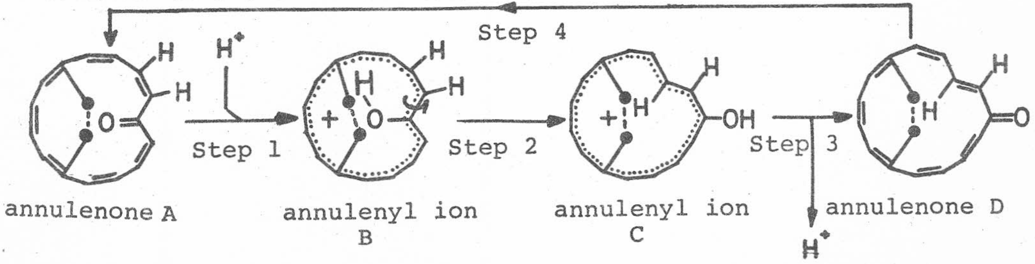
This cycle is of interest in connection with a real biological cycle, proton pump cycle of bacteriorhodopsin *(2)*.

DESCRIPTORS

Annulenes
annulenone and annulenyl ion cycle, construction of.

Nuclear magnetic resonance
of protonated annulenone,

Protonation and Proton transfer reaction
of annulenone and deprotonation of annulenyl ion,



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Abstractors: A. Graovac and N. Trinajstić

published in
Croatica Chemica Acta 53 (4) 643 – 647 (1980)

	Serial	LITERATURE TYPE	A20	643 – 647	PAGES	
	Analytic	BIBLIOGR. LEVEL	A21	July 3, 1979	RECEIPT	DATE
	547.65	UDC	A22	January 1981	PUBLICAT.	
A01	YU 0011–1643	ISSN	A23	English	TEXT	LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat. Chem. Acta*	SHORT TITLE	A45	10	REFERENCES	
				–	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		2	FIGURES	
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper		
A07	*CCA – 1250*	OTHER IDENTIFIC.				

A08

THERMAL REARRANGEMENTS OF AROMATIC COMPOUNDS. II. ISOMERIZATION OF AZULENE-3*a*-^{13}C TO NAPHTHALENE-^{13}C

A11 *L. T. Scott, M. A. Kirms, and M. A. Minton*

A14 Department of Chemistry, University of Nevada, Reno, Nevada 89557, U.S.A.

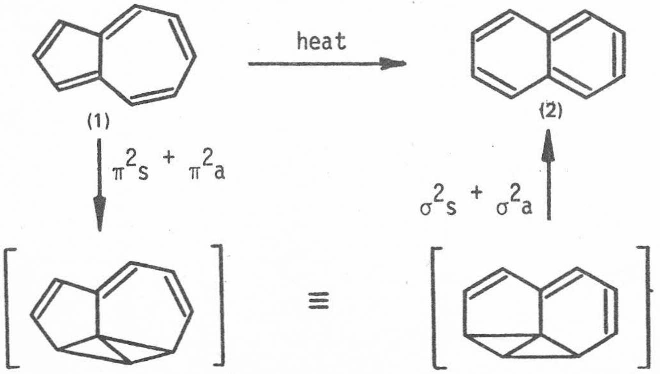
DESCRIPTORS

Aromatic compounds
thermal rearrangement of,

Isomerization
thermal, of azulene to naphthalene,

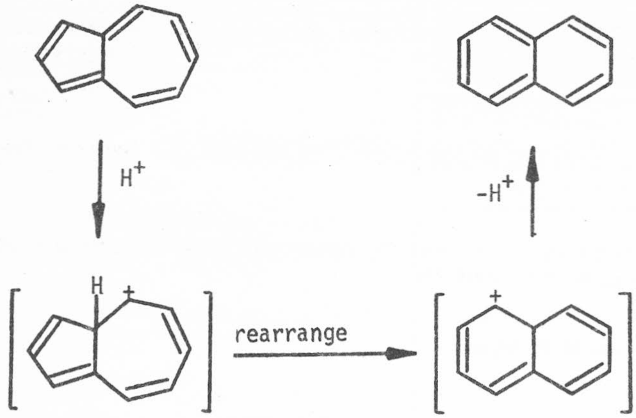
Rearrangement
skeletal, of aromatic compounds,

