

ALL-BENZENOID SYSTEMS:

DISTRIBUTION OF K , THE NUMBER OF KEKULÉ STRUCTURES,
IN BENZENOID HYDROCARBONS. XI

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(received: March 1990)

Abstract: The 239 normal benzenoids with $h \leq 7$, where h is the number of hexagons, are depicted and supplied with K values. Here K is the number of Kekulé structures. The distributions of K for the catacondensed and normal pericondensed benzenoids for $h \leq 11$ are given. Table and diagram forms are employed. Diagrams are also given for all-benzenoids, which were studied for $h \leq 18$ (catacondensed up to $h=22$). Maximal K numbers are discussed for all-benzenoids (which all are normal) and the normal benzenoids in general. Average K numbers from the mentioned distributions of K for normal benzenoids are compared with averages from the corresponding subset of all-benzenoids. In all cases the averages for all-benzenoids are higher than those for normal benzenoids. This provides a quantitative justification for referring to the all-benzenoid hydrocarbons as particularly stable systems chemically.

INTRODUCTION

Fully benzenoids¹⁻³ or all-benzenoids⁴⁻⁶ (the term adopted here) are known to be especially stable hydrocarbons, as is manifested by their high numbers of Kekulé structures (K) in relation to the numbers of hexagons (h). Here we shall demonstrate this feature in a quantitative way by means of "Kekulé structure statistics".⁷⁻¹¹

Definitions: A benzenoid (system) is defined as a geometrically planar, simply connected polyhex. It may be either Kekuléan or non-Kekuléan. The Kekuléan systems (which possess Kekulé structures) are divided into *essentially disconnected* (resp. *normal*) depending on whether they have (resp. have not) fixed bonds in their Kekulé structures. The *neo* classification (normal n ; essentially disconnected ε ; non-Kekuléan o) takes into account all benzenoid systems.

It has been proved¹² that all-benzenoid systems are normal (n) in the frames of the *neo* classification.¹³ We shall compare some average K values for all-benzenoids with given h values, viz. $\langle K_{\text{all}}(h) \rangle$, with the corresponding averages of normal benzenoids, viz. $\langle K_n(h) \rangle$. It seems reasonable in this way to consider the all-benzenoids as a subset of normal benzenoids only, not including the essentially disconnected (e) systems. For the e systems, namely, the K numbers behave "unnormally" in the following way. Assume that an e system with h' hexagons has K' Kekulé structures. For perylene, for instance, $h' = 5$, $K' = 9$. Then there exist e systems with $K=K'$ for any $h \geq h'$. Thus, for instance, there are e systems with $K=9$ for any $h \geq 5$. The n benzenoids, on the other hand, have a lower limit of K depending on h , which is $K_{\min} = h+1$. Therefore there are no normal benzenoids with $K=9$ for $h \geq 9$. (For $h=9$ there are 21 e benzenoids with $K=9$.) The "normal" behaviour for K numbers is that they (loosely speaking) increase with increasing h . Precisely: Let $B_n(h+1)$ be a normal benzenoid with $h+1$ hexagons generated from a normal benzenoid with h hexagons, viz. $B_n(h)$. Then for the K numbers: $K\{B_n(h+1)\} > K\{B_n(h)\}$.

After this discussion it is not very surprising that the average K value is decreased when essentially disconnected benzenoids are included.⁹ Our comparison of all-benzenoids with the set of normal benzenoids will therefore be more significant than it would be if the essentially disconnected systems were included.

Before we do this comparison we need a preparation dealing with the whole set of normal benzenoids. A considerable amount of facts is known about these systems in supplement of the previously published material.⁷⁻¹¹ In particular we have determined the K distributions for catacondensed systems (which are normal benzenoids) and normal pericondensed systems separately for all $h \leq 11$. We will find this separation especially useful when dealing with the all-benzenoids.

As a matter of fact the largest part of this work is devoted to normal benzenoids in general. The last (relatively short) sections include "all-benzenoid statistics".

FORMS OF NORMAL BENZENOIDS

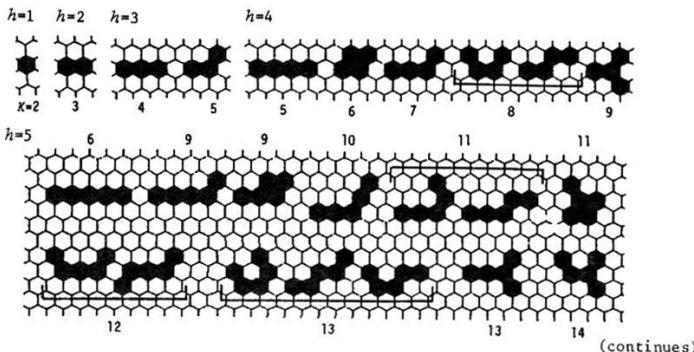
The forms of all benzenoids for $h \leq 5$ have been depicted by several authors.¹⁴⁻¹⁶ The pictures up to $h=4$ are reproduced in a review.¹⁷ In further publications the range of h was extended to 6,^{18,19} and to 7.²⁰ We

are interested in listings of benzenoids with K numbers indicated of the type as was displayed for $h \leq 4$ in another review.²¹ All benzenoids for $h \leq 9$ are depicted in a book²² and supplied with K numbers. In fact also the corresponding mammoth listing of the 30086 forms for $h=10$ has been reported²³ as unpublished data. These listings^{22,23} do not take the *neo* classification into account, while we are especially interested in the normal (n) benzenoids and their K numbers. All benzenoids classified according to *neo* and supplied with K numbers have been published for $h \leq 5$,⁸ and $h \leq 6$.²⁴ In continuation of this material we show in Fig. 1 the 167 forms of normal benzenoids with $h=7$ ordered according to increasing K numbers and with the K numbers themselves indicated. For the sake of completeness the figure also contains the 72 forms for $h \leq 6$.

