PREDICTING THE NUMBER OF HEXAGONAL SYSTEMS WITH 24 AND 25 HEXAGONS

Frédéric Chyzak[1], **Ivan Gutman**[2], **and Peter Paule**[3]

[1] *INRIA-Rocquencourt, B.P. 105, F–78153 Le Chesnay Cedex, France*

[2] *Faculty of Science, University of Kragujevac, P.O. Box 60, YU–34000 Kragujevac, Yugoslavia*

[3] *Research Institute for Symbolic Computation, Johannes Kepler University Linz, A–4040 Linz, Austria*

Abstract

We predict the number of hexagonal systems consisting of 24 and 25 hexagons to be $H_{24} = 122237774262384$ and $H_{25} = 606259305418149$, with 6 and 5 significant digits, respectively. Further estimates for H_n up to $n = 31$ are also given.

Hexagonal Systems

Informally speaking, a *hexagonal system* can be viewed as a connected arrangement of hexagonal cells packed in the same way as the typical honeycomb arrangement in a beehive. More formally, it is a finite connected plane graph with no cut-vertices, in which all interior regions are mutually congruent regular hexagons [1]. Hexagonal systems have from time to time attracted the attention of mathematicians (and were named "*hexagonal animals*", "*honeycomb systems*", "*polyhexes*", etc.), in connection with statistical physics and applications to lattice gas models [2, 3, 4]. But the main interest in them comes from chemistry: hexagonal systems are the natural graph representations of *benzenoid hydrocarbons*, whence the names "*benzenoid graphs*", "*benzenoid systems*", and "*fusenes*" used in the chemical literature. An enormous literature exists on various chemical applications of hexagonal systems. We refer to [5, 6] for details and references.

One of the classical problems in the theory of hexagonal systems is their enumeration. In what follows, the number of non-isomorphic hexagonal systems consisting of n hexagons is denoted by H_n, where "non-isomorphic" means viewed up to translations, rotations, and symmetries. This in turn is equal to the number of n-cyclic benzenoid hydrocarbons. The first few values of H_n are given in Table 1.

The enumeration of hexagonal systems according to area stands as one of the most challenging unsolved problems of combinatorial theory (cf. Section 10.8.5 in [7]). In spite of numerous attempts, no one was successful in applying Pólya's theory [7, 8, 9] or any other technique of combinatorics to find H_n or, at least, in establishing the asymptotic behavior

n	1	2	3	4	5	6
H_n	1	1	3	7	22	81
n	7	8	9	10	11	12
H_n	331	1435	6505	30086	141229	669584
n	13	14	15	16	17	
H_n	3198256	15367577	74207910	359863778	1751594643	

Table 1: Numbers H_n of hexagonal systems with n hexagons $(1 \leq n \leq 17)$

of H_n as n goes to infinity. Consequently, the only way to evaluate H_n is to use a (more or less) brute-force computer-assisted constructive enumeration; details of these methods are outlined in the book [10], in the reviews [11, 12], and elsewhere [13, 14, 15, 16, 17, 18]. Recently, some very efficient algorithms for the construction and counting of hexagonal systems were designed [17, 18], but even with them the calculation of H_n is extremely time- and memory-consuming. For instance, in order to obtain H_{22}, more than 300 days of CPU time were needed; the analogous calculation of H_{23} required 2.4 years of CPU time [18].

The values of H_n for n between 13 and 16 were first reported in 1990 by Knop *et al.* (H_{13} and H_{14} in [13], H_{15} and H_{16} in [14]). Three years later Tošić *et al.* arrived at H_{17} [15, 16]. With this the limit of the performance of the currently available computers had been reached, and further progress had to wait until a completely new algorithm was developed by Caporossi and Hansen [17] and further enhanced by Brinkmann [18]. This enabled the determination of H_{18} to H_{21} [17] as well as H_{22} and H_{23} [18]. It seems to be unlikely that the application of the same technique will be feasible in the case of $n \geq 24$.

It is a natural idea to somehow use the information contained in the sequence H_1, $H_2, \ldots, H_n$ to predict, at least approximately, the value of H_{n+1}. Early attempts in this direction [19, 20] were based on the assumption (without any theoretical justification, but in analogy with other results in graph enumeration) that for n being large enough, H_n can be approximated by some simple elementary function of n. This function was designed so as to depend on a few (usually two) adjustable parameters, the values of which were then determined from $H_1, H_2, \ldots, H_n$. The resulting values of H_{n+1} were eventually shown [13] to be quite accurate, but—of course—far from being exact. The same analysis was later applied to sequences of isomer counts of other homologous series of interest in chemistry [21, 22].