Thermal rearrangements, though commonplace among unsaturated aliphatic hydrocarbons *(1)*, have only rarely been observed in completely aromatic systems *(2)*. The thermal isomerization of azulene (1) to naphthalene (2) undoubtedly qualifies as the oldest and best known example of such a skeletal reorganization and has stood as a mechanistic puzzle for many decades *(2)*. In particular, the question has arisen *(3)* as to whether or not this rearrangement occurs *via* sequential, concerted, pericyclic reactions analogous to those which so often prevail in nonaromatic systems. Scheme 1 depicts one of possible mechanism *(3)*.



Scheme 1

The simplicity and symmetry-allowed nature of this mechanism make it most appealing. But the ^{13}C-nmr spectrum of naphthalene product has shown that the ^{13}C-label originating in the angular position of azulene are found after isomerization over γ, α, and β positions of naphthalene in a ratio 3:2:1, respectively. Therefore, no single pathway, including the bicyclobutane mechanism, proposed until now could account for the results of this experiment. Scheme 2, however, illustrates the authors' proposal for the thermal rearrangement of azulene to naphthalene.



Scheme 2

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Abstractor: N. Trinajstić

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	Serial	LITERATURE TYPE	A20	649 – 658	PAGES	
	Analytic	BIBLIOGR. LEVEL	A21	Sept. 3, 1979	RECEIPT	DATE
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A01	YU 0011–1643	ISSN	A23	English	TEXT	LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat.Chem.Acta*	SHORT TITLE	A45	29	REFERENCES	
				–	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		5	FIGURES	
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper		
A07	*CCA – 1251*	OTHER IDENTIFIC.				

A08

BONDING IN FUNCTIONALIZED AZIRIDINES: NITROGEN–15 AND CARBON–13 STUDIES

A11

P. Tarburton, J. P. Edasery, C. A. Kingsbury, V. W. Day, C. S. Day, D. S. Soriano, K. F. Podraza, I. Tavaniepour, and N. H. Cromwell

A14

Department of Chemistry, University of Nebraska, Lincoln, Nebraska 68588, U.S.A.

DESCRIPTORS

Aziridines
structure of,

Hyperconjugation
in aziridines, stereoelectronic interactions in relation to,

Two isomeric pairs of *cis*- and *trans*-1-cyclohexyl-2-phenyl-3-benzoylaziridines have been synthesized: (a) with a nitrogen-15 labelled nitrogen, and (b) with carbon-13 labelled ring carbons. The carbon-13 to X (where X = nitrogen-15, carbon-13 or hydrogen-1) spin-spin coupling constants were measured and interpreted in terms of stereoelectronic effects. X-ray crystallographic data of *cis*- and *trans*-1-cyclohexyl-2-phenyl-3-(*p*-toluyl)aziridines appear in good agreement with their NMR data and theoretical calculations based on INDO method *(1)*.

Bonding is discussed for the three-ring itself (NMR studies) and for its substituents (X-ray studies). It is concluded that stereochemical interaction of the Van der Waals type is an important determinant of aziridine bond length. Three-ring to carbonyl hyperconjugation is correlated with stereoelectronic interactions in the *trans* isomer.

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Abstractor: N. Trinajstić

published in
Croatica Chemica Acta 53 (4) 659 – 665 (1980)

	Serial	LITERATURE TYPE	A20	659 – 665	PAGES	
	Analytic	BIBLIOGR. LEVEL	A21	Sept. 3, 1979	RECEIPT	DATE
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A01	YU 0011–1643	ISSN	A23	English	TEXT	LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY	
A03	*Croat. Chem. Acta*	SHORT TITLE	A45	13	REFERENCES	
				–	TABLES	
A05	53 (1980)	VOL. NO. (YEAR)		2	FIGURES	
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper		
A07	*CCA – 1252*	OTHER IDENTIFIC.				

