Distribution of K, the Number of Kekulé Structures in Benzenoid Hydrocarbons Part IV. Benzenoids with 10 and 11 Hexagons

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Z. Naturforsch. **41**, 1429–1430 (1986); received September 15, 1986

An approximate asymptotic formula is derived for the number of normal benzenoids. For this category and h (number of hexagons) = 10 and 11 all numbers of Kekulé structures were computer and systematized.

Introduction

The benzenoid hydrocarbons [1] have been enumerated some time ago for $h = 10$ [2], where h is the number of hexagons. Recently the number of catacondensed benzenoids and the total number of benzenoids have been determined by Doroslovački and Tošić according to a private communication quoted by Gutman [3]. In the present work we have deduced the numbers 4803 and 21 804 for the normal pericondensed benzenoids of $h = 10$ and 11, respectively. For precise definitions of the different classes of benzenoids, see, e.g. [4]. In the present work we report further details for the $h = 10$ and 11 benzenoids with special emphasis on their number of Kekulé structures (K).

The normal pericondensed benzenoids of $h = 11$ together with the catacondensed systems constitute the 42919 normal systems of benzenoids; the corresponding figure for $h = 10$ is 10375. The number of essentially disconnected benzenoids [5] as well as non-Kekuléans is so far unknown for $h = 11$.

Approximate Asymptote

The knowledge of the number of normal benzenoids for all h values through 11 makes it feasible to derive an approximate asymptotic formula for these numbers, say N_h. It is expected to acquire the same degree of accuracy as the corresponding Gutman [3] formulas for the number of catacondensed benzenoids (C_h) and all benzenoids (B_h). It was found:

$$N_h \approx 0.0242\, h^{-0.9}(4.5)^h .$$

The largest difference from the exact value, viz. 74, occurs at $h = 11$. For comparison Gutman's [3] formulas give the differences 69 and 801 for C_h and B_h, respectively.

Distribution of K

The numbers of Kekulé structures (K) for normal benzenoids have been studied intensively. The complete distributions have been reported for $h = 1, \ldots, 6$ [4, 6] $h = 7$ [6], $h = 8$ and 9 [7]. Figure 1 shows a diagram of the corresponding distribution for $h = 10$. A list of the actual numbers is too voluminous to be given here. That is also the case of a full report on the K distribution for $h = 11$, for which $12 \leqq K \leqq 302$. Therefore we only give some averages of the K numbers.

Average K Values and Related Quantities

A kind of Kekulé structure statistics was introduced previously [7], where the average K values for

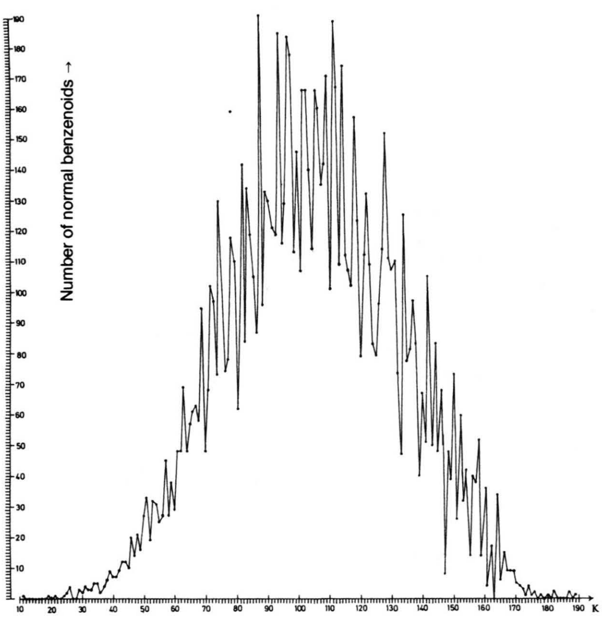

Fig. 1. Distribution of K for all normal benzenoids with $h = 10$.

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Table 1. Average K values and related quantities*.

h	$\langle K \rangle$			$K_{max}(h-1)$
	cat	np	n	
10	116.7	90.12	104.4	110
11	185.0	141.4	162.8	189
h	$(\ln \langle K \rangle)/h$			
	cat	np	n	
10	0.476	0.450	0.465	
11	0.475	0.450	0.463	

* Abbreviations: cat catacondensed; n normal; np normal pericondensed.

normal benzenoids, say $\langle K^{\mathrm{n}} \rangle$, seem to be the most interesting. The list for h up to 9 [7] is supplemented by $h = 10$ and 11 in Table 1. Also the averages for catacondensed, $\langle K^{\mathrm{cat}} \rangle$, and normal pericondensed, $\langle K^{\mathrm{np}} \rangle$, were computed separately. These two classes together constitute all the normal benzenoids. The quantity $(\ln \langle K \rangle)/h$ was found to be of particular interest [7] and seems to approach a limiting value, especially when the average for all normal benzenoids is taken. The present extension to $h = 10$ and 11 does not contradict this behaviour, but it has not been proved mathematically.

Average and maximum K values

It was observed [7] that the quantity $\langle K^n \rangle$ for a given $h \leqq 9$ falls very near the maximum K for one unit less, i.e. $K_{max}(h-1)$, but constantly somewhat above. For $h = 10$ we find (cf. Table 1) that $\langle K^n \rangle$ for the first time comes slightly below $K_{max}(9)$, and the tendency is enhanced for $h = 11$.

Concluding Remarks

The classification of all the 141 229 benzenoids with 11 hexagons is a formidable task, but it is especially interesting because of the concealed non-Kekuléans [8], which appear among them for the first time, i.e. for the lowest possible h value. These systems with no Kekulé structures have the same number of black and white vertices [9]. The existence of such systems was pointed out in the cited paper [9], where two of them are depicted. More examples have been found later [10, 11]. Altogether eight concealed non-Kekuléans with $h = 11$ [8] have been detected, but it has not been proved that no more of them exist. Neither in the present work this particular problem has been solved, but some steps have been taken in that direction.

Acknowledgement

Financial support to BNC from The Norwegian Research Council for Science and the Humanities is gratefully acknowledged.

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