In this paper we report the results of an analogous approach, which, however, is much less arbitrary. Indeed, the class of sequences in which the approximation is searched for is much larger than those classes used so far, and allows for as many parameters as needed. The method is reminiscent of the methods of differential approximants [23] and algebraic approximants [24] used in statistical mechanics, and possesses the sound theoretical and algorithmic foundation of *holonomic functions.* This is the topic of the end of the introduction, which to a certain extend is independent from the rest of the text.

Holonomic Guessing

Being faced with the first five entries 0, 1, 3, 6, and 10 of an infinite sequence of numbers, an obvious guess for the sixth one would be 15. One could even propose the formula $n(n+1)/2$

for the nth entry, but this refined guess cannot be proved unless further information is provided. For instance, such a proof would become an easy task if we knew in addition that we are dealing with the sums of the first n nonnegative integers.

Over the years various computer algebra tools have been developed in order to assist this process of *guessing and proving*. As far as guessing is concerned, this is reflected by the success of Sloane's classical book [25] and its enlarged revision [26]. Each book is basically a table of sequences of integers, collected from all branches of mathematics and sciences. The sequences are arranged in numerical order, and come each with a brief description and references. The mere existence of these "dictionaries" has allowed for a new process of research: after generating the first numbers of a sequence of combinatorial interest, one identifies them with the aid of the tables. The work by Sloane and Plouffe has recently found an electronic and algorithmic supplement [27]: the tables are now electronically available for human search; additionally the on-line system now has a facility where it will algorithmically try to guess a formula or to relate the input sequence to a tabulated one. In particular, the counting sequence of hexagonal systems is now to be found there (known as sequences number A000228, A018190, and A038148). With regard to proving, we only mention Zeilberger's "holonomic systems approach to special function identities" [28] and the developments described in [29].

In this article, the aspect of computer-assisted *holonomic guessing* plays the central role. The first systematic presentation of the underlying theory of univariate holonomic functions has been given by Stanley [30]. The first implementation of these ideas was realized in the form of the Maple package GFUN by Salvy and Zimmermann [31]; it is now used as part of [27]. Another package named GENERATINGFUNCTIONS provides Mathematica users with the same functionality [32].

A detailed description of holonomic theory (e.g., closure properties of holonomic functions, etc.) would go far beyond the scope of this note. Therefore we restrict to introduce only those notions that are relevant to the understanding of the method to be used for predicting the values H_{24} and H_{25}.

For many counting sequences (a_n), the ordinary generating function and its exponential counterpart,

$$\sum_{n=0}^{\infty} a_n x^n \qquad \text{and} \qquad \sum_{n=0}^{\infty} \frac{a_n x^n}{n!},$$

respectively, are *holonomic*, which means that such a function or series satisfies a linear differential equation with polynomial coefficients. Examples of holonomic functions include many familiar power series such as algebraic functions (functions that are solution of a polynomial equation), the exponential function e^x, logarithmic function $\log(1+x)$, and trigonometric functions like $\sin x$. For example, if b_n denotes the number of binary planar trees with $n+1$ leaves (with the convention $b_0 = 1$), then the ordinary generating function of the sequence (b_n) is holonomic since

$$\sum_{n=0}^{\infty} b_n x^n = \frac{1-\sqrt{1-4x}}{2x}$$

is algebraic.

It is not difficult to prove that the series $\sum_{n=0}^{\infty} a_n x^n$ is holonomic if and only if the sequence (a_n) satisfies a linear recurrence with polynomial coefficents, i.e.,

$$p_0(n)a_n + p_1(n)a_{n+1} + \cdots + p_d(n)a_{n+d} = 0,$$

where the p_i's are polynomials in the indeterminate n. This serves as a motivation to call the sequence (a_n) *holonomic* in this case. Algorithmically it is easy to convert each representation—differential equation and recurrence—into the other. Furthermore, both representations serve as the basis for computer-assisted guessing. For example, let us assume that we came up with the first six binary tree numbers $(b_0, b_1, b_2, b_3, b_4, b_5) = (1, 1, 2, 5, 14, 42)$. Then we could use GFUN (or GENERATINGFUNCTIONS) to automatically guess the recurrence

$$(n + 2)b_{n+1} - 2(2n + 1)b_n = 0.$$

The procedure to produce this guess is essentially based on a simple coefficient comparison method (namely differential Padé-Hermite approximants) for which one has to bound in advance the order of the recurrence and the degree of the polynomial coefficients involved: the product "order times degree" is essentially the number of undetermined coefficients used by the method.

