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STRICTLY PERICONDENSED BENZENOID ISOMERS

Jerry Ray Dias
Department of Chemistry
University of Missouri
Kansas City, MO 64110, USA

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Abstract

Systematic treatment of isomers of benzenoid hydrocarbons led to the discovery of constant-isomer benzenoid series where the series with the same isomer number have a one-to-one topological correspondence of their benzenoid membership.

Introduction

The enumeration of even carbon nonradical benzenoid hydrocarbons is of practical interest to experimental chemistry, and our work in this area has evolved several important concepts and related terminology[1-3]. Numerous computerized results have since appeared after our conceptual approach had been published[4]. However, many of these papers deal with excessively large hypothetical systems of little practical value and published in a form of little use to the practicing chemist. The work of Knop and coworkers remains the single most important resource to practicing chemists[5]. Strictly pericondensed benzenoids have all their internal third degree vertices mutually connected, have no catacondensed appendages, a minimal number of bay regions, and have no triplet of bay regions (fjords).

Discussion

The motivation for this paper is to present an extention of the numerical results of Stojmenovic and coworkers[6] far beyond the formula of $C_{112}H_{26}$ using our prior depictions and algorthim to enumerate strictly pericondensed benzenoids[3]. While presenting a more or less historical review, S.J. Cyvin and coworkers[7] have used our methodologies and prior depictions[8] guided by the numerical results of Stojmenovic and coworkers[6] to improve our enumeration results which were already improved by us[3]. Unfortunately, because the numerical data of Stojmenovic and coworkers ended at $C_{112}H_{26}$, Cyvin and coworkers were unable to go beyond this point. It is always easier to solve a problem when you already have the answer. Although, references 17 and 18 of this recent paper[7] cite the computer data of Stojmenovic and coworkers as the original source, our data should have been cited explicitly in this MATCH paper[7].

Tables 1 and 2 greatly extend the isomer data for our constant-isomer series, and Table 3 provides additional data for adjacent strictly pericondensed benzenoids. The algorithm used to evolve this data has already been detailed elsewhere[3]. Table 1 contains particularly important data since these even carbon strictly pericondensed benzenoids are speculated to be ultimate pyrolytic carbonization products. Since the benzenoids formulas in Tables 1 to 3 cannot correspond to benzenoid systems with helicenic components or benzenoid-related systems with holes (circulenes), these isomer numbers are <u>totally unambiguous</u>.

Table 1. Constant Isomer Series of Even Strictly Pericondensed Benzenoids.

Series	No. of Isomers	Series	No. of Isomers
$C_{10}H_8$	1	$C_{40}H_{16}$	3(1)
$C_{32}H_{14}$		$C_{76}H_{22}$	
$C_{66}H_{20}$		$C_{128}H_{28}$	
$C_{112}H_{26}$		:::	
$C_{170}H_{32}$		$C_{50}H_{18}$	7(2)
:::		$C_{92}H_{24}$	
$C_{16}H_{10}$	1	$C_{146}H_{30}$	
$C_{42}H_{16}$		:::	
$C_{80}H_{22}$		$C_{62}H_{20}$	12(4)
$C_{130}H_{28}$		$C_{108}H_{26}$	
:::		$C_{166}H_{32}$	
$C_{22}H_{12}$	2(1)[a]	$C_{236}H_{38}$	
$C_{52}H_{18}$		:::	
$C_{94}H_{24}$		$C_{76}H_{22}$	12(4)
$C_{148}H_{30}$		$C_{126}H_{28}$	
:::		$C_{188}H_{34}$	
$C_{24}H_{12}$	1	:::	
$C_{54}H_{18}$		$C_{90}H_{24}$	27(12)
$C_{96}H_{24}$		$C_{144}H_{30}$	
$C_{150}H_{30}$		$C_{210}H_{36}$	
:::		:::	
$C_{30}H_{14}$	3(1)	$C_{106}H_{26}$	38(19)
$C_{64}H_{20}$		$C_{164}H_{32}$	
$C_{110}H_{26}$		$C_{234}H_{38}$	
$C_{168}H_{32}$		:::	
:::			

a) The number of less stable diradical isomers is given in parentheses.

