A Survey and New Results on Computer Enumeration of Polyhex and Fusene Hydrocarbons

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After a short historic review, we briefly describe a new algorithm for constructive enumeration of polyhex and fusene hydrocarbons. In this process our algorithm also enumerates isomers and symmetry groups of molecules (which implies enumeration of enantiomers). Contrary to previous methods often based on the boundary code or its variants (which records orientation of edges along the boundary) or on the DAST code, which uses a rigid dualist graph (whose vertices are associated with faces and edges with adjacency between them), the proposed algorithm proceeds in two phases. First inner dual graphs are enumerated; then molecules obtained from each of them by specifying angles between adjacent edges are obtained. Favorable computational results are reported. The new algorithm is so fast that output of the structures is by far the most time-consuming part of the process. It thus contributes to enumeration in chemistry, a topic studied for over a century, and is useful in library making, QSAR/QSPR, and synthesis studies.

INTRODUCTION

Since the XIXth century, counting and enumeration of molecules from various families have been important activities in mathematical chemistry. Many authors have presented methods and results so obtained. The reader may consult Balaban et al,[1] Dias,[2] Gutman and Cyvin,[3] Balaban,[4] Balasubramanian,[5] Hosoya,[6] Knop et al.,[7] Mercier et al.,[8] Trinajstić et al.,[9] Bonchev and Rouvray,[10,11] and Cyvin et al.[12]

Counting molecules of a family means finding how many there are. In the mathematical literature the word **enumeration** is also used for just determining the number of structures. Listing all molecules or **constructively** enumerating them implies giving a concise description of each molecule, such as a code. This is of course useful in library making. Moreover, exhaustive lists of molecules can help in synthesis both for finding targets and input molecules. Molecular codes can be used when studying some property described by an invariant, to determine minimum, maximum, and average values of this invariant. When the set is very large, one may also use the codes to select randomly a subset of molecules in order to obtain a good estimate of the invariant. Note that selection is easy to do at the time the molecules are listed, e.g. by keeping the code of any new molecule with a given probability.

Constructively enumerating polyhex and fusene hydrocarbons has attracted much attention since the 1960s. The new algorithm described here is so fast that writing the structures—to a file or a pipe read by another program—is by far the most time-consuming part of the computer program based on it. Using e.g. an adjacency list as the code for the fusene hydrocarbons, already for 15 hexagons a C-program just reading the data from a pipe (to be exact: just consisting of the line *while ((c = getc(stdin)) ! = EOF);*) takes about 85% of the time of the generation program constructing, coding, and writing the structures and more than 220 times as long as needed to form the structures in memory. The relative amount of time needed for reading and writing even increases with the number of hexagons. So assuming the same codes to be outputted, there is simply not much room for improvement, and we have a good reason to believe that this algorithm is the endpoint in a long series of algorithms proposed for listing polyhex and fusene hydrocarbons. We take this as an occasion to survey the most important methods for constructive enumeration presented in this series of algorithms.

For the nonconstructive enumeration of polyhex hydrocarbons recent work by Vöge, Guttmann, and Jensen (see ref 13) may well be regarded as a breakthrough. They developed a nonconstructive method to count benzenoids and gave the number of structures with up to 35 hexagons. For the nonconstructive enumeration of fusene hydrocarbons no method appears to have been published so far.

While the molecules considered here have only carbon and (omitted) hydrogen atoms, chemical graph enumeration also addresses the problem of heteroatoms, through labeled graphs. The proposed algorithm could be extended for such a purpose in future work.

DEFINITIONS

A **polyhex** is a set of congruent regular hexagons arranged in the plane such that any two of them either share exactly

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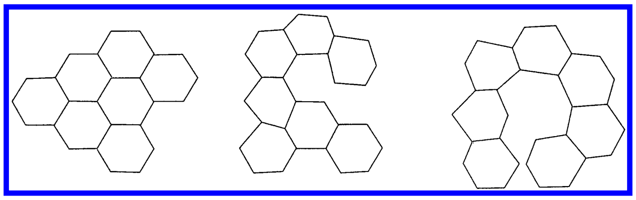

Figure 1. A polyhex, a fusene that is isomorphic to a polyhex and a fusene that is not isomorphic to a polyhex.

one edge or are distinct.[14,15] For **fusenes**[16] the requirement that the hexagons are pairwise congruent and regular is dropped. Instead they are allowed to be just topological hexagons, that is, they may be deformed. Since we are interested in combinatorial isomorphism classes, we will not distinguish between a fusene that is isomorphic to a polyhex and the isomorphic polyhex. So polyhexes are a subset of the set of fusenes.

In this paper, we consider only simply connected polyhexes and fusenes. They correspond to planar polyhex hydrocarbons (or benzenoids) respectively to general polycyclic hydrocarbons such as e.g. helicenes. For conciseness, we refer to them below simply as polyhexes and fusenes. We will first review the algorithms proposed for the enumeration of polyhexes and afterward those proposed for fusenes.

POLYHEXES

The Boundary Code Algorithm. Knop et al.[17] proposed an algorithm based on the *boundary code*, which appears to be the first computer code for polyhexes. The boundary code is computed as follows: embed the polyhex to be coded in the hexagonal lattice with some edges vertical. Beginning at any edge, follow the boundary clockwise noting the orientation of successive edges with a digit 1 to 6 where 1 corresponds to a vertical edge pointing upward, and so on. Then proceed to a circular shift to get the lexicographically maximum code. Due to the symmetry of the hexagonal lattice there are still 12 possibilities: 6 rotations and 1 reflection. The boundary code is the lexicographically maximum code among those so obtained.

Polyhexes with h hexagons are generated by adding one hexagon to those with $h - 1$ hexagons in all possible ways. They are coded, the codes are sorted, and the redundant ones are deleted. This approach led to the enumeration of polyhexes with $h = 10$[17], $h = 11$[18], and $h = 12$[19] hexagons. It is demanding both in computing time and in memory.