DISTRIBUTION OF K FOR NORMAL BENZENOIDS

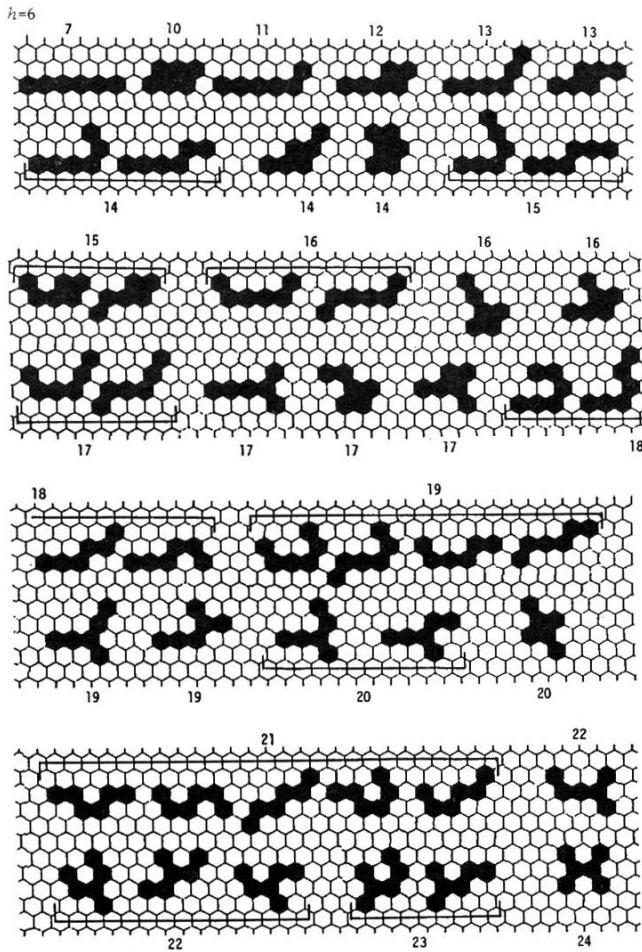
A distribution of K for a given h indicates the numbers of benzenoids with the different K values. The distributions of K for normal benzenoids have been given in terms of diagrams for $3 \leq h \leq 6$,⁷ $h=7$,^{7,24} $h=8$ and 9 ,²⁴ and $h=10$.¹⁰ Tables of numerical values are also available, especially for the distribution of K for normal benzenoids with $h=10$.²⁴

We have produced the distributions of K for catacondensed and normal pericondensed benzenoids separately and introduced a procedure for computer-generation of the diagrams. They are shown in Figs. 2a-2e. Also included are the curves for normal benzenoids in total. The hand-drawings for h up to 10 are reproduced, while the curve for $h=11$ is given for the first time.



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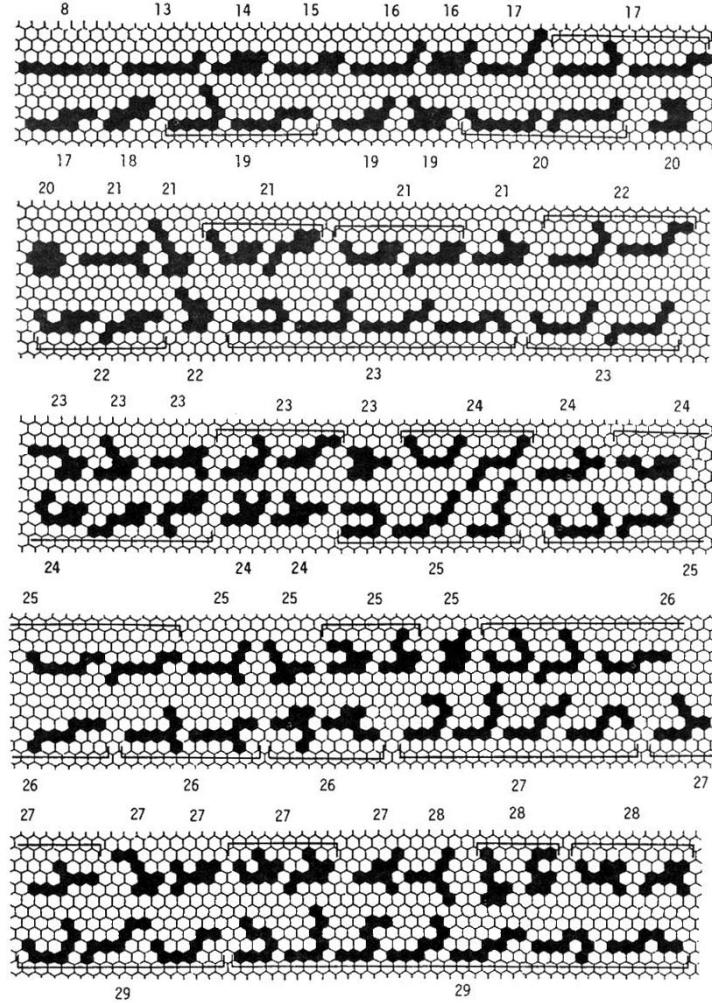
Fig. 1 (continued)



(continues)

Fig. 1 (continued)

$h=7$



(continues)

Fig. 1 (continued)

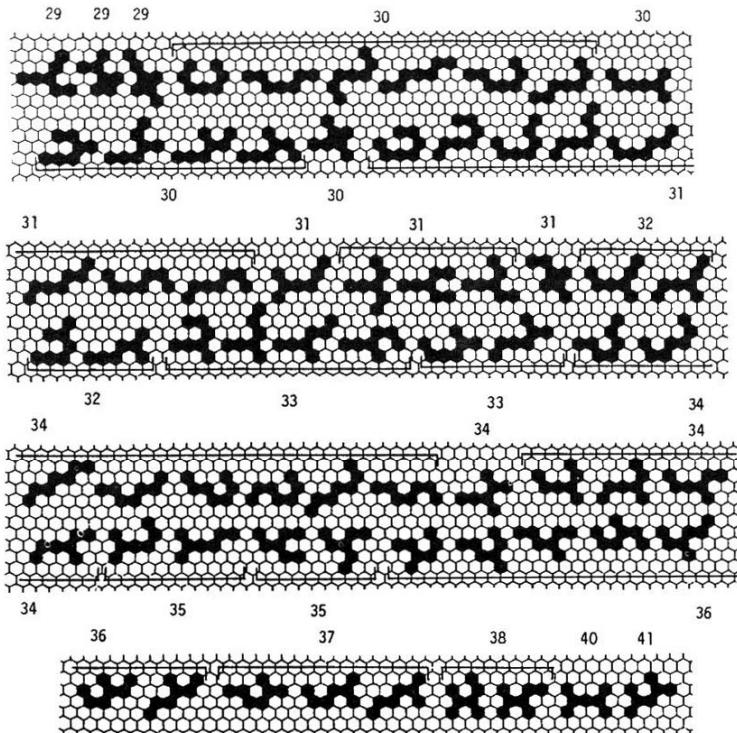


Fig. 1. All normal benzenoids with $h \leq 7$. K numbers are indicated. Bracketed systems are isoarithmetic.

