

ESSENTIALLY DISCONNECTED BENZENOIDS:

DISTRIBUTION OF K , THE NUMBER OF KEKULÉ STRUCTURES,
IN BENZENOID HYDROCARBONS - VII

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Abstract: The distributions of the number of Kekulé structures for essentially disconnected benzenoids are extended to systems with 10 and 11 hexagons.

The "anatomy" of essentially disconnected "hexagonal animals" was discussed in the preceding article.¹ It should be consulted for definitions and the results of enumerations. The present work deals with the distributions of K for essentially disconnected benzenoids, where K is the number of Kekulé structures. A distribution of K describes the number of systems with a given h as a function of K , say $N_h(K)$.

The distributions of K for a set of normal benzenoids and a set of essentially disconnected benzenoids are known to be substantially different.²

GENERAL PROPERTIES OF K

For the class of essentially disconnected benzenoids the number of systems with a given K , viz.

$$N(K) = \sum_h N_h(K)$$

is either zero or infinite. The allowed K values, which give nonvanishing $N_h(K)$, may be written $p \cdot q$, where p and q are integers greater than two. The first allowed K values are 9, 12, 15, 16, 18, 20, 21, 24, 25 and 27.

Let an allowed K value be realized at $h_{\min}(K)$ as the lowest h value. For $K=9$, for instance, $h_{\min}(9)=5$. Furthermore, $K=9$ is also realized for all $h > 5$. In general, a given K value is always realized for all $h \geq h_{\min}(K)$.

From the previously published material² it is found:

K	$h_{\min}(K)$
9	5
12, 15	6
$16 \leq K \leq 25$	7
$27 \leq K \leq 42$	8

At the first sight one might also believe that $h_{\min}(K) = 9$ for $44 \leq K \leq 70$. This is true only for the allowed K values within this interval except $K=68$ (which also is allowed). For this value one finds (see the next section) $h_{\min}(68) = 10$.

DISTRIBUTION OF K

Table 1 summarizes the distributions of K for $h = 5, 6, 7, 8, 9$.² It is extended by the corresponding material for $h=10$ and 11, which implies the 3732 ($h=10$) and 19960 ($h=11$) systems.¹

From Table 1 also an extension of the $h_{\min}(K)$ values is feasible. Firstly, one finds $h_{\min}(K) = 10$ for $K=68$ and $72 \leq K \leq 115$. Secondly, $h_{\min}(K) = 11$ for most of the allowed values within the interval $116 \leq K \leq 196$, but with the exception of $K=188$ and 195. A closer inspection has shown that $h_{\min}(188) = h_{\min}(195) = 12$. This is documented by the below examples.

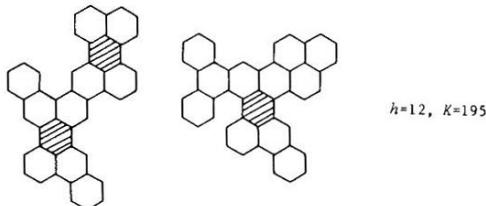
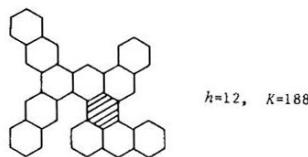


Table 1. Distributions of K , viz. $N_h(K)$, for essentially disconnected benzenoids with $5 \leq h \leq 11$.

K	$h=5$	6	7	8	9	10	11	K	$h=10$	11	K	$h=11$
9	1	1	3	7	21	64	210	76	37	133	133	147
12		1	2	6	22	74	253	77	65	202	135	154
15		1	4	9	29	99	338	78	51	202	136	156
16			2	4	9	28	92	80	43	212	138	116
18			1	5	14	54	204	81	46	287	140	78
20			2	7	19	63	217	84	65	356	141	109
21			4	8	26	83	278	85	37	172	143	120
24			3	7	25	91	328	87	51	168	144	195
25			2	6	19	50	158	88	56	211	145	101
27				11	24	80	307	90	71	368	147	205
28				7	17	53	178	91	52	174	148	9
30				5	22	74	279	92	6	125	150	172
32				5	10	32	127	93	49	199	152	108
33				9	27	73	239	95	42	190	153	53
35				8	26	77	245	96	34	276	154	62
36				4	38	108	406	98	8	126	155	97
39				7	24	70	208	99	17	353	156	96
40				5	23	66	235	100	10	172	159	43
42				1	26	81	273	102	36	183	160	52
44					17	54	154	104	35	182	161	23
45					37	132	453	105	32	386	162	42
48					24	97	296	108	17	304	165	97
49					17	37	117	110	12	142	168	93
50					6	28	94	111	5	153	169	54
51					19	64	162	112	5	186	170	72
52					13	46	143	114	2	119	171	32
54					18	62	261	115	6	147	174	34
55					18	79	224	116		89	175	18
56					22	74	232	117		300	176	30
57					21	69	196	119		124	177	22
60					13	103	393	120		335	180	54
63					12	135	398	121		85	182	14
64					9	34	134	123		185	183	5
65					14	67	205	124		87	184	15
66					6	59	208	125		115	185	10
68					0	32	125	126		245	186	6
69					3	69	172	128		77	190	4
70					2	58	220	129		125	192	3
72						134	408	130		110	196	2
75						89	300	132		182		