The DAST Algorithm. Müller et al.[20] proposed an algorithm exploiting the DAST (Dualist Angle-Restricted Spanning Tree) code,[21] which is based on the *dualist approach* associated with any polyhex.[22] This approach is obtained by embedding the polyhex in the regular hexagonal lattice associating a vertex with the center of each hexagon and joining vertices corresponding to hexagons with a common edge. Note that the dualist graph is rigid, *i.e.*, angles between adjacent edges are fixed; therefore, it is not an abstract graph in the graph theoretic sense. Due to rigidity of angles, any spanning tree of the dualist graph completely defines the polyhex. The proposed algorithm proceeds by enumeration of representative spanning trees of dualists with h vertices obtained by adding a vertex to those with $h - 1$ vertices. These trees are canonically coded by choosing starting hexagons in every possible way and canonically choosing one of the codes. Again codes are sorted and redundant ones deleted. This more powerful method led to the enumeration of polyhexes with $h = 13$[20], $h = 14$[23], $h = 15$[21], and $h = 16$[14] hexagons. Demands on memory are still high.

The DAST algorithm increased the size of the largest set of polyhexes generated by a factor of about 550.

The Cage Algorithm. Tosic et al.[24,15] proposed an entirely different approach following ideas presented in ref 40, which does not require storing and sorting long lists of codes, but unfortunately is not able to output nonredundant lists without additional routines that would decrease the performance. So this approach is on the boundary line of constructive enumeration.

They first compute the number of isomorphism classes of all polyhexes with nontrivial symmetry group by a method due to Redelmeier:[40] Redelmeier lists polyominoes which can be considered square analogues of polyhexes with the exception that holes in the patch are allowed. Fixed polyominoes are polyominoes in the square lattice with two fixed polyominoes being considered equivalent if and only if a translational symmetry maps one onto the other. Polyominoes with a prescribed symmetry group are constructed by adding squares simultaneously at all positions equivalent under the prescribed symmetry operations or are computed from numbers for smaller classes. E.g. the polyominoes with n squares and a reflection symmetry not fixing any face correspond to fixed polyominoes with $n/2$ squares. Starting with the richer groups, the numbers of polyominoes with a symmetry exactly a subgroup of the richer group can be computed by subtracting the number of polyominoes with a richer group determined before.

So the last group to be considered is the trivial group. Redelmeier constructs all fixed polyominoes by rooting them in a way that the leftmost square in the lowest row is fixed at a certain square in the lattice and successively constructing larger polyominoes from smaller ones.

Since for every group it is well-known how often a structure occurs as a fixed polyominoe and the numbers of structures in every symmetry class are known, it is easy to compute the number of free—that is isomorphic polyominoes.

After constructing the symmetric polyhexes, which is not described in detail, Tosic et al. use a slightly different method than Redelmeier: They install an equilateral triangular region of the hexagonal lattice and construct all benzenoids that are *properly* placed inside this region—that is touch the left and lower side of the triangle—by constructing all possible boundaries of such patches. Since the number of different (proper) placements of a polyhex inside the cage is known exactly (e.g. 12 possibilities for C_s), it is easy to compute the number of nonisomorphic benzenoids with trivial group from the total counts and the counts for the nontrivial groups computed before. Note that no isomorphism rejection is done and also space requirement is moderate.

To the present authors it seems that using Redelmeier's method also for the second part might have resulted in a faster algorithm.

The Cage algorithm increased the size of the largest set of polyhexes generated by a factor of about 5.

THE BOUNDARY EDGES CODE ALGORITHM

Caporossi and Hansen[25] proposed an algorithm based on the *boundary edges code*[26] which for polyhexes is equivalent to the PC-2 code of Herndon and Bruce[27] and *reverse search* or the *canonical construction path* method like described in refs 28 and 29. The boundary edges code of a polyhex is obtained by embedding it in the hexagonal lattice, beginning at a vertex of degree 3 of the boundary (which exists if $h \geq 2$) and following this boundary clockwise noting the number of traversed edges of each successive hexagon. Note that the same hexagon can appear up to 3 times in the code. Then a circular shift and possibly a reversal are made to get the lexicographically maximal code. Following the principles for isomorphism rejection, each polyhex with h hexagons (the *son*) is constructed from a unique polyhex with $h - 1$ hexagons (the father). The rule defining the father is that it is obtained by removing the hexagon corresponding to the first digit in the boundary edges code of the son. This entails a difficulty, as in some rare cases, the removal of this hexagon disconnects the polyhex (in other words, some polyhexes, called *orphans*, have no father). However, this can only occur for $h > 28$[25]. This approach has led to the enumeration of polyhexes with $h = 18$ to $h = 21$ hexagons, increasing the size of the largest set of polyhexes enumerated by a factor of over 600. In this paper, we will further rise this size by another factor of about 125.

FUSENES

Less attention appears to have been devoted to the enumeration of fusenes than of polyhexes. After, not always correct, hand computations by various authors, Cyvin et al.[16] presented results for the enumeration of fusenes with up to 9 hexagons. Brunvoll et al.[30] extended this enumeration to $h = 15$. Beginning with minimal nonplanar fusenes the authors examine all possible additions of one hexagon at a time. In this way, they obtain by hand the number of fusenes with $h = 10$ hexagons. Moreover they give the number of fusenes with up to $h = 15$ hexagons without giving details on the algorithm used or the program which implements it. Caporossi, Hansen, and Zheng[31] adapted the enumeration method for polyhexes based on the boundary edges code. In this case, orphans can occur when $h \geq 20$, for $h = 20$ there are exactly 4 of them. Another difficulty arises: the boundary code can be extended to fusenes, which, when embedded in the hexagonal lattice may have superposed hexagons. Surprisingly the boundary edges code does not necessarily uniquely define a fusene;[32] however, the smallest pair of fusenes with the same code have 25 hexagons. This approach led to the enumeration of fusenes with 20 hexagons. This increased the size of the largest set of fusenes generated by a factor of about 4100. In this paper, we will further raise this size by another factor of about 25 000.