Table [1] (cont'd)

Series	No. of Isomers	Series	No. of Isomers
$C_{124}H_{28}$	38(19)		
$C_{186}H_{34}$			
$C_{260}H_{40}$			
:::			
$C_{142}H_{30}$	86(47)	$C_{230}H_{38}$	616
$C_{208}H_{36}$		$C_{312}H_{44}$	
$C_{286}H_{42}$		$C_{406}H_{50}$	
:::		:::	
$C_{162}H_{32}$	128(71)[b]	$C_{256}H_{40}$	616
$C_{232}H_{38}$		$C_{342}H_{46}$	
$C_{314}H_{44}$		$C_{440}H_{52}$	
:::		:::	
$C_{184}H_{34}$	128(71)	$C_{282}H_{42}$	1265
$C_{256}H_{40}$		$C_{372}H_{48}$	
$C_{344}H_{46}$		$C_{474}H_{54}$	
:::		:::	
$C_{206}H_{36}$	428[c]	$C_{310}H_{44}$	∿1800
$C_{284}H_{42}$		$C_{404}H_{50}$	
$C_{374}H_{48}$		:::	
:::		$C_{340}H_{46}$	∿1800[b]
		$C_{438}H_{52}$	
		:::	

b) Predicted values on induction.

c) Sum of radical and nonradical isomers is underlined.

Table [2]. Constant Isomer Series of Odd Strictly Pericondensed Benzenoids.

Series	No. of Isomers	Series	No. of Isomers
$C_{13}H_9$	1	$C_{69}H_{21}$	13[b]
$C_{37}H_{15}$		$C_{117}H_{27}$	
$C_{73}H_{21}$		$C_{177}H_{33}$	
$C_{121}H_{27}$		:::	
:::			
$C_{19}H_{11}$	1	$C_{83}H_{23}$	20[b]
$C_{47}H_{17}$		$C_{135}H_{29}$	
$C_{87}H_{23}$		$C_{199}H_{35}$	
$C_{139}H_{29}$		:::	
:::			
$C_{27}H_{13}$	1	$C_{99}H_{25}$	20
$C_{59}H_{19}$		$C_{155}H_{31}$	
$C_{103}H_{25}$		$C_{223}H_{37}$	
$C_{159}H_{31}$		:::	
:::			
$C_{35}H_{15}$	2	$C_{115}H_{27}$	48
$C_{71}H_{21}$		$C_{175}H_{33}$	
$C_{119}H_{27}$		$C_{247}H_{39}$	
$C_{179}H_{33}$		:::	
:::			
$C_{45}H_{17}$	4[a]	$C_{133}H_{29}$	74
$C_{85}H_{23}$		$C_{197}H_{35}$	
$C_{137}H_{29}$		$C_{273}H_{41}$	
$C_{201}H_{35}$		:::	
:::			
$C_{57}H_{19}$	4	$C_{153}H_{31}$	74
$C_{101}H_{25}$		$C_{221}H_{37}$	
$C_{157}H_{31}$		$C_{301}H_{43}$	
$C_{225}H_{37}$		:::	
:::			

a) In the previous enumeration , one structure was inadvertently overlooked.

b) These two series were published with undetected misprints .

Table 2. (cont'd)

Series	No. of Isomers	Series	No. of Isomers
$C_{173}H_{33}$	174	$C_{243}H_{39}$	550
$C_{245}H_{39}$		$C_{327}H_{45}$	
$C_{329}H_{45}$		$C_{423}H_{51}$	
...		...	
$C_{195}H_{35}$	258	$C_{269}H_{41}$	796
$C_{271}H_{41}$		$C_{357}H_{47}$	
$C_{359}H_{47}$		$C_{457}H_{53}$	
...		...	
$C_{219}H_{37}$	258	$C_{297}H_{43}$	796[c]
$C_{299}H_{43}$		$C_{389}H_{49}$	
$C_{391}H_{49}$		$C_{493}H_{55}$	
...		...	

c) Predicted value based on induction.

Table 3. Number of Isomers of Near-Staircase Edge Strictly Peri-condensed Benzenoids

Formula	No. of Isomers[a,b]
$C_{111}H_{27}$	490
$C_{113}H_{27}$	167
$C_{129}H_{29}$	730
$C_{131}H_{29}$	251
$C_{149}H_{31}$	761
$C_{151}H_{31}$	255
$C_{171}H_{33}$	542
$C_{193}H_{35}$	787
$C_{217}H_{37}$	793
$C_{58}H_{20}$	85(44)
$C_{72}H_{22}$	103(53)
$C_{74}H_{22}$	36(17)
$C_{86}H_{24}$	79(42)
$C_{104}H_{26}$	121(65)
$C_{120}H_{28}$	561
$C_{122}H_{28}$	125(69)
$C_{138}H_{30}$	1160
$C_{140}H_{30}$	413
$C_{156}H_{32}$	1688
$C_{160}H_{32}$	600
$C_{180}H_{34}$	1733
$C_{182}H_{34}$	610
$C_{204}H_{36}$	1247
$C_{228}H_{38}$	1781
$C_{254}H_{40}$	1793

a) The number of less stable diradical isomers is given in parentheses.

b) The sum of radical and nonradical isomers is underlined.

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