The curves (Fig. 2) give a general idea of the behaviour of the distributions of K under consideration. Sometimes it is useful to have the exact numbers. A complete information to this effect (for $h \leq 11$) is supplied in Table 1.

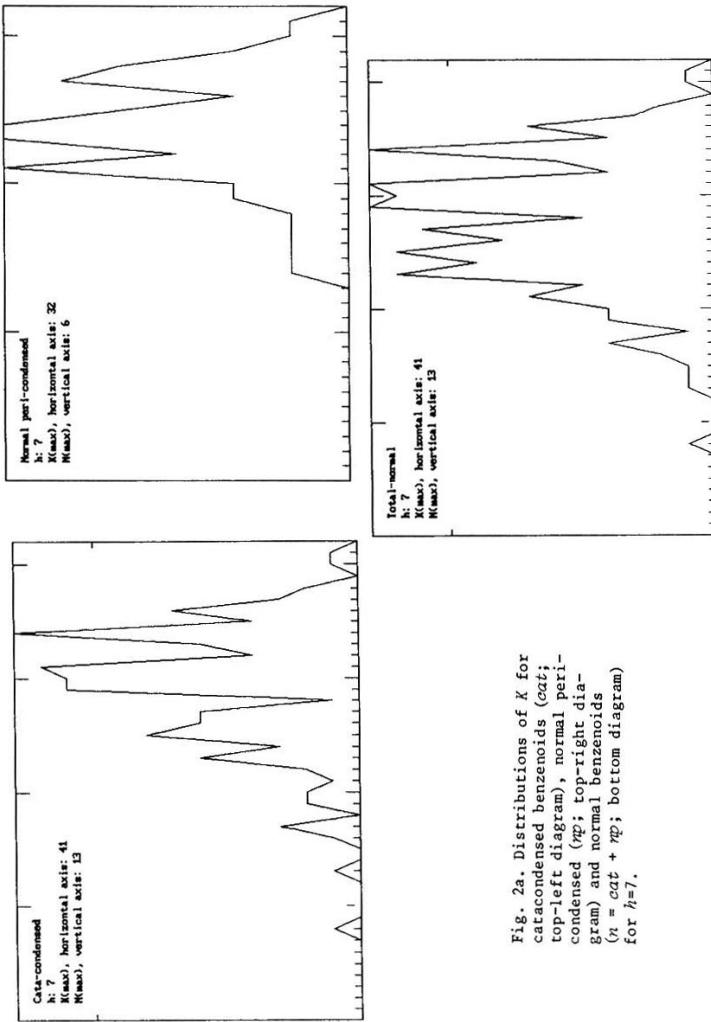


Fig. 2a. Distributions of K for catacondensed benzenoids (cat; top-left diagram), normal pericondensed ($\#p$; top-right diagram) and normal benzenoids ($n = cat + \#p$; bottom diagram) for $h=7$.

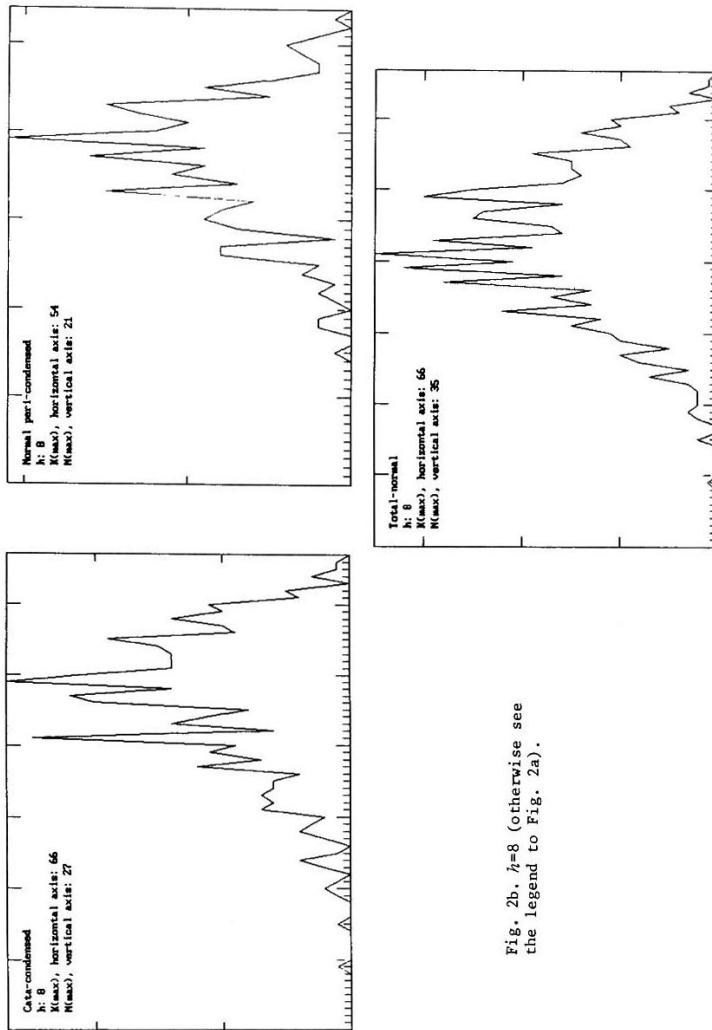


Fig. 2b, $h=8$ (otherwise see
the legend to Fig. 2a).