THE NEW APPROACH

Our new approach constructs fusenes and filters them for benzenoids in the case where only this subclass is of interest. For a lot of problems filtering the output is not very efficient. In particular it is so when only a small amount of the graphs listed have the desired property. In our case the number of nonisomorphic structures listed per second is of course much larger if all fusenes are of interest, but even after filtering for polyhexes more than 1 000 000 nonisomorphic structures per second remain (on a 700 MHz Pentium PC with Linux Operating system).

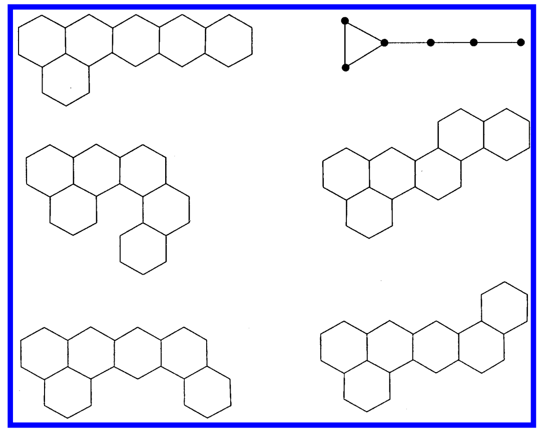

Figure 2. A fusene, its inner dual, and some other fusenes with the same inner dual.

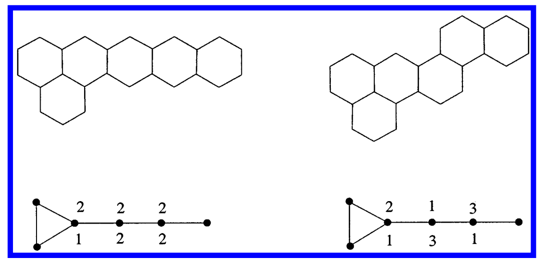

Figure 3. Two fusenes with the same inner dual and their labeled inner duals.

Checking whether a fusene fits into the hexagonal lattice is of course an easy task, so we will only describe our algorithm for the construction of fusenes here. As for the methods in the historic review, we will give the main ideas here and refer the reader to ref 33 for a more detailed description.

We represent fusenes as labeled inner duals. The inner dual of a fusene is obtained by associating a vertex with every hexagon and connecting two such vertices if the corresponding hexagons share an edge. The inner dual of a fusene does not describe a fusene uniquely as can be seen in Figure 2.

To uniquely describe a fusene, we must assign labels to the vertices, each time they are traversed when following the boundary, giving the numbers of edges of the hexagon in the boundary cycle at the corresponding place. Since in those cases when a hexagon occurs only once in the boundary, this number is given by $6 - deg(v)$ with $deg(v)$ the degree of the corresponding vertex in the inner dual, we can omit the labels for these vertices. See Figure 3 for an example.

The class of graphs that are inner duals of fusenes can easily be characterized. A planar graph embedded in the plane is the inner dual of a fusene, if and only if it is *(i)* connected, *(ii)* all bounded faces of G are triangles, *(iii)* all inner vertices (vertices not on the boundary) have degree 6, and *(iv)* the number t_v of times a vertex v appears on the boundary of G plus its degree d_v is at most 6: $t_v + d_v \leq 6$.

These graphs can be easily constructed by adding one point at a time. To avoid the generation of isomorphic copies, we applied McKay's *canonical construction path method*.[34]

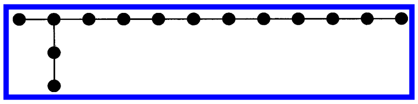

Figure 4. An inner dual of a fusene with 14 hexagons allowing $3^{10} = 59\,049$ labelings.

To construct fusenes, or to be exact, labeled inner duals, from these graphs, we have to assign labels to the vertices that occur more than once in the boundary in a way that the degree plus the sum of labels equals 6. Isomorphism rejection is done by the homomorphism principle described e.g. in ref 35 or—as part as a survey paper on isomorphism rejection methods—in ref 36.

It is easy to see why this gives such a fast algorithm: assume that two isomorphic labeled inner duals are constructed. Then this isomorphism induces an isomorphism of the underlying inner duals. Since we have only one element from every isomorphism class of inner duals, it must be an automorphism and in fact a nontrivial one, because otherwise we would have the same labeling twice, which must of course be avoided. But this implies that from inner duals with trivial symmetry, we can never construct isomorphic fusenes. So in these cases we need not run any checks on the labeled inner duals. In Figure 4 an example is shown where we can construct 59 049 fusenes without having to run any checks on them. Since the ratio of inner duals with trivial group grows very fast, the vast majority of fusenes can be accepted without any test. The ratio of inner duals with trivial group is already 99.9994% for fusenes with 26 hexagons—each of them with more than 7000 different labelings in average.

NUMERICAL RESULTS

The main new results obtained are the numbers of polyhexes up to 24 hexagons and fusenes up to 26. For polyhexes with $h = 22$ and 23 and fusenes with $22 \leq h \leq 25$, to check results, computations were done independently in Bielefeld and in Montreal, on a series of computers in each place. Results were in full agreement. For polyhexes with $h = 24$ and fusenes with $23 \leq h \leq 26$, computations were done in part in Bielefeld and in part in Montreal.

To further check the correctness and study the new algorithm performance, computations of known values were reproduced and agreed in all cases with those of refs 20−25. Values obtained for polyhexes are reported in Table 1, while those for fusenes are given in Table 2. The number of polyhexes with h hexagons are given in column 2. In total the set of polyhexes constructively enumerated is about 150 times larger than done before i.e. for $h \leq 21$.