A08

CYCLOBUTENE – FUSED AROMATIC MOLECULES

A11

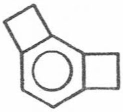
R. P. Thummel

A14

Department of Chemistry, University of Houston, Houston, Texas 77004, U.S.A.

The Diels-Alder cycloaddition of dimethyl-1,2-cyclobutenedicarboxylate to a 1,3-diene results in the formation of an adduct which can subsequently be decarboxylated and dehydrogenated to provide a cyclobutene-fused benzenoid system *(1,2)*. The use of appropriate dienes has led to the preparation of a series of *para-* and *meta-* bis-annelated benzenes including 1, 2, and higher homologs. Variations in the ^1H and ^{13}C nmr and in the UV spectra are found to be a function of the size of the annelated rings as well as their relative orientation.

1



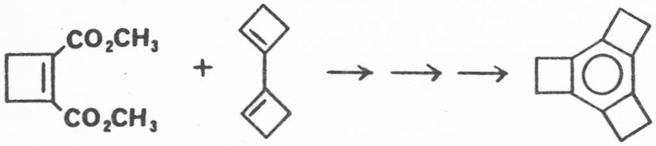
2

A similar approach has been employed in a preparation of the very elusive tricyclobutabenzene (5) which may represent the missing link between 1,5,9-cyclododecatriyne and 6-radialene. Tricyclobutabenzene is a stable crystalline material whose physical properties are quite consistent with higher homologs. An X-ray structure of the perfluoro analog of 5 shows no evidence for any bond alternation.

DESCRIPTORS

Aromatic compounds
cyclobutene-fused benzenoid system, properties of

Diels–Alder reaction
of dimethyl-1,2-cyclobutene-dicarboxylate and 1,3-diene,



3 4 5

A double-barreled application of the Diels-Alder approach has led to the synthesis of naphtho[*b,e*]dicyclobutene (6). The physical properties *(3)* of this molecule will also be compared to higher homologs.

6

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Abstractor: N. Trinajstić

published in
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	Serial	LITERATURE TYPE	A20	667 – 673	PAGES
	Analytic	BIBLIOGR. LEVEL	A21	Oct. 19, 1979	RECEIPT DATE
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A01	YU 0011–1643	ISSN	A23	English	TEXT LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY LANG
A03	*Croat. Chem. Acta*	SHORT TITLE	A45	9	REFERENCES
				–	TABLES
A05	53 (1980)	VOL. NO. (YEAR)		1	FIGURES
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION	Conference Paper	
A07	*CCA – 1253*	OTHER IDENTIFIC.			

A08

ZERO–FIELD SPLITTING PARAMETERS D OF MACROCYCLIC SYSTEMS

A11

H. Vogler

A14

MPI für Medizinische Forschung, Abteilung Organische Chemie, D-6900 Heidelberg, Germany

The macrocyclic systems studied were annulenes and corannulenes.

There is considerable interest in the chemical and physical properties of annulenes *(1)*, *i.e.* completely conjugated monocarbocyclic polyenes, the ring size being indicated by a number in brackets. It is well known that [4*n* + 2]- and [4*n*]annulenes can be classified as aromatic and antiaromatic concerning their ground state stabilities *(2)* and magnetic properties as proton chemical shifts *(1,3)* or diamagnetic exaltations *(4)*. Corannulenes *(5)* consist of two perimeters which are connected by radial bonds. Considering benzenoid alternant corannulenes the inner and the outer annulene are always of the same type and differ by 12 carbon atoms. Up to now only three members of this class of compounds have been synthesized, *i.e.* pyrene, coronene and kekulene *(6)*.