As mentioned above, additional information is needed in order to prove such a guess. For instance, if one knows in advance that the generating function is algebraic, which implies the existence of a holonomic recurrence, then one only needs to know an upper bound for its order. Or, if the holonomic nature is not known in advance, one might observe the convolution recurrence

$$b_n = \sum_{k=0}^{n-1} b_k b_{n-k-1}.$$

In this case transforming the conjectured recurrence of order 1 into the closed form

$$b_n = \frac{1}{n+1}\binom{2n}{n}$$

and substituting it into the convolution formula leads to the verification of a binomial identity. This could again be left to the computer by appying a symbolic summation procedure from [29]. (The numbers b_n above are the well-known Catalan numbers, often denoted by C_n.)

Concerning the problem of enumerating hexagonal systems, we do not know up to now whether the corresponding generating function of (H_n) is holonomic or not. Therefore we would need additional information to actually prove the accuracy of our guess, which can only be considered as a "holonomic approximation". The information we use for our holonomic guessing solely consists in the values of H_n that have been computed so far. In order to provide further evidence, we present a detailed analysis of the stability of the prediction scheme.

Holonomic guessing could also be considered as a kind of computer-assisted "heuristic reasoning", meant in the spirit of Pólya. According to his dictionary of heuristics [33]: *"We are often obliged to use heuristic reasoning. We shall attain complete certainty when we shall have obtained the complete solution, but before obtaining certainty we must often be satisfied with a more or less plausible guess."*

In the present article we use the Maple package GFUN. Analogous procedures are available to Mathematica users [32] and could have been used as well.

1 Warming Up: Predicting the Number of Hexagonal Systems with n Hexagons for n between 18 and 23

When Tošić *et al.* gave the value 1751594643 for H_{17} [15, 16], only the values of H_1, H_2, $\ldots$, H_{16} were known. All those results are summarized in Table 1. Using these initial 17 numbers as exclusive information about the sequence (H_n), we proceed to guess a linear recurrence satisfied by a holonomic approximation of the sequence. By means of it we then predict further numbers H_n of hexagonal systems when $18 \leq n \leq 23$, before comparing them with the actual values already known at present.

Prediction Scheme

We use the following prediction scheme:

Step 1. Load the package (as part of the standard distribution of Maple V Release 5), enter the list of numbers known after Tošić *et al.*, and set up a few package parameters.

```
with(share): with(gfun):
L:=[1,1,3,7,22,81,331,1435,6505,30086,141229,669584,
    3198256,15367577,74207910,359863778,1751594643]:
gfun['minordereqn']:=1: gfun['maxordereqn']:=2:
gfun['mindegcoeff']:=0: gfun['maxdegcoeff']:=20:
```

Specifically, we require the package to consider equations of order 1 or 2 with polynomial coefficients of degree between 0 and 10.

Step 2. *Guess* a recurrence satisfied by the sequence which starts with the values above:

```
rec17:=listtorec(L,u(n));
```

which outputs:

$$\texttt{rec17} := [\{p_0(n)u(n) + p_1(n)u(n+1) + p_2(n)u(n+2), u(0) = 1, u(1) = 1\}, \texttt{ogf}]$$

where each p_i above is a polynomial of degree 5 in n with integer coefficients of 52 digits. The explicit values are available in Appendix A.

Step 3. Convert this recurrence into a procedure which computes the nth term of the sequence:

```
pr17:=rectoproc(op(1,rec17),u(n));
```

Remarkably, the output procedure `pr17`, which is too large to be displayed here, has been *automatically generated* by Gfun. Additionally, Gfun *automatically optimized* it, in the sense of minimizing the number of arithmetical operations used in the procedure.

n	18	19	20
H'_n	8553612149	41892180909	205710300568
H_n	8553649747	41892642772	205714411986
$-\delta_n$	$4.4 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	$2.0 \cdot 10^{-5}$
n	21	22	23
H'_n	1012535580260	4994621421396	24686078283303
H_n	1012565172403	4994807695197	24687124900540
$-\delta_n$	$2.9 \cdot 10^{-5}$	$3.7 \cdot 10^{-5}$	$4.2 \cdot 10^{-5}$

Table 2: Predicted numbers H'_n of hexagonal systems with n hexagons, actual numbers H_n, and corresponding relative errors $-\delta_n = -(H'_n - H_n)/H_n$ of prediction $(18 \leq n \leq 23)$

Step 4. Compute *predicted values* for hexagonal systems with 18 to 23 hexagons. The predicted values H'_n are in fact rational numbers rounded to the nearest integer. Rather than displaying the Maple output, as obtained by the command

```
seq(i=trunc(pr17(i-1)+1/2),i=18..23);
```

we give the predicted results in Table 2.