Table 3 gives values for ratios of numbers of polyhexes with h and $h - 1$ hexagons. These ratios appear to be roughly equal to 5 and increase with h, 4.63 for $h = 10$ and 4.95 for $h = 24$.

Values for the number of dual graphs are given in column 4 of Table 3, and the number of such graphs having a nontrivial symmetry group in column 5. The number of dual graphs appears to be much smaller than the number of planar polyhexes and decreases proportionally when h increases: there are about 20 planar polyhexes per dual graph on average when $h = 10$ and 1100 when $h = 24$. Only a small portion of these dual graphs have nontrivial symmetry groups, and, again, this proportion decreases sharply when h increases as shown in column 6: 15% of dual graphs have nontrivial symmetry when $h = 10$ and about 0.0022% when $h = 24$. As noted above, this is an important factor in explaining the algorithm's good performance: for most polyhexes, as the dual graph has only trivial symmetry, no symmetry tests need be performed to avoid redundancy. Computing times are given in column 8 of Table 1. All enumerations up to $h = 21$ were done on a 700 MHz linux PC computer and on a heterogeneous set of computers from $h = 22$ to 24. As a very large set of polyhexes are enumerated, total computing times are considerable, for the largest values of h. A heterogeneous pool of computers was used in batch mode, mostly at night, to achieve the enumeration which would otherwise have lasted many years. Table 1 (and 2) also gives the number of polyhexes (and fusenes) generated per second. Interestingly, this number increases with h, despite the fact that polyhexes get larger. The increase in time due to generation of codes is thus more than compensated by the decrease in time for symmetry testing when h increases. The set of polyhexes with $h = 20$

Table 1. Number of Polyhexes, Total CPU Time Required on a 700 MHz Linux PC, and Average Number of Polyhexes Per Second According to h (*) Indicates Results Obtained from a Mixed Set of Very Different Computers[a]

H	*N*(*h*)	CPU time	polyhexes per second
10	30086	0.026″	1145315.25
11	141229	0.1″	1409710.61
12	669584	0.39″	1728333.36
13	3198256	1.55″	2066361.52
14	15367577	6.77″	2269002.79
15	74207910	29.85″	2485966.29
16	359863778	2′12.99″	2705975.87
17	1751594643	10′11.38″	2864968.76
18	8553649747	47′57.87″	2972215.53
19	41892642772	3h43′39.77″	3121710.54
20	205714411986	17h47′18.57″	3212351.85
21	1012565172403	3d15h26′42.78″	3216506.40
22(*)	4994807695197		
23(*)	24687124900540		
24(*)	122238208783203		

[a] In this case CPU time and generation rate is not consistent and is therefore omitted.

Table 2. Number of Fusenes, Total CPU Time Required on a 700 MHz Linux PC, and Average Number of Fusenes Per Second According to h (*) Indicates Results Obtained from a Mixed Set of Very Different Computers[a]

H	*N*(*h*)	CPU time	fusenes per second
10	33836	0.02″	1770714.85
11	166246	0.07″	2460934.95
12	829987	0.21″	3938641.22
13	4197273	0.81″	5185698.42
14	21456444	3.34″	6415651.05
15	110716585	14.21″	7787941.50
16	576027737	1′2.34″	9239180.77
17	3018986040	4′42.83″	10674061.31
18	15927330105	22′3.31″	12035977.15
19	84530870455	1h45′31.46″	13350923.88
20	451069339063	8h39′15.85″	14477839.03
21	2418927725532	1d19h30′11.44″	15445408.39
22(*)	13030938290472		
23(*)	70492771581350		
24(*)	382816374644336		
25(*)	2086362209298079		
26(*)	11408580755666756		

[a] In this case CPU time and generation rate is so dependent on the machine that it does not give any information and is therefore omitted.

Table 3. Number of Planar Polyhexes ($N(h)$), Ratio $N(h)/N(h-1)$, Number of Dual Graphs (DG), Ratio $N(h)/DG(h)$, Number of Dual Graphs with Nontrivial Symmetry (SDG), and Ratio SDG/DG in Percents According to h

H	$N(h)$	$\frac{N(h)}{N(h\text{-}1)}$	dual graphs	$\frac{N(h)}{DG(h)}$	S D G	$\frac{SDG}{DG}$
10	30086	4.62	1477	20.36	230	15.57
11	141229	4.69	4918	28.71	427	8.68
12	669584	4.74	16956	39.48	861	5.07
13	3198256	4.77	59494	53.75	1588	2.66
14	15367577	4.80	212364	72.36	3194	1.50
15	74207910	4.82	766753	96.78	5923	0.77
16	359863778	4.84	2796876	128.66	11963	0.42
17	1751594643	4.86	10284793	170.31	22144	0.21
18	8553649747	4.88	38096072	224.53	45009	0.11
19	41892642772	4.89	141998218	295.02	83605	0.05
20	205714411986	4.91	532301941	386.46	170059	0.03
21	1012565172403	4.92	2005638293	504.86	317341	0.01
22	4994807695197	4.93	7592441954	657.87	647393	0.008
23	24687124900540	4.94	28865031086	855.26	1210548	0.004
24	122238208783203	4.95	110174528925	1109.50	2477096	0.002