Table 2. Average K values.

h	n	e	$n+e$	$n+e+o$
1	2 ^a	.	2 ^a	2 ^a
2	3 ^a	.	3 ^a	3 ^a
3	4.5 ^a	.	4.5 ^a	3 ^a
4	7.17 ^a	.	7.17 ^a	6.14 ^a
5	11.21 ^a	9 ^a	11.07 ^a	7.55 ^a
6	17.5 ^a	12 ^a	17.18 ^a	10.81 ^a
7	27.46 ^a	17.70 ^a	26.28 ^a	15.08 ^a
8	42.83 ^a	25.53 ^a	40.09 ^a	21.35 ^a
9	66.94 ^a	37.58 ^a	60.64 ^a	30.04 ^a
10	104.40 ^b	55.00	91.33	42.82
11	162.83 ^b	84.99	136.86	60.93

^aB.N. Cyvin, J. Brunvoll, S.J. Cyvin and I. Gutman, Match 21, 301 (1986).^bWith one decimal in: S.J. Cyvin, J. Brunvoll and B.N. Cyvin, Z. Naturforsch. 41a, 1429 (1986).Table 3. Values of $(\ln K)/h$.

h	n	e	$n+e$	$n+e+o$
1	0.6931 ^{a,b}	.	0.6931 ^b	0.6931 ^b
2	0.5493 ^{a,b}	.	0.5493 ^b	0.5493 ^b
3	0.5014 ^{a,b}	.	0.5014 ^b	0.3662 ^b
4	0.4924 ^{a,b}	.	0.4924 ^b	0.4538 ^b
5	0.4834 ^{a,b}	0.4394 ^b	0.4808 ^b	0.4042 ^b
6	0.4770 ^{a,b}	0.4142 ^b	0.4739 ^b	0.3968 ^b
7	0.4733 ^{a,b}	0.4105 ^b	0.4670 ^b	0.3877 ^b
8	0.4697 ^{a,b}	0.4050 ^b	0.4614 ^b	0.3826 ^b
9	0.4671 ^{a,b}	0.4029 ^b	0.4561 ^b	0.3781 ^b
10	0.4648 ^c	0.4007	0.4514	0.3757
11	0.4630 ^c	0.4039	0.4472	0.3736

^aWith three decimals in: B.N. Cyvin, J. Brunvoll, S.J. Cyvin and I. Gutman, Match 21, 301 (1986).^bCurve in: B.N. Cyvin, J. Brunvoll, S.J. Cyvin and I. Gutman, Match 21, 301 (1986).^cWith three decimals in: S.J. Cyvin, J. Brunvoll and B.N. Cyvin, Z. Naturforsch. 41a, 1429 (1986).

AVERAGE K VALUES AND RELATED QUANTITIES, $(\ln\langle K \rangle)/h$

We are now able to extend the previous material^{2,3} concerning the title quantities. One of the cited papers² should be consulted for the definitions. Table 2 shows the deduced average K values, viz. $\langle K \rangle$. The corresponding values of $(\ln\langle K \rangle)/h$ are collected in Table 3. The recent results of enumeration of benzenoids, which were needed in these deductions, are available from the consolidated report by fourteen authors.⁴

By means of the data of Table 3 the curves in Fig. 4 of Ref. 2 may be extended by two units in h . The curves marked n , $n+e$ and $n+e+o$ continue the trend of a slight decrease with increasing h . For e , somewhat unexpectedly, the curve is found to increase from $h=10$ to $h=11$. It is clear that one should be very careful before assuming a hypothetic limit value for anyone of these curves when $h \rightarrow \infty$.

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