Comparison to Recent Results

The numbers obtained in *Step 4* of the previous scheme match *with good accuracy* those obtained by Caporossi and Hansen [17], and by Brinkmann, Caporossi and Hansen [18]. Indeed, the heavy computations described in [18, 17] proved the numbers H_n of hexagonal systems to be those given in Table 2. The table also gives the corresponding relative error

$$\delta_n = \frac{H'_n - H_n}{H_n}$$

of the predicted values H'_n.

In order to perform the calculations of `rec17`, `pr17`, and the estimates, *not more than 3 seconds of CPU time were needed.*

Note that other parameter settings could have been used in Step 1 above. Let us repeat that the number of undetermined coefficients used by the method is essentially the product “order times degree”. The algorithm tries to detect equations with a small number of non-zero coefficients in the search space described by the parameters. The other setting

```
gfun['minordereqn']:=0: gfun['maxordereqn']:=20:
gfun['mindegcoeff']:=0: gfun['maxdegcoeff']:=2:
```

yields another equation with low polynomial degree but high order (specifically: order 8 instead of 2, degree 1 instead of 5, 25-digit instead of 52-digit integers). The latter recurrence results in different predicted numbers, which however approximate the actual ones with essentially the same good accuracy. This is why we will not discuss the choice of parameter settings any further.

n	4	5	6	7	8	9	10	11	12	13	14	15	16	17
order	2	2	2	2	2	2	2	2	1	2	2	1	2	2
degree	1	1	2	2	2	3	3	3	5	4	4	7	5	5
digits	1	1	3	4	5	9	13	17	26	28	33	47	48	52
n	18	19	20	21	22	23								
order	1	2	2	1	2	2								
degree	8	6	6	10	7	7								
digits	69	70	78	103	104	116								

Table 3: Parameters for the recurrence obtained by the scheme at nth stage $(4 \leq n \leq 23)$

2 Predicting the Number of Hexagonal Systems with 24 or More Hexagons

In the previous section, we started from a list of known values for the H_n (up to $n = 17$), and derived a *single* recurrence to predict *several* further values (up to $n = 23$). In this section, we follow a more incremental strategy: from a list of known or already predicted values for $H_1, \ldots, H_n$, we derive a recurrence to predict a *single* further value for H_{n+1}. Adjoining it to the initial list, we then iterate the process ℓ times, ending with *several* recurrences, one for each value predicted for $H_{n+1}, \ldots, H_{n+\ell}$.

Prior to this, we provide good numerical evidence for the stability of our incremental prediction scheme, which makes it possible to obtain values for H_{24} and H_{25} of credibly good accuracy.

Stability of the Prediction Scheme

Using all known values $H_1, \ldots, H_n$ for a number $n \leq 23$, one can predict the numbers H_{n+p} for $p \geq 1$ following the same scheme as previously outlined for $n = 17$. This is readily implemented in Maple:

```
L:=[1,1,3,7,22,81,331,1435,6505,30086,141229,669584,
    3198256,15367577,74207910,359863778,1751594643,
    8553649747,41892642772,205714411986,1012565172403,
    4994807695197,24687124900540]:
gfun['minordereqn']:=1: gfun['maxordereqn']:=2:
gfun['mindegcoeff']:=0: gfun['maxdegcoeff']:=20:
for i from 4 to nops(L) do
    rec[i]:=listtorec(L[1..i],u(n));
    pr[i]:=rectoproc(op(1,rec[i]),u(n))
od:
```