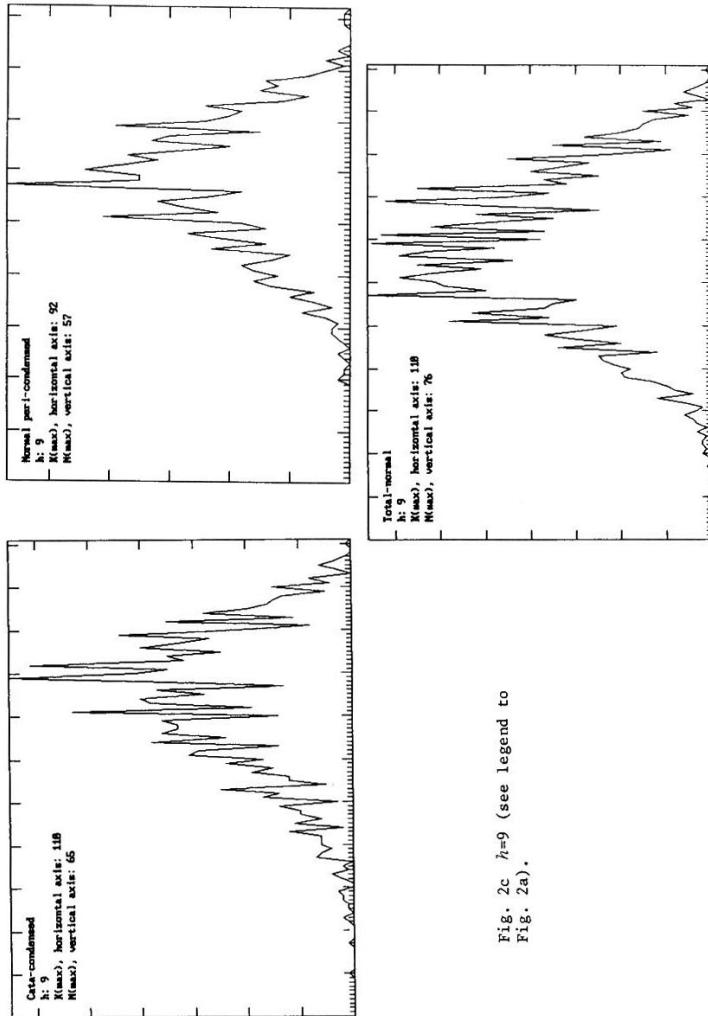


Fig. 2c $h=9$ (see legend to
Fig. 2a).

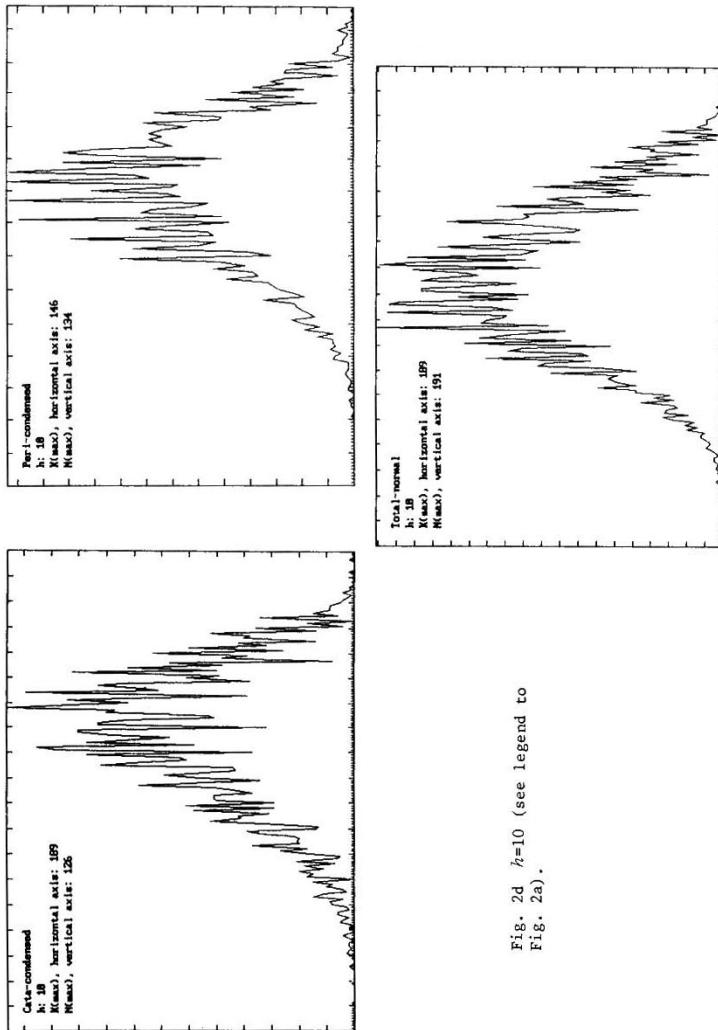


Fig. 2d $h=10$ (see legend to
Fig. 2a).