Table 4. Benzenoids with 21 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{59}H_{19}$	1					1	
$C_{60}H_{20}$	47			1	1	7	38
$C_{61}H_{21}$	587	2	2			12	571
$C_{62}H_{22}$	3838			3	13	70	3752
$C_{63}H_{23}$	18876					36	18840
$C_{64}H_{24}$	79472	1	4	5	45	235	79182
$C_{65}H_{25}$	296025					167	295858
$C_{66}H_{26}$	1029521			8	188	867	1028458
$C_{67}H_{27}$	3352432	1	21			517	3351893
$C_{68}H_{28}$	10337238			12	587	2453	10334186
$C_{69}H_{29}$	30314357					1262	30313095
$C_{70}H_{30}$	84877350	1	44	16	1588	6150	84869551
$C_{71}H_{31}$	225927887					3642	225924245
$C_{72}H_{32}$	573384355			16	4547	16214	573363578
$C_{73}H_{33}$	1384916403	2	103			8863	1384907435
$C_{74}H_{34}$	3175427434			42	11377	37733	3175378282
$C_{75}H_{35}$	6874424366					18149	6874406217
$C_{76}H_{36}$	14033798842	1	232	31	24111	75274	14033699193
$C_{77}H_{37}$	26842275823					34783	26842241040
$C_{78}H_{38}$	47720986689			43	47515	138929	47720800202
$C_{79}H_{39}$	78025561519		480			60330	78025500709
$C_{80}H_{40}$	116224121999			45	85645	239646	116223796663
$C_{81}H_{41}$	154775144598					82662	154775061936
$C_{82}H_{42}$	179004609494	2	577	73	124260	335306	179004149276
$C_{83}H_{43}$	171367411124					74046	171367337078
$C_{84}H_{44}$	127557881410			30	117943	311055	127557452382
$C_{85}H_{45}$	65842485473		460			33940	65842451073
$C_{86}H_{46}$	18806505243			40	61547	152826	18806290830
total	1012565172403	10	1923	365	479367	1635175	1012563055563

hexagons was enumerated in about 18 h and that one with $h = 21$ in about 3 days and 15 h of computer time. Comparing these results with the best previous ones (Caporossi and Hansen[25]) leads to the following conclusion: for $h = 20$, previous results with a Pentium II 266 took about 23 days, so the new algorithm appears to be roughly 10 times quicker, but this factor increases with h. The reason is that, as mentioned before, the average computing time per polyhex decreases when h grows with the new algorithm while it increased linearly with the previous one.

A further analysis of results for polyhexes with $h = 21$, 22, and 23 and fusenes with $h = 22$, 23, 24, 25, and 26 is given in Tables 4−7 and in Tables 8−12, respectively: numbers of polyhexes are broken down by isomers and by symmetry classes (only columns corresponding to classes of symmetry for which there exists at least one polyhex with h hexagons are given).

DISCUSSION

A novel approach has been proposed for the enumeration of planar polyhexes. It works at two levels: enumeration of dual graphs and enumeration of planar polyhexes for each inner dual. An algorithm based on this approach has been used to enumerate for the first time planar polyhexes with $h = 22$, 23, and 24 hexagons. The set of polyhexes with $h \le 24$ so enumerated contains over 150 billion molecules and is more than 150 times larger than the largest one previously enumerated.[25] A formula for estimating the number $N(h)$ of polyhexes with h hexagons has been proposed some time ago by Aboav and Gutman.[37] As shown in ref 25, predictions are close to real values for $h \le 17$ but appear to underestimate the real values when $h > 17$. Recently, Chyzak, Gutman, and Paule[38] explored a novel and more powerful approach to the estimation of $N(h)$. This approach uses values

Table 5. Benzenoids with 22 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{62}H_{20}$	16			1	2	4	9
$C_{63}H_{21}$	290		1			8	281
$C_{64}H_{22}$	2467			3	32	56	2376
$C_{65}H_{23}$	13652					54	13598
$C_{66}H_{24}$	62027	3	2	3	138	211	61670
$C_{67}H_{25}$	247989					178	247811
$C_{68}H_{26}$	903415			6	510	770	902129
$C_{69}H_{27}$	3066067		8			493	3065566
$C_{70}H_{28}$	9893810			16	1627	2349	9889818
$C_{71}H_{29}$	30276022					1193	30274829
$C_{72}H_{30}$	88445658	4	21	19	4641	6479	88434494
$C_{73}H_{31}$	247093330					2788	247090542
$C_{74}H_{32}$	660724668			24	12646	16960	660695038
$C_{75}H_{33}$	1685369866	1	58			5908	1685363899
$C_{76}H_{34}$	4107270241			30	31360	40657	4107198194
$C_{77}H_{35}$	9536543476					11169	9536532307
$C_{78}H_{36}$	21028831864	6	149	30	70888	89378	21028671413
$C_{79}H_{37}$	43844651607					19138	43844632469
$C_{80}H_{38}$	86215717266			50	144276	176325	86215396615
$C_{81}H_{39}$	158793911206		234			27984	158793882988
$C_{82}H_{40}$	271745847969			90	261789	311332	271745274758
$C_{83}H_{41}$	427742492665					36524	427742456141
$C_{84}H_{42}$	612649644824	18	512	62	409747	478536	612648755949
$C_{85}H_{43}$	782779458259					35025	782779423234
$C_{86}H_{44}$	866100354968			163	524600	599661	866099230544
$C_{87}H_{45}$	792069689506		767			20387	792069668352
$C_{88}H_{46}$	562684058255			37	462848	517568	562683077802
$C_{89}H_{47}$	277402920664						277402920664
$C_{90}H_{48}$	75380203150	9	755	81	232842	251310	75379718153
total	4994807695197	41	2507	615	2157946	2652445	4994802881643