Setting the order and degree parameters as indicated in the Maple code above, the recurrences obtained are of small order (1 or 2), but involve polynomials in n of degree linear in n (typically, $\lfloor n/3 \rfloor$) and integers of (experimentally) $O(n \ln n)$ digits. This is summarized in Table 3. Denote by $H_n^{(p)}$ the value for H_{n+p} predicted p steps ahead by the

n	10	11	12	13	14	15
$p=1$	$9.9\cdot10^{-4}$	$4.8\cdot10^{-3}$	$7.8\cdot10^{-4}$	$-1.2\cdot10^{-5}$	$-4.3\cdot10^{-5}$	$1.6\cdot10^{-5}$
$p=2$	$7.2\cdot10^{-3}$	$1.6\cdot10^{-2}$	$3.1\cdot10^{-3}$	$-9.3\cdot10^{-5}$	$-1.8\cdot10^{-4}$	$7.1\cdot10^{-5}$
n	16	17	18	19	20	21
$p=1$	$-2.0\cdot10^{-6}$	$4.4\cdot10^{-6}$	$-5.2\cdot10^{-6}$	$8.6\cdot10^{-6}$	$-1.9\cdot10^{-6}$	$3.7\cdot10^{-6}$
$p=2$	$-3.8\cdot10^{-6}$	$1.1\cdot10^{-5}$	$-1.9\cdot10^{-5}$	$3.4\cdot10^{-5}$	$-6.7\cdot10^{-6}$	$2.0\cdot10^{-5}$
n	22					
$p=1$	$-7.6\cdot10^{-7}$					

Table 4: Relative errors $-\delta_n^{(p)}$ of prediction $(1 \le p \le 2,\ \ 4 \le n \le 22)$

scheme at the nth stage (i.e., by using the known H_k's for $1 \le k \le n$). This value $H_n^{(p)}$ is obtained as the result of the following Maple command (again, a rational number rounded to the nearest integer):

```
trunc(pr[n](n+p-1)+1/2);
```

Here, n and p are replaced by the corresponding integers.

The comparison of the estimate $H_n^{(p)}$ with the actual value H_{n+p} is achieved via the relative error

$$\delta_n^{(p)} = \frac{H_n^{(p)} - H_{n+p}}{H_{n+p}},$$

which is given in Table 4. Our calculations suggest that for a fixed p, each sequence of the absolute value $|\delta_n^{(p)}|$ of the errors made when predicting p steps ahead decreases with (possibly) some small oscillation.

The errors $\delta_n^{(p)}$ for higher values of p are given in Table 7 (Appendix B). The same remark about their decrease with small oscillation applies to values of p up to 8. Besides, the data in the table also strongly suggests a slow and monotonic variation of $-\delta_n^{(p)}$ with the parameter p (at least when n is greater than 8). More specifically, when $n \ge 8$ the ratio $\mu_n = \delta_n^{(8)}/\delta_n^{(1)}$ never exceeds a few hundreds.

Predictions

Following our calculation scheme and the recurrence computed for $n = 23$, we obtain the predictions for the next values of H_n that are given in Table 5. Note that the predicted values $H_n'' = H_n^{(1)}$ for $n > 23$ have been obtained by defining $H_n^{(p)}$ by the recurrence computed using the known values H_1 to H_{23} together with the *successively predicted ones* $H_{23}^{(1)}, H_{24}^{(1)}, \ldots, H_{n-1}^{(1)}$.

The validity of these predictions for $n = 24$ and $n = 25$ is suggested by the stability of the scheme, as described in the previous section (see Table 4). A similar analysis of Table 7 vindicates the further values and the bounds on the errors to be found in Table 5.

In order to perform the calculations of the recurrences, evaluation procedures, and estimates for each n between 1 and 23, *not more than 60 seconds of CPU time were needed.*

n	24	25	26
H''_n	122237774262384	606259305418149	3011424390300379
error	10^{-6}	10^{-5}	10^{-5}
n	27	28	29
H''_n	14979449994317356	74608167670480920	372053203099446920
error	10^{-5}	10^{-4}	10^{-4}
n	30	31	
H''_n	1857452345893521033	9283108148442320346	
error	10^{-3}	10^{-3}	

Table 5: Predicted numbers H''_n of hexagonal systems with n hexagons and presumable relative error bounds $(24 \leq n \leq 31)$

n	5	6	7	8	9	10	11	12	13
ρ_n	3.682	4.086	4.335	4.533	4.625	4.694	4.741	4.776	4.805
n	14	15	16	17	18	19	20	21	22
ρ_n	4.829	4.849	4.867	4.883	4.898	4.911	4.922	4.933	4.943
n	23	24	25	26	27	28	29	30	
ρ_n	4.951	4.960	4.967	4.974	4.981	4.987	4.992	4.998	

Table 6: Observed ratios $\rho_n = H_{n+1}/H_n$ $(5 \leq n \leq 22)$, as well as predicted ratios $\rho''_n = H''_{n+1}/H''_n$ $(23 \leq n \leq 30)$

Again, the other parameter setting suggested at the end of Section 1 yields a different recurrence (order 11 instead of 2, degree 1 instead of 7, 46-digit instead of 116-digit integers). However, the numbers predicted by this alternative recurrence remain close to the ones in Table 5.