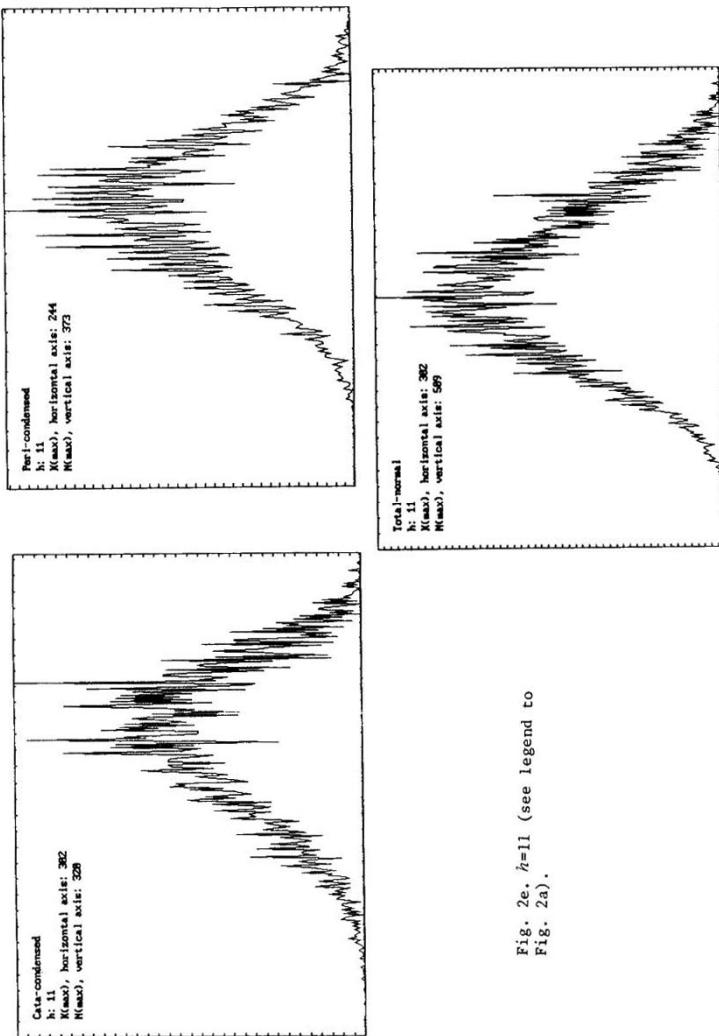


Fig. 2e. $h=11$ (see legend to
Fig. 2a).

Table 1. Numbers of catacondensed (*cat*) and normal pericondensed (*np*) benzenoids with $h \leq 11$ at given K numbers.

K	$h=1$		$h=2$		$h=3$		$h=4$		$h=5$		$h=6$		$h=7$		$h=8$		
	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	
2	1																
3		1															
4			1														
5			1	1	0												
6				0	1	1	0										
7			1	0	0	0	0	1	0								
8			2	0	0	0	0	0	0	1	0						
9			1	0	1	1	0	0	0	0	0	1	0				
10				1	0	0	1	0	1	0	0	0	0	1	0	0	
11							2	1	1	0	0	0	0	0	0	0	
12							2	0	0	1	0	0	0	0	0	0	
13							4	0	1	1	1	1	0	0	0	0	
14							1	0	2	2	0	1	0	0	0	0	
15									2	2	0	1	1	1	1	1	
16									2	2	1	1	0	0	0	0	
17									3	2	3	1	0	0	0	0	
18									4	0	0	1	0	0	2	2	
19									6	0	2	2	1	2	2	2	
20									2	1	2	2	2	2	0	0	
<hr/>			<hr/>			<hr/>			<hr/>			<hr/>			<hr/>		
K	$h=6$		$h=7$		$h=8$		K	$h=7$		$h=8$		K	$h=8$		K	$h=8$	
	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>		<i>cat</i>	<i>np</i>	<i>cat</i>	<i>np</i>		<i>cat</i>	<i>np</i>		<i>cat</i>	<i>np</i>
21	5	0	1	6	1	1	41	1	0	25	10	61	4	0			
22	4	0	2	3	0	2	42			6	13	62	5	0			
23	2	0	6	6	2	1	43			14	15	63	0	0			
24	1	0	3	6	4	3	44			11	5	64	3	0			
25			8	4	1	2	45			8	9	65	1	0			
26			6	2	0	8	46			20	5	66	1	0			
27			6	5	2	8	47			22	2						
28			1	4	4	1	48			14	2						
29			11	2	3	7	49			27	3						
30			11	1	2	9	50			21	4						
31			12	1	7	8	51			14	2						
32			4	0	6	6	52			14	0						
33			6	0	7	15	53			14	1						
34			13	0	6	7	54			15	0						
35			4	0	6	11	55			19	0						
36			7	0	4	9	56			9	0						
37			3	0	12	16	57			10	0						
38			2	0	7	9	58			14	0						
39			0	0	11	21	59			10	0						
40			1	0	9	12	60			11	0						

(continues)

Table 1 (continued)

K	h=9				h=10				h=11				K	h=9				h=10				h=11			
	cat		np		cat		np		cat		np			cat		np		cat		np		cat		np	
	10	1	0			0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
19	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
21	0	1	0	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	1	2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	1	0	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
27	2	1	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
28	2	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
29	3	3	1	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
30	0	3	0	2	0	2	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
31	0	2	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
32	2	4	2	1	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
33	4	8	1	2	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
34	1	3	2	3	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
35	2	6	2	3	2	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
36	0	10	0	2	3	2	3	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
37	7	6	2	2	2	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
38	6	13	4	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
39	4	16	1	8	2	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
40	6	12	0	7	0	2	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
41	6	16	2	5	2	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
42	6	18	0	9	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
43	12	13	5	7	4	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
44	2	10	4	8	1	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
45	11	23	2	8	0	8	0	8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
46	6	14	6	14	0	5	0	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
47	10	21	6	8	2	7	0	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
48	10	27	2	19	0	4	0	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
49	14	14	3	13	5	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
50	3	18	8	19	2	11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
51	17	41	9	24	2	6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
52	14	22	4	15	2	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
53	25	28	15	17	4	5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
54	5	32	11	20	6	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
55	12	23	3	22	2	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
56	12	18	4	23	2	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
57	19	57	10	35	3	17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
58	15	35	8	19	6	14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
59	24	35	15	23	10	21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
60	17	44	0	29	4	19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(continues)

Table 1 (continued)