Table 6. Benzenoids with 23 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{64}H_{20}$	4			1		2	1
$C_{65}H_{21}$	126					9	117
$C_{66}H_{22}$	1448			3	6	33	1406
$C_{67}H_{23}$	9349					38	9311
$C_{68}H_{24}$	47167			3	45	235	46884
$C_{69}H_{25}$	200545					124	200421
$C_{70}H_{26}$	771061			6	145	704	770206
$C_{71}H_{27}$	2745113					435	2744678
$C_{72}H_{28}$	9185903			13	510	2283	9183097
$C_{73}H_{29}$	29232372					1437	29230935
$C_{74}H_{30}$	89047381			19	1706	6954	89038702
$C_{75}H_{31}$	259056456					3628	259052828
$C_{76}H_{32}$	723113653			24	4697	17864	723091068
$C_{77}H_{33}$	1936428286					9528	1936418758
$C_{78}H_{34}$	4970254505			35	12446	43798	4970198226
$C_{79}H_{35}$	12200281933					24237	12200257696
$C_{80}H_{36}$	28643742341			45	32297	106293	28643603706
$C_{81}H_{37}$	64109618941					53593	64109565348
$C_{82}H_{38}$	136335211131			79	73731	228216	136334909105
$C_{83}H_{39}$	274374476732					104754	274374371978
$C_{84}H_{40}$	520693871834			70	147440	431864	520693292460
$C_{85}H_{41}$	925231748273					188701	925231559572
$C_{86}H_{42}$	1527029503977			108	274532	760883	1527028468454
$C_{87}H_{43}$	2317626216529					300925	2317625915604
$C_{88}H_{44}$	3196330255841			70	454304	1212591	3196328588876
$C_{89}H_{45}$	3924113646972					373411	3924113273561
$C_{90}H_{46}$	4161661164458			169	594505	1536669	4161659033115
$C_{91}H_{47}$	3643586919511					305586	3643586613925
$C_{92}H_{48}$	2476073860335				514849	1298746	2476072046740
$C_{93}H_{49}$	1168340063265					129710	1168339933555
$C_{94}H_{50}$	302754225098			103	245895	586556	302753392544
total	24687124900540			748	2357108	7729807	24687114812877

of the whole sequence $N(k)$ for $k < h$ and the theory of *univariate holonomic functions*.[38] Based upon values of $N(h)$ for $h = 1$ *to* 21 from refs 20−25 and values of $N(22)$ and $N(23)$ from a preliminary presentation of this paper Chizak et al.[38] predict that $N(24) = 122237774262384$ and $N(25) = 6062593054148149$, with six and five significant digits, respectively. As the real value of $N(24)$ is 122238208783203, the first prediction is correct, with the stated accuracy.

Clearly the approach of this paper could be applied to the enumeration of many other classes of molecules. With the

Table 7. Polyhexes with 24 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{66}H_{20}$	1			1			
$C_{67}H_{21}$	43		1			2	40
$C_{68}H_{22}$	789			2	18	34	735
$C_{69}H_{23}$	6124					37	6087
$C_{70}H_{24}$	34324	2	6	2	107	173	34034
$C_{71}H_{25}$	157989					155	157834
$C_{72}H_{26}$	643859			7	427	657	642768
$C_{73}H_{27}$	2389044		16			482	2388546
$C_{74}H_{28}$	8341018			12	1490	2206	8337310
$C_{75}H_{29}$	27543406					1334	27542072
$C_{76}H_{30}$	86809987	3	40	23	4590	6510	86798821
$C_{77}H_{31}$	262398390					3315	262395075
$C_{78}H_{32}$	762002033			30	13298	18208	761970497
$C_{79}H_{33}$	2123950040		133			7804	2123942103
$C_{80}H_{34}$	5696736534			23	35971	47329	5696653211
$C_{81}H_{35}$	14682481766					16914	14682464852
$C_{82}H_{36}$	36317312851	1	283	53	90268	114779	36317107467
$C_{83}H_{37}$	86051673983					33879	86051640104
$C_{84}H_{38}$	195126389101			52	209337	258280	195125921432
$C_{85}H_{39}$	421970853293	5	630			60786	421970791872
$C_{86}H_{40}$	867366149134			105	443940	532865	867365172224
$C_{87}H_{41}$	1687976789804					98070	1687976691734
$C_{88}H_{42}$	3096731853207	2	1279	124	846043	987689	3096730018070
$C_{89}H_{43}$	5317534069199					137195	5317533932004
$C_{90}H_{44}$	8477771216467			206	1440863	1641862	8477768133536
$C_{91}H_{45}$	12423582389694	3	2283			166882	12423582220526
$C_{92}H_{46}$	16519224289831			135	2105423	2358366	16519219825907
$C_{93}H_{47}$	19514318126449					146898	19514317979551
$C_{94}H_{48}$	19872186264006		2471	307	2482288	2723100	19872181055840
$C_{95}H_{49}$	16688966939777					77267	16688966862510
$C_{96}H_{50}$	10871927816586			42	2018188	2164650	10871923633706
$C_{97}H_{51}$	4919263363368		1727				4919263361641
$C_{98}H_{52}$	1218239791106			113	931601	966300	1218237893092
total	122238208783203	16	8869	1237	10623852	12574028	122238185575201

Table 8. Fusenes with 22 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{62}H_{20}$	16			1	2	4	9
$C_{63}H_{21}$	290		1			8	281
$C_{64}H_{22}$	2467			3	32	56	2376
$C_{65}H_{23}$	13652					54	13598
$C_{66}H_{24}$	62059	3	2	3	138	212	61701
$C_{67}H_{25}$	249560					187	249373
$C_{68}H_{26}$	922044			6	510	783	920745
$C_{69}H_{27}$	3199475		8			533	3198934
$C_{70}H_{28}$	10640364			17	1630	2535	10636182
$C_{71}H_{29}$	33789373					1352	33788021
$C_{72}H_{30}$	102950093	4	21	19	4757	7484	102937808
$C_{73}H_{31}$	301331020					3391	301327629
$C_{74}H_{32}$	847281192			26	13276	21245	847246645
$C_{75}H_{33}$	2279612359	2	60			8067	2279604230
$C_{76}H_{34}$	5877688301			32	34345	55794	5877598130
$C_{77}H_{35}$	14473565043					16692	14473548351
$C_{78}H_{36}$	33915807920	6	160	40	81379	135190	33915591145
$C_{79}H_{37}$	75278121292					31411	75278089881
$C_{80}H_{38}$	157842852130			54	173257	291344	157842387475
$C_{81}H_{39}$	310233169716		281			52815	310233116620
$C_{82}H_{40}$	566811884929			131	332556	574364	566810977878
$C_{83}H_{41}$	952681353673					76282	952681277391
$C_{84}H_{42}$	1456866469815	20	655	70	549920	971115	1456864948035
$C_{85}H_{43}$	1982805876265					76761	1982805799504
$C_{86}H_{44}$	2329329491408			277	737676	1342969	2329327410486
$C_{87}H_{45}$	2255574110204		1003			51319	2255574057882
$C_{88}H_{46}$	1704767353642			51	683310	1274425	1704765395856
$C_{89}H_{47}$	904573028990						904573028990
$C_{90}H_{48}$	276327463180	15	1102	188	375524	751033	276326335318
total	13030938290472	50	3293	918	2988312	5747425	13030929550474