3 Exponential Asymptotic Part

A natural idea is to consider the ratio $\rho_n = H_{n+1}/H_n$ of two successive terms of the sequence of observed numbers of hexagonal systems. Table 6 provides further evidence to corroborate the conjecture of Aboav and Gutman that the limiting value is remarkably close (or exactly equal) to 5 [20].

In the same vein, we observed that each predicted recurrence of the $H_n^{(p)}$ for fixed n asymptotically behaves exponentially, namely $H_n^{(p)} \sim K_n \alpha_n^p$ for a constant K_n and a parameter α_n that is an explicit algebraic number close to, but greater than 5. Furthermore, the greater n is, the closer to 5 the exponential parameter α_n is.

Acknowledgement

The work of F.C. and P.P. has been partially supported by the SFB grant F1305 of the Austrian Science Foundation (FWF). I.G. thanks the Johannes Kepler University in Linz (Austria) for a grant that enabled him to spend one month there in the year 1999.

A Explicit Value for the Recurrence of Section 1

The second-order recurrence in Step 2 of the prediction scheme described in Section 1 involves the following polynomials of degree 5 in n with integer coefficients of 52 digits:

$$\begin{aligned}
p_0 = &-1867772898049832297838775598964134957166764980189512 \\
&- 1088455682940707996869729155113288248493317254822003 6n \\
&+ 1272153387865028752855490296494935672276973325034951 0n^2 \\
&- 3253475329234326006503819920315214439352035172000985n^3 \\
&+ 3181010063168573064122469538508900000133224356894 42n^4 \\
&- 1094296786346068067492485775565713435084795742277 9n^5,
\end{aligned}$$

$$\begin{aligned}
p_1 = &\ 5111812422122801926839613693662870834533658464707872 \\
&+ 3546978801554295139510518187541933947524020432378 4n \\
&- 3367129112115264514741892953382392619519869487897336n^2 \\
&+ 7702884436701516186518213901391711247856711639703 16n^3 \\
&- 1749796213747597881059183004330035092409900235230 8n^4 \\
&- 3188835391221555958813481750811329757447934182008n^5,
\end{aligned}$$

$$\begin{aligned}
p_2 = &-1081346508024323209666946031566245292455631161506120 \\
&+ 1825732298678477187904364773808202001052192802042 90n \\
&+ 2966722753925751047553877198957564982939143473202 31n^2 \\
&- 5073225809747136025689451949247199360023820761503 6n^3 \\
&- 7073106935049620643525597754441192257088974124079n^4 \\
&+ 1027640238414335110389952660120536662439679446914n^5.
\end{aligned}$$

B More Numerical Results Supporting the Prediction Accuracy

Table 7 is an extended version of Table 4. It suggests that the calculation method proposed in this paper is very stable, far beyond the prediction of the first next two values H_{24} and H_{25} of the sequence.

References

[1] Sachs, H. Perfect matchings in hexagonal systems. *Combinatorica 4*, 1 (1984), 89–99.

[2] Baxter, R. J. Hard hexagons: exact solution. *J. Phys. A 13*, 3 (1980), L61–L70.

[3] Baxter, R. J. *Exactly Solved Models in Statistical Mechanics.* Academic Press, London, 1982.

[4] Andrews, G. E., and Baxter, R. J. A motivated proof of the Rogers-Ramanujan identities. *Amer. Math. Monthly 96*, 5 (1989), 401–409.

[5] Gutman, I., and Cyvin, S. J. *Introduction to the Theory of Benzenoid Hydrocarbons.* Springer-Verlag, Berlin, 1989.

n	4	5	6	7	8	9
$p=1$	0.22	0.24	$3.6 \cdot 10^{-2}$	$-2.7 \cdot 10^{-2}$	$4.7 \cdot 10^{-2}$	$-7.5 \cdot 10^{-3}$
$p=2$	0.47	0.42	$9.0 \cdot 10^{-2}$	$1.3 \cdot 10^{-2}$	0.22	$-2.2 \cdot 10^{-2}$
$p=3$	0.68	0.60	0.16	3.7	0.65	$-4.2 \cdot 10^{-2}$
$p=4$	0.81	0.72	0.22	44.	1.6	$-6.7 \cdot 10^{-2}$
$p=5$	0.90	0.81	0.28	320.	3.3	$-9.6 \cdot 10^{-2}$
$p=6$	0.94	0.87	0.33	1800.	6.3	0.13
$p=7$	0.97	0.91	0.38	8000.	11.	0.17
$p=8$	0.98	0.94	0.43	31000.	17.	0.20
μ_n	4.4	3.9	12.	$-.11 \cdot 10^{7}$	360.	26.