The triplet zero-field splitting parameters D of [4*n*]- and [4*n* + 2]-annulenes are calculated within a pi-model *(7)*. The zero-field splitting (ZFS) parameter D is a measure of the magnetic dipole-dipole interaction of the two unpaired electrons of the triplet state.

DESCRIPTORS

Annulenes
zero-field splitting parameters calculation of,

Bond length
alternation in annulenes compared with ground state properties,

The dependence of parameter D on *n* and the degree of bond lengths alternation is compared with that of ground state properties like magnetic ring currents. Furthermore it is shown that corannulenes which consist of two concentric perimeters with connecting radial bonds cannot be regarded as macrocyclic annulenoid systems in the triplet state.

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Abstractor: N. Trinajstić

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	Serial	LITERATURE TYPE	A20	675 – 685	PAGES
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A01	YU 0011–1643	ISSN	A23	English	TEXT LANG
A02	CCACAA	CODEN	A24	Croat. Engl.	SUMMARY LANG
A03	*Croat.Chem.Acta*	SHORT TITLE	A45	31	REFERENCES
				1	TABLES
A05	53 (1980)	VOL. NO. (YEAR)		12	FIGURES
A06	No. 4	ISSUE NO.	CAT. OF CONTRIBUTION		Conference Paper
A07	*CCA – 1254*	OTHER IDENTIFIC.			

A08

POSITION DEPENDENCE OF SCF SCREENED POTENTIAL IN SEVERAL NONBENZENOID AROMATIC HYDROCARBONS CONTAINING A FOUR–MEMBERED RING

A11

H. Yamaguchi, K. Ninomiya, and M. Ogata

A14

Department of Chemistry, Faculty of Science, Kumamoto University, Kumamoto 860, Japan

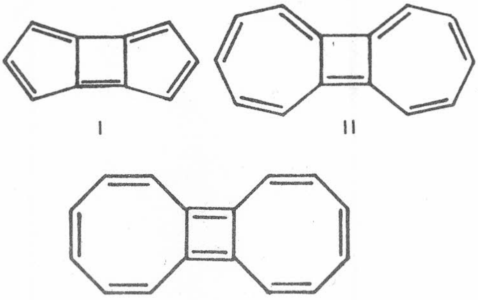
DESCRIPTORS

The electronic structures of nonbenzenoid aromatic hydrocarbons containing a four-membered ring have been of interest since Lin and Krantz provided the first physical evidence for the structure of cyclobutadiene *(1)*.

The position dependence of the SCF screened potential in several nonbenzenoid aromatic hydrocarbons containing a four-membered ring (Scheme 1) has been investigated using the SCF screened potential MO CI method *(2,3)*.

Aromatic hydrocarbons, properties
nonbenzenoid systems, MO calculations,

Molecular orbital
SCF screened potential in nonbenzenoid systems, position dependence of,



Scheme 1

The starting bond distortions, belonging to the A_g, B_{1g}, and B_{3u} representations, all converge into the unique self-consistent set of bond lengths belonging to the molecular symmetry group D_{2h}, while the distortions belonging to B_{2u} converge into another set of bond lengths belonging to C_{2v}.

From the dependence of the SCF screened potential for a number that indicates the kind of screened potential, it can be seen that there is only one kind of screened potential at each of the numbers in the D_{2h} structure and at the even numbers in the C_{2v} structure. However, under the influence of the bond-length alternation, there are two kinds of screened potentials, screening and anti-screening, at the odd numbers in the C_{2v} structure. Such characteristics of the screened potentials in the C_{2v} structure show a tendency similar to those of the polyene ($C_{10}H_{12}$).

From the above results, it may be concluded that molecules I, II, and III have polyolefinic character.

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Abstractor: N. Trinajstić

DOCUMENTA CHEMICA YUGOSLAVICA

CROATICA CHEMICA ACTA

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Zagreb, 25. siječnja 1981.

SADRŽAJ

Prilozi

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