previous enumeration method, enumeration is more difficult than for planar polyhexes because when using the BE code, orphans (that cannot be generated due with the specific enumeration tree) appear already when $h = 20$[31], and, as mentioned above, there are pairs of distinct helicenes with the same BE code,[32] from $h = 25$ onward. Following

Table 9. Fusenes with 23 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{64}H_{20}$	4			1		2	1
$C_{65}H_{21}$	126					9	117
$C_{66}H_{22}$	1448			3	6	33	1406
$C_{67}H_{23}$	9349					38	9311
$C_{68}H_{24}$	47171			3	45	236	46887
$C_{69}H_{25}$	201113					126	200987
$C_{70}H_{26}$	781183			6	145	723	780309
$C_{71}H_{27}$	2831856					473	2831383
$C_{72}H_{28}$	9727293			13	510	2416	9724354
$C_{73}H_{29}$	32003229					1658	32001571
$C_{74}H_{30}$	101412837			19	1739	7813	101403266
$C_{75}H_{31}$	308365006					4675	308360331
$C_{76}H_{32}$	903199293			28	4906	21575	903172784
$C_{77}H_{33}$	2547079997					13325	2547066672
$C_{78}H_{34}$	6905474303			37	13450	57298	6905403518
$C_{79}H_{35}$	17951229551					36963	17951192588
$C_{80}H_{36}$	44746799814			55	36524	152858	44746610377
$C_{81}H_{37}$	106538616373					90391	106538525982
$C_{82}H_{38}$	241417796285			92	87242	357015	241417351936
$C_{83}H_{39}$	518467103666					192587	518466911079
$C_{84}H_{40}$	1051271149216			91	182817	737545	1051270228763
$C_{85}H_{41}$	1996752230986					381508	1996751849478
$C_{86}H_{42}$	3523516200300			139	361188	1434489	3523514404484
$C_{87}H_{43}$	5717346564789					667157	5717345897632
$C_{88}H_{44}$	8424666093927			114	632578	2507225	8424662954010
$C_{89}H_{45}$	11021745857204					895538	11021744961666
$C_{90}H_{46}$	12418764521506			256	856492	3385348	12418760279410
$C_{91}H_{47}$	11531707595904					777673	11531706818231
$C_{92}H_{48}$	8359646974100				755737	3022948	8359643195415
$C_{93}H_{49}$	4261485821599					342738	4261485478861
$C_{94}H_{50}$	1245935891922			188	375524	1502284	1245934013926
total	70492771581350			1045	3308903	16594667	70492751676735

Table 10. Fusenes with 24 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{66}H_{20}$	1			1			
$C_{67}H_{21}$	43		1			2	40
$C_{68}H_{22}$	789			2	18	34	735
$C_{69}H_{23}$	6124					37	6087
$C_{70}H_{24}$	34324	2	6	2	107	173	34034
$C_{71}H_{25}$	158144					159	157985
$C_{72}H_{26}$	648833			7	427	666	647733
$C_{73}H_{27}$	2441952		16			511	2441425
$C_{74}H_{28}$	8716742			12	1490	2296	8712944
$C_{75}H_{29}$	29650651					1478	29649173
$C_{76}H_{30}$	96903418	3	40	23	4649	7214	96891489
$C_{77}H_{31}$	305367060					3895	305363165
$C_{78}H_{32}$	928636403			36	13793	21797	928600777
$C_{79}H_{33}$	2720423258	1	135			9910	2720413212
$C_{80}H_{34}$	7694135780			23	38582	61343	7694035832
$C_{81}H_{35}$	20972750996					23747	20972727249
$C_{82}H_{36}$	55001434461	1	303	62	100944	163459	55001169692
$C_{83}H_{37}$	138483894649					53104	138483841545
$C_{84}H_{38}$	334388076753			58	246047	404174	334387426474
$C_{85}H_{39}$	771242974577	6	701			104341	771242869529
$C_{86}H_{40}$	1693160752488			151	548966	919206	1693159284165
$C_{87}H_{41}$	3523443608933					187655	3523443421278
$C_{88}H_{42}$	6918072102201	3	1508	160	1103167	1873536	6918069123827
$C_{89}H_{43}$	12716032056937					299207	12716031757730
$C_{90}H_{44}$	21702739655309			336	1994983	3472005	21702734187985
$C_{91}H_{45}$	34034966854177	9	2859			399364	34034966451945
$C_{92}H_{46}$	48377948880959			193	3083825	5482884	48377940314057
$C_{93}H_{47}$	60923773326726					370173	60923772956553
$C_{94}H_{48}$	65964838261853		3087	478	3819606	6989479	65964827449203
$C_{95}H_{49}$	58858357937056					223977	58858357713079
$C_{96}H_{50}$	41010359983640			51	3274338	6140178	41010350569073
$C_{97}H_{51}$	20119936936041		2219				20119936933822
$C_{98}H_{52}$	5640868033058			188	1664015	3328030	5640863040825
total	382816374644336	25	10875	1783	15894957	30544034	382816328192662

enumeration of fusenes to $h = 15$ by Brunvoll et al.,[39] the BE code and orderly generation were used to enumerate such molecules with $h \leq 20$.[31] In another paper[33] the two-level approach described here is applied to the counting of fusenes