n	10	11	12	13	14	15
$p=1$	$9.9 \cdot 10^{-4}$	$4.8 \cdot 10^{-3}$	$7.8 \cdot 10^{-4}$	$-1.2 \cdot 10^{-5}$	$-4.3 \cdot 10^{-5}$	$1.6 \cdot 10^{-5}$
$p=2$	$7.2 \cdot 10^{-3}$	$1.6 \cdot 10^{-2}$	$3.1 \cdot 10^{-3}$	$-9.3 \cdot 10^{-5}$	$-1.8 \cdot 10^{-4}$	$7.1 \cdot 10^{-5}$
$p=3$	$2.1 \cdot 10^{-2}$	$3.5 \cdot 10^{-2}$	$7.5 \cdot 10^{-3}$	$-3.0 \cdot 10^{-4}$	$-4.4 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$
$p=4$	$4.3 \cdot 10^{-2}$	$6.2 \cdot 10^{-2}$	$1.4 \cdot 10^{-2}$	$-6.9 \cdot 10^{-4}$	$-8.5 \cdot 10^{-4}$	$3.9 \cdot 10^{-4}$
$p=5$	$7.5 \cdot 10^{-2}$	$9.9 \cdot 10^{-2}$	$2.4 \cdot 10^{-2}$	$-1.3 \cdot 10^{-3}$	$-1.4 \cdot 10^{-3}$	$6.9 \cdot 10^{-4}$
$p=6$	0.12	0.14	$3.6 \cdot 10^{-2}$	$-2.1 \cdot 10^{-3}$	$-2.2 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$
$p=7$	0.17	0.19	$5.0 \cdot 10^{-2}$	$-3.2 \cdot 10^{-3}$	$-3.1 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$
$p=8$	0.22	0.25	$6.7 \cdot 10^{-2}$	$-4.5 \cdot 10^{-3}$	$-4.3 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$
μ_n	220.	53.	87.	370.	99.	140.

n	16	17	18	19	20	21
$p=1$	$-2.0 \cdot 10^{-6}$	$4.4 \cdot 10^{-6}$	$-5.2 \cdot 10^{-6}$	$8.6 \cdot 10^{-6}$	$-1.9 \cdot 10^{-6}$	$3.7 \cdot 10^{-6}$
$p=2$	$-3.8 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	$-1.9 \cdot 10^{-5}$	$3.4 \cdot 10^{-5}$	$-6.7 \cdot 10^{-6}$	$2.0 \cdot 10^{-5}$
$p=3$	$-8.8 \cdot 10^{-6}$	$2.0 \cdot 10^{-5}$	$-4.6 \cdot 10^{-5}$	$8.3 \cdot 10^{-5}$	$-1.6 \cdot 10^{-5}$	
$p=4$	$-1.7 \cdot 10^{-5}$	$2.9 \cdot 10^{-5}$	$-9.0 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$		
$p=5$	$-3.0 \cdot 10^{-5}$	$3.7 \cdot 10^{-5}$	$-1.6 \cdot 10^{-4}$			
$p=6$	$-4.9 \cdot 10^{-5}$	$4.2 \cdot 10^{-5}$				
$p=7$	$-7.3 \cdot 10^{-5}$					

n	22
$p=1$	$-7.6 \cdot 10^{-7}$

Table 7: Error $-\delta_n^{(p)}$ of the prediction and measure $\mu_n = \delta_n^{(8)}/\delta_n^{(1)}$ of its variation with p $(1 \le p \le 8,\ \ 4 \le n \le 23)$

[6] Gutman, I. Topological properties of benzenoid systems. *Topics Curr. Chem. 162* (1992), 1–28.

[7] Harary, F., and Palmer, E. M. *Graphical Enumeration.* Academic Press, New York, 1973.

[8] Pólya, G., and Read, R. C. *Combinatorial Enumeration of Groups, Graphs, and Chemical Compounds.* Springer-Verlag, New York, 1987.

[9] Kerber, A. *Algebraic Combinatorics via Finite Group Actions.* BI Wissenschaftsverlag, Mannheim-Wien-Zürich, 1991.

