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Use of Small Computers for Large Computations: Enumeration of Polyhex Hydrocarbons

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The enumeration of polyhex hydrocarbons with up to 16 hexagons is reported. These results are now for the first time available.

Recently in this journal Tošić and Kovačević[1] reported generation and enumeration of unbranched catacondensed benzenoids with up to $h = 20$ (h is the number of hexagons in the benzenoid hydrocarbon). There have also been other papers in this journal on enumeration of benzenoid hydrocarbons.[2-4] However, all these papers (and others in the literature[5]) are incomplete in the sense that they did not give the total numbers of benzenoid hydrocarbons for $h \geq 13$. The reason is that the enumeration of benzenoid hydrocarbons is a difficult combinatorial problem.[6] It is also a computationally involved problem.[5,7]

Since we have successfully developed a very powerful algorithm for enumeration of hexagonal structures,[8] we wish to supplement the above studies with counts of polyhex hydrocarbons with up to $h = 16$. Polyhex hydrocarbons are graph theoretically represented by polyhexes.[9] Polyhexes are hexagonal systems that may be obtained by any combination of regular hexagons such that two hexagons have exactly one common edge or are disjoint. Benzenoid hydrocarbons represent a subset of polyhex hydrocarbons[10] and are graph theoretically depicted by benzenoid graphs.[9] Benzenoid graphs are those polyhexes that are 1-factorable structures.[11] A 1-factorable polyhex corresponds to a polyhex hydrocarbon with Kekulé structure(s).[12] Most of the papers reporting the enumeration of hexagonal structures did not distinguish be-

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Table I. Enumeration of Polyhexes with up to $h = 16$

h	planar polyhexes without holes	planar polyhexes with holes: single hole	planar polyhexes with holes: multiple holes	CPU time: days	h	min	s
1	1						0.44
2	1						0.44
3	3						0.44
4	7						0.44
5	22						0.60
6	81						1.26
7	331						4.67
8	1435	1					20.87
9	6505	5				1	40.13
10	30086	43				8	12.90
11	141229	283				40	52.17
12	669584	1954			3	24	1.80
13	3198256	12363	1		17	4	32.50
14	15367577	76283	11	3	14	4	24.76
15	74207910	453946	149	18	3	13	34.70
16	359863778	2641506	1618	91	7	24	33.69

tween the terms polyhex and benzenoid.

Our algorithm for enumeration of polyhexes is based on the DAST (the dualist angle-restricted spanning tree) code.[13] This code is founded on the graph-theoretical concept of the weighted spanning tree of dualist.[14] A computer program for enumerating polyhex hydrocarbons using our algorithm is detailed elsewhere.[8] Counts of planar polyhex hydrocarbons with and without holes with up to $h = 16$ are given in Table I. In the table we also give CPU time needed to complete computation for each h. For example, the required CPU time for the enumeration of polyhexes with 16 hexagons was 91 days, 7 h, 24 min, and 33.69 s.

Computations have been carried out on the Siemens PCD3D (20 MHz, 386-AT). We deliberately did not use our supercomputer to show that these types of combinatorial computations can be completed on the personal computer, if one is willing to spend some time to design carefully an efficient computational algorithm and if one can spare a PC for continuous computations over a long period of time.

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Molecular Topological Index

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The molecular topological index (MTI) has been systematically tested for counterexamples (two or more nonisomorphic structures with the same MTI number). The analysis was carried out for alkane trees with up to 16 atoms. The search for counterexamples was positive: The first pair of alkane trees with identical MTI numbers was found in the octane family. The more disturbing finding was that two nonisomorphic alkane trees of different sizes may also possess the same MTI value. An attempt to redefine the MTI in terms of only the distance matrix and the valency matrix was abortive.

Schultz[1] has recently introduced in this journal a novel topological (or, more correctly, graph-theoretical) descriptor for characterization of alkanes by an integer. This descriptor was named by its originator the molecular topological index (MTI). The MTI appears to be an attractive graph-theoretical descriptor that is easy to compute and has structural significance. The important questions, Are the MTI numbers unique?, and, if the answer is positive, What are the smallest graphs for which MTI is not unique?, however, were not considered by Schultz. He only stated that the MTI is a highly discriminative descriptor. In this paper we will try to answer these questions.

The MTI is based on the adjacency ($N \times N$) matrix A, the distance ($N \times N$) matrix D, and the valency ($1 \times N$) matrix v of an alkane. The sum of the elements e_i ($i = 1, 2, ..., N$)

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