Table 11. Fusenes with 25 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{69}H_{21}$	13	1				3	9
$C_{70}H_{22}$	377			2	4	24	347
$C_{71}H_{23}$	3735					29	3706
$C_{72}H_{24}$	24118	2	1	5	25	131	23953
$C_{73}H_{25}$	120554					114	120440
$C_{74}H_{26}$	524277			6	132	670	523469
$C_{75}H_{27}$	2072796	1	8			423	2072364
$C_{76}H_{28}$	7651202			10	473	2307	7648412
$C_{77}H_{29}$	26860896					1353	26859543
$C_{78}H_{30}$	90685646	1	25	19	1469	6814	90677317
$C_{79}H_{31}$	294562963					4581	294558382
$C_{80}H_{32}$	924559738			31	4894	21998	924532815
$C_{81}H_{33}$	2806148724	1	48			13890	2806134785
$C_{82}H_{34}$	8234470707			47	14744	64640	8234391276
$C_{83}H_{35}$	23337273144					38789	23337234355
$C_{84}H_{36}$	63922633920	8	177	62	39776	170723	63922423173
$C_{85}H_{37}$	168852094677					104802	168851989875
$C_{86}H_{38}$	429385902834			91	105267	441222	429385356254
$C_{87}H_{39}$	1049084647460	3	419			269058	1049084377980
$C_{88}H_{40}$	2457887660324			97	265094	1095003	2457886300130
$C_{89}H_{41}$	5500452610149					610892	5500451999257
$C_{90}H_{42}$	11716813721258	18	972	196	591209	2398941	11716810729918
$C_{91}H_{43}$	23655553846218					1239007	23655552607211
$C_{92}H_{44}$	45030114059836			226	1185497	4754880	45030108119233
$C_{93}H_{45}$	80199532579866		1769			2316724	80199530261373
$C_{94}H_{46}$	132546287292835			264	2215965	8787858	132546276288748
$C_{95}H_{47}$	201096822793187					3726026	201096819067161
$C_{96}H_{48}$	276029896848327	38	3688	355	3569692	14143599	276029879130949
$C_{97}H_{49}$	335065018786608					4553620	335065014232988
$C_{98}H_{50}$	349233191892987			349	4408744	17450804	349233170033090
$C_{99}H_{51}$	299986425679336		4933			3642533	299986422031870
$C_{100}H_{52}$	201275032921426			274	3597040	14388434	201275014935678
total	2086362209298079	88	16675	2222	17664040	88408597	2086362103206444

Table 12. Fusenes with 26 Hexagons According to Symmetry and Isomers

isomer	number	D3h	C3h	D2h	C2h	C2v	Cs
$C_{71}H_{21}$	2						2
$C_{72}H_{22}$	156			1	8	16	131
$C_{73}H_{23}$	2146					21	2125
$C_{74}H_{24}$	16114			5	75	129	15905
$C_{75}H_{25}$	89291					121	89170
$C_{76}H_{26}$	415026			9	346	553	414118
$C_{77}H_{27}$	1717641					462	1717179
$C_{78}H_{28}$	6602604			8	1284	2001	6599311
$C_{79}H_{29}$	23948010					1454	23946556
$C_{80}H_{30}$	83104146			13	4408	6808	83092917
$C_{81}H_{31}$	277944743					4111	277940632
$C_{82}H_{32}$	899003741			32	13534	21081	898969094
$C_{83}H_{33}$	2811003293					11349	2810991944
$C_{84}H_{34}$	8518689591			45	40148	63181	8518586217
$C_{85}H_{35}$	25009679327					29269	25009650058
$C_{86}H_{36}$	71087726820			91	113583	180890	71087432256
$C_{87}H_{37}$	195452591330					71268	195452520062
$C_{88}H_{38}$	519649522494			92	299614	481635	519648741153
$C_{89}H_{39}$	1332948639137					163071	1332948476066
$C_{90}H_{40}$	3293047426892			145	744570	1217590	3293045464587
$C_{91}H_{41}$	7819020933152					344829	7819020588323
$C_{92}H_{42}$	17799952888030			163	1718108	2848636	17799948321123
$C_{93}H_{43}$	38703513605586					647233	38703512958353
$C_{94}H_{44}$	80096907623043			275	3628442	6121628	80096897872698
$C_{95}H_{45}$	157059721995634					1113172	157059720882462
$C_{96}H_{46}$	290179001174842			258	6915782	11846227	290178982412575
$C_{97}H_{47}$	501328642753301					1677481	501328641075820
$C_{98}H_{48}$	803168051569463			766	11810625	20694386	803168019063686
$C_{99}H_{49}$	1179974918629309					2076402	1179974916552907
$C_{100}H_{50}$	1565694336418938			292	17106283	30600504	1565694288711859
total	11408580755666756			4311	85259905	163717519	11408580506685021

with up to $h = 26$. The task is somewhat easier than for planar polyhexes as testing planarity is not needed. Other classes of molecules which could be enumerated in a similar way are listed in the detailed survey of Cyvin et al.[12]

The question of further progress remains, as usual, open. Of course, larger sets of polyhexes could (and probably will) be enumerated with more powerful computers, but the algorithmic progress should be judged separately. It then appears that the present approach eliminates most of the time spent on symmetry testing, as there are few dual graphs compared to polyhexes, and those dual graphs which have nontrivial symmetry are a small portion of them.

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