[10] Trinajstić, N., Nikolić, S., Knop, J. V., Müller, W. R., and Szymanski, K. *Computational Chemical Graph Theory: Characterization, Enumeration and Generation of Chemical Structures by Computer Methods.* Horwood, New-York, 1991.

[11] Cyvin, B. N., Brunvoll, J., and Cyvin, S. J. Enumeration of benzenoid systems and other polyhexes. *Topics Curr. Chem. 162* (1992), 65–180.

[12] Brunvoll, J., Cyvin, B. N., and Cyvin, S. J. Benzenoid chemical isomers and their enumeration. *Topics Curr. Chem. 162* (1992), 181–221.

[13] Müller, W. R., Szymanski, K., Knop, J. V., Nikolić, S., and Trinajstić, N. On the enumeration and generation of polyhex hydrocarbons. *J. Comput. Chem. 11*, 2 (1990), 223–235.

[14] Knop, J. V., Müller, W. R., Szymanski, K., and Trinajstić, N. Use of small computers for large computations: enumeration of polyhex hydrocarbons. *J. Chem. Inf. Comput. Sci. 30* (1990), 159–160.

[15] Mašulović, D., Tošić, R., Cyvin, B. N., and Cyvin, S. J. Supplement to the Düsseldorf-Zagreb numbers for polyhexes. *Commun. Math. Chem. 29* (1993), 165–166.

[16] Tošić, R., Mašulović, D., Stojmenović, I., Brunvoll, J., Cyvin, S. J., and Cyvin, B. N. Enumeration of polyhex hydrocarbons to $h = 17$. *J. Chem. Inf. Comput. Sci. 35* (1995), 181–187.

[17] Caporossi, G., and Hansen, P. Enumeration of polyhex hydrocarbons to $h = 21$. *J. Chem. Inf. Comput. Sci. 38* (1998), 610–619.

[18] Brinkmann, G., Caporossi, G., and Hansen, P. Mathematics, chemistry and record hunting. To be published, 1999.

[19] Gutman, I. Number of benzenoid hydrocarbons. *Z. Naturforsch. A 41*, 8 (1986), 1089–1090.

[20] Aboav, D., and Gutman, I. Estimation of the number of benzenoid hydrocarbons. *Chem. Phys. Lett. 148* (1988), 90–92.

[21] Cioslowski, J. Series analysis methods in enumeration of chemical isomers. *Theor. Chim. Acta 76* (1989), 47–51.

[22] Aboav, D., and Gutman, I. Estimation of the number of unbranched catacondensed benzenoid hydrocarbons. *J. Serb. Chem. Soc. 54* (1989), 249–251.

[23] Guttmann, A. J. Asymptotic analysis of power-series expansions. In *Phase Transitions and Critical Phenomena*, vol. 13. Academic Press, London, 1989, pp. 1–234.

[24] Brak, R., and Guttmann, A. J. Algebraic approximants: a new method of series analysis. *J. Phys. A 23*, 24 (1990), L1331–L1337.

[25] Sloane, N. J. A. *A Handbook of Integer Sequences.* Academic Press, New York-London, 1973.

[26] Sloane, N. J. A., and Plouffe, S. *The Encyclopedia of Integer Sequences.* Academic Press, San Diego, CA, 1995.

[27] Sloane, N. J. A. Sloane's on-line encyclopedia of integer sequences. Available on the web from the URL `http://www.research.att.com/~njas/sequences/`.

[28] Zeilberger, D. A holonomic systems approach to special functions identities. *J. Comput. Appl. Math. 32*, 3 (1990), 321–368.

[29] Petkovšek, M., Wilf, H. S., and Zeilberger, D. $A = B$. Peters, Wellesley, MA, 1996.

[30] Stanley, R. P. Differentiably finite power series. *European J. Combin. 1*, 2 (1980), 175–188.

[31] Salvy, B., and Zimmermann, P. Gfun: a Maple package for the manipulation of generating and holonomic functions in one variable. *ACM Trans. Math. Softw. 20*, 2 (1994), 163–177.

[32] Mallinger, C. *Algorithmic Manipulations and Transformations of Univariate Holonomic Functions and Sequences.* Master thesis, RISC, Johannes Kepler Universität Linz, Austria, Aug. 1996. Available at the URL:

`http://www.risc.uni-linz.ac.at/research/combinat/risc/publications/`.

[33] Pólya, G. *How to Solve It*, second ed. Princeton University Press, Princeton, NJ, 1988.