Open problem

Algebraic solution for the numbers of staggered conformers of alkanes

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The enumeration of alkane isomers has very long traditions. In particular, the studies on constitutional isomers of alkanes are well known through several reviews [1–5] of the relevant history. As chemical graphs [4], the alkane isomers are represented by trees in which the degree of any vertex does not exceed four (quartic trees [6]). The enumeration of free (unrooted) quartic trees, corresponding to the constitutional alkane isomers C_nH_{2n+2}, started with Cayley [7,8]. The work of Flavitzky [9], which predates Cayley, is often overlooked. It deals with rooted quartic trees, corresponding to constitutional alcohol isomers of the form $C_nH_{2n+1}OH$. Since Flavitzky and Cayley, a great deal of work has been done on the enumeration of constitutional isomers of alkanes. The problem was eventually solved satisfactorily for all chemical purposes, and the solution has been expressed in different ways: by recursive algorithms [10,11], in terms of generating functions [12,13], and on the basis of combinatorial summations [14]. The amount of numerical data from computer programmings, which are available, is overwhelming [3,4,13–17]. In contrast to these extensive studies, very little work has been done on the enumeration of alkane conformers (conformational isomers), although this kind of enumeration is supposed to be of even greater interest in chemistry than the enumeration of alkane constitutional isomers.

A staggered alkane conformer as a chemical graph [4] shall presently be referred to as an *alkanoid* (not to be confused with alkaloid). An alkanoid is an angle-restricted tree which can be embedded in the diamond lattice [18–20].

A complete mathematical solution for the numbers of nonisomorphic *unbranched* alkanoids has been given by Funck [21]. In this work, which was ahead of its time, it is not referred explicitly to graph theory. The work passed unnoticed among graph theoreticians and mathematical chemists, who later performed similar enumerations. In fact, Balaban [22] rediscovered Funck's solution eighteen

years later. An alternative approach, referred to as graphical enumeration, is due to Randić [23]. Balaban [22] pointed out the interesting one-to-one correspondence between unbranched alkanoids and unbranched catafusenes [24]. Harary and Read [25] have furnished the solution for catafusenes in total (unbranched + branched) and presented the result as a complicated generating function. It is tempting to investigate whether their methods could be used to deduce an algebraic solution for the numbers of nonisomorphic alkanoids in total (including the *branched* systems). So far, only some rudimentary results [22,26] are available for the numbers of branched alkanoids.

Overlapping systems have to be tolerated. In an overlapping system at least two vertices occupy the same site in the diamond lattice. Such systems are also included in the numbers from Funck [21] and from Balaban [22] for unbranched alkanoids. The corresponding systems among catafusenes are the catacondensed helicenes. They are included in the Harary–Read [25] numbers and particularly in the algebraic solution for unbranched catafusenes by Balaban and Harary [24].

In summary, the open problem is this: Deduce an algebraic solution for the numbers of nonisomorphic alkanoids, corresponding to staggered alkane conformers (C_nH_{2n+2}), which can be embedded in a diamond lattice.

The present author is interested even in partial solutions of the problem, e.g. for specific symmetries. It was ascertained that sixteen symmetry groups are possible for the branched alkanoids, viz.: T_d, T, D_{3d}, D_3, S_6, C_{3v}, C_3, D_{2d}, D_2, S_4, C_{2h}, C_{2v}, C_2, C_s, C_i, C_1.

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