K	h=10				h=11				K	h=10				h=11				
	cat		np		cat		np			cat		np		cat		np		
	—	—	—	—	—	—	—	—		—	—	—	—	—	—	—	—	
111	108	81	49	258	141	49	2	85	373	171	4	0	127	178				
112	115	52	20	129	142	102	3	136	227	172	3	0	179	147				
113	58	51	104	151	143	50	0	94	198	173	1	0	179	175				
114	97	77	43	218	144	82	1	85	318	174	4	0	176	261				
115	80	32	57	144	145	48	0	106	181	175	1	0	154	108				
116	67	40	56	172	146	67	1	138	180	176	2	0	137	156				
117	88	14	40	263	147	8	0	84	342	177	0	0	204	219				
118	100	57	98	132	148	48	0	150	213	178	1	0	275	142				
119	100	23	50	137	149	39	0	161	243	179	0	0	168	133				
120	32	47	51	251	150	73	0	117	317	180	1	0	148	181				
121	93	19	85	153	151	26	0	144	225	181	0	0	232	136				
122	93	39	65	142	152	60	0	103	215	182	2	0	155	95				
123	82	27	48	328	153	32	0	114	325	183	0	0	227	169				
124	51	32	60	180	154	42	0	119	125	184	0	0	77	134				
125	53	26	76	154	155	14	0	159	226	185	0	0	153	135				
126	90	6	38	234	156	40	0	128	271	186	0	0	309	138				
127	87	27	116	224	157	38	0	177	261	187	2	0	199	81				
128	126	26	53	179	158	52	0	164	189	188	0	0	219	119				
129	103	8	62	338	159	14	0	172	337	189	1	0	152	89				
130	82	25	92	151	160	36	0	106	188	190			151	139				
131	104	6	80	222	161	4	0	120	157	191			151	104				
132	72	1	67	254	162	17	0	139	323	192			240	123				
133	39	8	80	186	163	0	0	154	216	193			188	67				
134	119	6	91	163	164	34	0	124	219	194			223	107				
135	71	6	59	263	165	6	0	137	199	195			154	55				
136	77	4	80	239	166	15	0	179	238	196			218	67				
137	93	4	122	245	167	9	0	204	178	197			162	81				
138	80	3	99	304	168	9	0	137	236	198			183	94				
139	38	2	103	229	169	9	0	175	136	199			212	39				
140	61	6	105	156	170	5	0	179	181	200			193	68				

(continues)

Table 1 (continued)

K	h=11			K	h=11			K	h=11			K	h=11		
	<i>cat</i>		<i>np</i>		<i>cat</i>		<i>np</i>		<i>cat</i>		<i>np</i>		<i>cat</i>		<i>np</i>
	—	—	—		—	—	—		—	—	—		—	—	—
201	114	75		231	66	0		261	8	0		291	0	0	
202	193	57		232	142	4		262	62	0		292	11	0	
203	112	54		233	151	6		263	18	0		293	1	0	
204	172	53		234	143	1		264	56	0		294	0	0	
205	154	32		235	82	3		265	2	0		295	0	0	
206	186	83		236	184	2		266	29	0		296	2	0	
207	274	2		237	28	3		267	7	0		297	3	0	
208	210	43		238	134	0		268	39	0		298	0	0	
209	138	29		239	31	0		269	38	0		299	0	0	
210	231	20		240	76	1		270	23	0		300	0	0	
211	156	2		241	93	1		271	1	0		301	0	0	
212	226	31		242	136	0		272	44	0		302	2	0	
213	168	11		243	96	1		273	3	0					
214	221	28		244	83	1		274	35	0					
215	156	15		245	37	0		275	10	0					
216	210	14		246	146	0		276	15	0					
217	107	3		247	26	0		277	9	0					
218	253	13		248	115	0		278	7	0					
219	166	8		249	117	0		279	7	0					
220	105	20		250	63	0		280	4	0					
221	98	7		251	22	0		281	0	0					
222	320	14		252	55	0		282	17	0					
223	134	13		253	27	0		283	3	0					
224	149	6		254	120	0		284	15	0					
225	123	2		255	39	0		285	1	0					
226	183	8		256	90	0		286	5	0					
227	182	12		257	16	0		287	0	0					
228	153	9		258	68	0		288	2	0					
229	90	4		259	58	0		289	1	0					
230	180	15		260	78	0		290	1	0					

ALL-BENZENOIDS (INTRODUCTORY)

It was pointed out that all-benzenoids form a subset of normal benzenoids. An advantage of studying the all-benzenoids separately is the practical possibility of carrying out the analyses to significantly larger h values. As Knop et al.²⁵ pointed out 18 systems represent the whole set of all-benzenoids for $h \leq 10$, while all benzenoids with $h \leq 10$ count 38472 systems. Also the number of the normal benzenoids with $h \leq 10$ is quite sizable, viz. 13788. In Fig. 1 the 239 normal benzenoids with $h \leq 7$ are depicted. Less than half of this number, exactly 114 systems, cover the all-benzenoids for $h \leq 13$ as depicted elsewhere.²⁶

The "statistical" data for all-benzenoids in the last three sections are all consistent with the previous computerized analysis of the systems.²⁶

DISTRIBUTIONS OF K FOR ALL-BENZENOIDS

The distributions of K for all-benzenoids with $h \leq 13$ are easily surveyed from Fig. 3 of Ref. 26. Already for $h=10$ we find a distinct separation between the K numbers for the pericondensed and catacondensed systems. The three pericondensed systems have K values around 100 (actually $100 \leq K \leq 104$), while the K values for the six catacondensed systems are found within 183 ± 6 . We may say that the K values form two "clusters". For $h=11$ the all-benzenoid systems, which all are pericondensed, have K values around 200 ($198 \leq K \leq 205$). The systems with $h=12$, which also are all pericondensed, exhibit again two clusters, viz. $K = 227 \pm 3$ and $K = 407 \pm 12$. It is not difficult to recognize these two clusters by the forms of the benzenoids. Those with the higher K values pertain to pyrenes with catacondensed appendages, while the lower K values are associated with a higher pericondensation. Finally we look at the pictures of all-benzenoids with $h=13$ (Fig. 3 of Ref. 26). In a "low resolution" there are three clusters: (1) the "cluster" consisting of one K value, viz. 250, (2) $K = 460 \pm 16$ and (3) $K = 827 \pm 36$. The last cluster (3) originates precisely from the catacondensed systems.

Fig. 3a (bottom diagram) shows the distribution of K for all-benzenoids with $h=13$. The three clusters described above are clearly recognized. In the top-row diagrams, where the K distributions for the catacondensed and pericondensed systems are given separately, the clusters are displayed under "higher resolution". The subsequent figures (Figs. 3b-3g) show the distributions of K for all-benzenoids with $h \leq 19$ (only catacondensed for $h=19$). Clusters are recognized in all cases. For $h=16$ we find again a complete separation between the K values for the pericondensed ($K \leq 2195$) and the catacondensed ($K \geq 3524$) systems.

