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Note

On Counting Polyhex Hydrocarbons*

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The counting of the number of P_h geometrically planar, without annulene-like holes, polyhex hydrocarbons with h hexagons, is reported with up to $h = 13$. The exact value of P_{13} is 3198256. This value is lower than the value (3201000) recently predicted.

This report was motivated by a recent paper of Aboav and Gutman[1] on the estimation of P_h, the number of polyhex hydrocarbons with h hexagons. They considered geometrically planar simply connected polyhex hydrocarbons. Aboav and Gutman produced a formula for rather accurate estimation of P_h with up to $h = 12$, and predicted P_{13} to be 3.201×10^6. They concluded their report by expressing hope that somebody will soon compute P_{13}. As soon as we read the above paper we computed P_h with up to $h = 13$. Here we report our results.

Our paper[2] in 1983 was amongst the first published reports on the computer enumeration of P_h, though there had been earlier reports in the chemical literature on the counting of certain classes of polyhex hydrocarbons such as cata-condensed polyhexes; the very first was a report by Balaban and Harary in 1968.[3] Since that time we tried to improve our algorithm, based on the boundary code,[2] for computation of P_h.[4–6] However, it was only recently[7,8] that we were able to devise an algorithm which is fast enough to tackle P_h with larger values ($h \geq 10$). The algorithm is based on a code in which every hexagon of a polyhex hydrocarbon is represented by a single digit from 0 to 7. Perhaps the easiest way of introducing this code is by the reconstruction of a polyhex from its code. The other way from the polyhex to the code is then simply governed by a set of rules[8] which enforce different people to select the same of the possible many digit sequences allowing the reconstruction of the same polyhex.

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The digit from 0 to 7 is merely a short notation for 3 bits (binary digits) each of which describes the absence or presence of a neighbouring hexagon in a specific direction relative to the direction from the starting hexagon. To reconstruct the same polyhex there must obviously be an arbitrary but fixed convention about the ordering of the 3 directions: 60° to the left, straightforward, 60° to the right and a mapping of them to the 3 bits, *e. g.* values 4, 1, 2, (see Figure 1). A similar idea was also discussed by Balaban and Harary.[3]

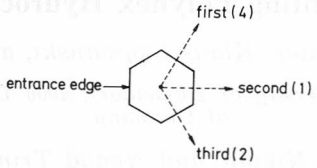
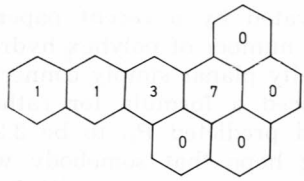


Figure 1. Ordering of directions and their weights (in parentheses).

If there are hexagons in all three directions, then the entry is maximum, *i. e.*, 7. If there are no hexagons in any of three directions, the entry is minimum, *i. e.*, 0. This code can never start with zero, except in one case, that is in the case of benzene whose code consists of only a single digit: 0. As an example we give in Figure 2 the code for benzo[uv]naphtho[2,1,8,7-defg]-pentacene.



CODE: 11370000

Figure 2. Labelling of each hexagon in benzo[u,v]naphtho[2,1,8,7-defg]pentacene and the corresponding code.

On the basis of this code we developed a computer algorithm for generating and counting geometrically planar simply connected polyhex hydrocarbons.[8] We spent 21378 seconds cpu time on a 6 mips computer in order to generate and enumerate P_h with up to $h = 13$. In Table I we give exact and estimated values of P_h ($h \leq 13$). For previous computations the reader is adviced to consult the consolidated report by Balaban et al.[9]

We did not confirm the prediction of Aboav and Gutman[1] for P_{13}, we obtained for $P_{13} = 3198256$, a number which is smaller than their value (3201000). They may perhaps now re-adjust the parameters in their approximate formula in order to make it more precise, because their argument that P_{20} or P_{30} may never be known exactly is valid. We are now trying to compute P_{14}, though a lot of cpu time will be needed for this computation. As the overal time expense of the algorithm is nearly proportional to the number of all hexagons in all generated polyhexes (and in effect such an expense — perhaps with a different constant factor — must be in any

TABLE I

Exact and estimated values of polyhex hydrocarbons with up to 13 hexagons. Estimated values are taken from Aboav and Gutman[1]

h	P_h (exact)	P_h (estimated)
1	1	
2	1	
3	3	
4	7	
5	22	
6	81	
7	331	339
8	1435	1454
9	6505	6502
10	30086	30088
11	141229	141185
12	669584	669787
13	3198256	3201000

algorithm), we will need for P_{14} about 6 times the cpu time for P_{13}, just as we needed for P_{13} about 5.5 times that for P_{12}.

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SAŽETAK

O prebrojavanju policikličkih ugljikovodika

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Prebrojeni su planarni policiklički ugljikovodici P_h bez anulenskih rupa, koji su sastavljeni od h benzenskih prstenova. Numerički su rezultati dobiveni po prvi puta do $h = 13$. Točna vrijednost za P_{13} je 3198256. To je nešto niža vrijednost od nedavno objavljene aproksimativne vrijednosti za P_{13} (3201000).