MAXIMAL K VALUES

Table 2 shows the maximal K numbers for $h \leq 11$, for the (normal) catacondensed (*cat*) and normal pericondensed (*per*) systems, in consistence with Table 1. The data for $h=12$ and 13 (*cat* only) were derived elsewhere.^{7,11} The

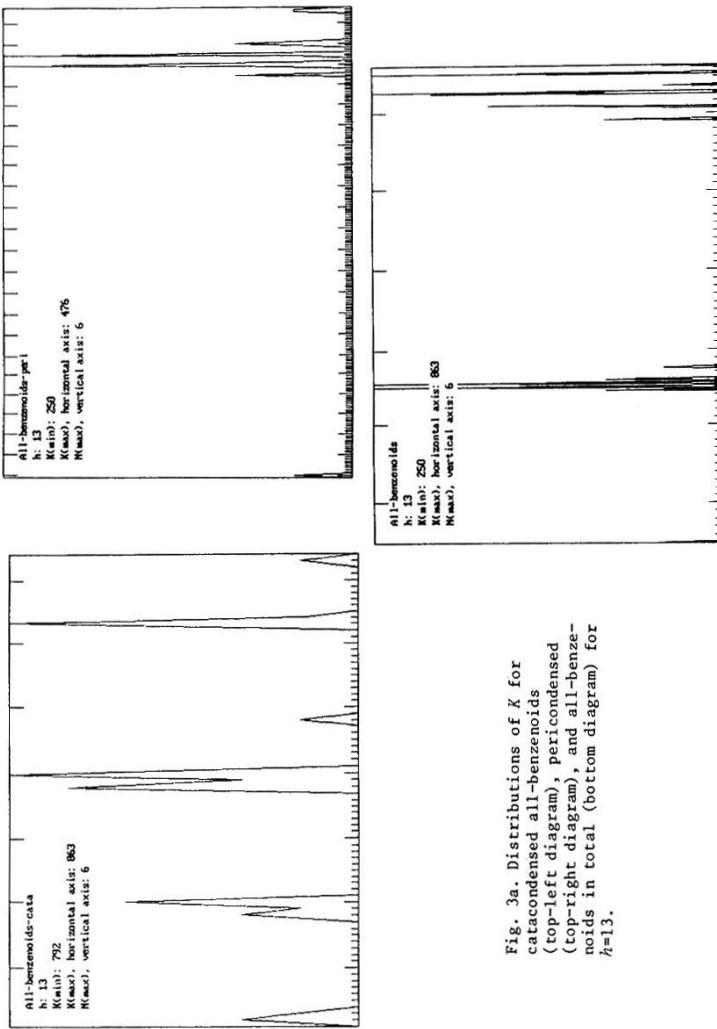


Fig. 3a. Distributions of K for cationcondensed all-benzenoids (top-left diagram), pericondensed (top-right diagram), and all-benzenoids in total (bottom diagram) for $h=13$.

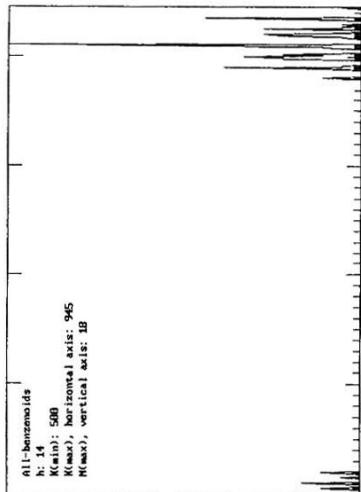
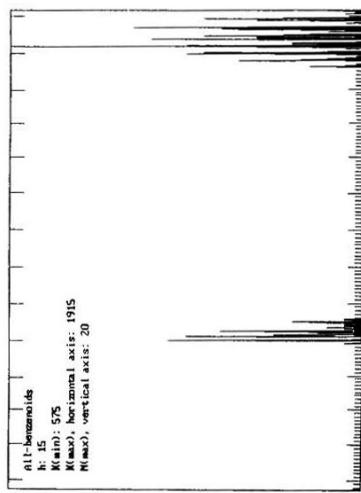


Fig. 3b. Distribution of K for (pericondensed) all-benzenoids with $h=14$.

Fig. 3c. Distribution of K for (pericondensed) all-benzenoids with $h=15$.

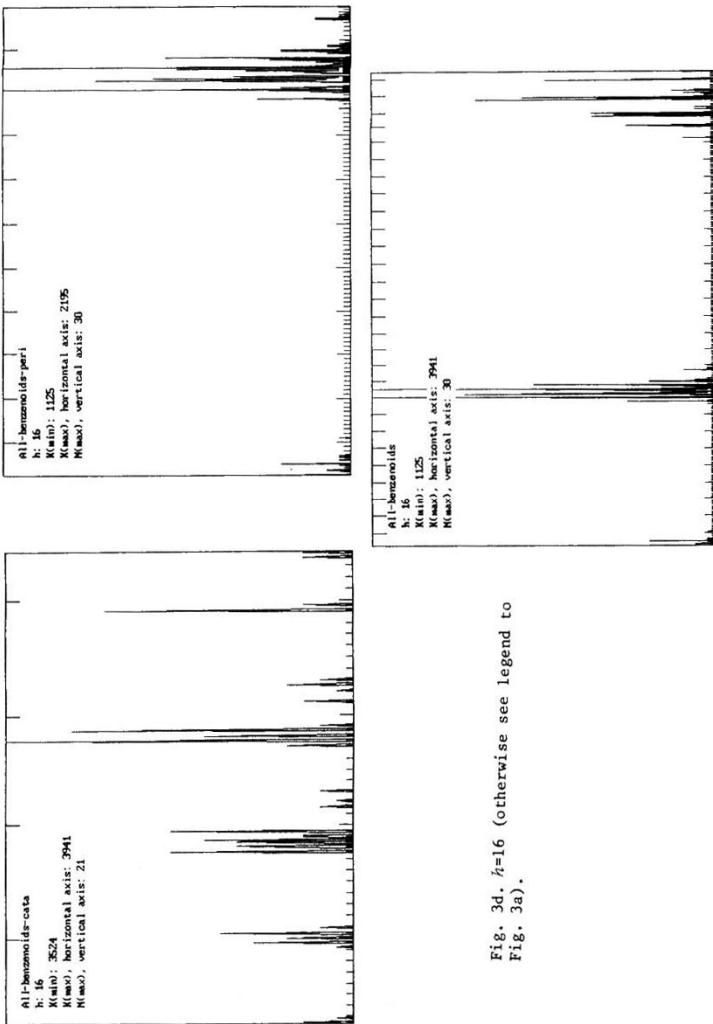


Fig. 3d, $\delta_1=16$ (otherwise see legend to Fig. 3a).

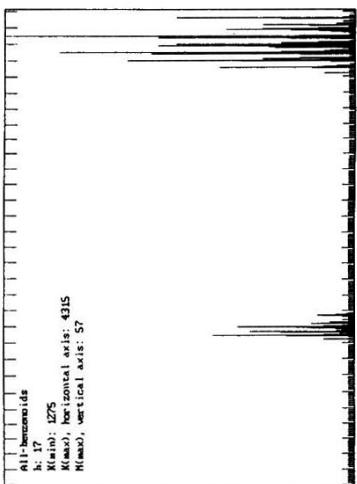
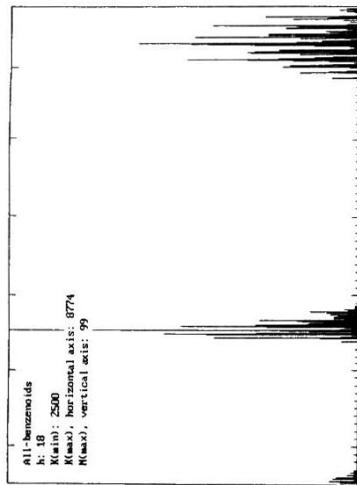


Fig. 3e. Distribution of K for (pericondensed) all-benzenoids with $h=17$.

Fig. 3f. Distribution of K for (pericondensed) all-benzenoids with $h=18$.

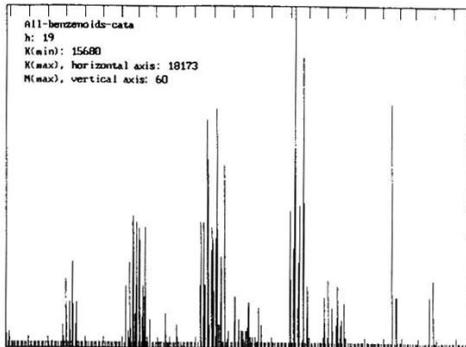


Fig. 3g. Distribution of K for catacondensed all-benzenoids with $h=19$.

corresponding maximal K numbers for all-benzenoids are included in Table 2; data up to $h=16$ (*cat* and *per*) and $h=19, 22$ (*cat* only) are available.²⁶

A well supported conjecture states that the system with $K = K_{\max}$ among normal benzenoids for a given h is a catacondensed system, branched for $h \geq 4$.^{7,11} Furthermore, these systems are all-benzenoids for $h = 1, 4, 7, 10, \dots$, i.e. every third h value. Table 2 is seen to be completely consistent with these conjectures.

The normal pericondensed systems with $K = K_{\max}$ are all-benzenoids for $h=6$ and 9 .⁷ It is believed that such a system in general consists of one pyrene subunit and otherwise catacondensed appendages; it has two internal vertices in total. Furthermore, we conjecture that the normal pericondensed systems with $K = K_{\max}$ are all-benzenoids for all $h = 6, 9, 12, \dots$, i.e. every third value. For the other h values we should expect that $K = K_{\max}$ among normal pericondensed benzenoids is realized for a system which is not an all-benzenoid. Table 2 meets this expectation for $h = 8, 10$ and 11 .

AVERAGE K VALUES

From the material of Table 1 we have computed the average K values, $\langle K \rangle$ for normal benzenoids, catacondensed and pericondensed separately, and for the total. The results are collected in Table 3, where the corresponding data for all-benzenoids are included. In every case we find $\langle K \rangle(\text{all-benzenoid}) \geq \langle K \rangle(\text{normal})$ when corresponding entries are compared (provided

Table 2. Values of K_{\max} for normal benzenoids and all-benzenoids (cat catacondensed; per pericondensed).

h	K_{\max} (normal)		K_{\max} (all-benzenoid)	
	cat	per	cat	per
1	2	-	2	-
2	3	-	-	-
3	5	-	-	-
4	9	6	9	-
5	14	11	-	-
6	24	20	-	20
7	41	31	41	-
8	66	53	-	45
9	110	91	-	91
10	189	146	189	104
11	302	214	-	205
12	504	419?	-	419
13	863	+	863	476
14	†	†	-	945
15	†	1915?	-	1915
16	3941?	†	3941	2195
17	†	†	-	4315
18	†	8774?	-	8774
19	18173?	†	18173	†
22	82991?	†	82991	†

† Unknown

that all-benzenoids exist in the particular case); the equality applies only to the trivial case of $h=1$. We find significant differences and believe that the rule is valid for all h . In conclusion we consider the above rule as a quantitative justification for the statement that all-benzenoid hydrocarbons are especially stable chemically.

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

Table 3. Average values of K for normal benzenoids and all-benzenoids (cat catacondensed; per pericondensed; tot total).

h	< K >(normal)			< K >(all-benzenoid)		
	cat	per	tot	cat	per	tot
1	2	-	2	2	-	2
2	3	-	3	-	-	-
3	4.5	-	4.5	-	-	-
4	7.4	6	7.17	9	-	9
5	11.41	10	11.21	-	-	-
6	18.36	14.92	17.5	-	20	20
7	29.12	23.47	27.46	40.5	-	40.5
8	46.36	36.58	42.83	-	45	45
9	73.52	57.53	66.94	-	90	90
10	116.70	90.12	104.40	184.17	101.67	156.67
11	184.99	141.36	162.83	-	202	202
12	†	†	†	-	382.17	382.17
13	†	†	†	827.91	446.56	660.65
14	†	†	†	-	867.70	867.70
15	†	†	†	-	1597.70	1597.70
16	†	†	†	3739.80	1982.01	2556.80
17	†	†	†	-	3752.70	3752.70
18	†	†	†	-	6585.03	6508.03
19	†	†	†	16871.33	†	†
22	†	†	†	76141.23	†	†

† Unknown

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