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Letter

Double bonds in fused hexacyclic systems

Sasan Karimi

Chemistry Department, Queensborough Community College, Bayside, NY 11364, USA
E-mail: skarimi@qcc.cuny.edu

Marty Lewinter

Mathematics Department, Purchase College, Purchase, NY 10577, USA

Julian Stauffer

High School Intel, 31 Woodland Rd., Bedford, NY 10506, USA

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If a hexacyclic graph, G, represents a benzenoid, a perfect matching corresponds to the location of double bonds (pi-bonds). We present an algorithm for counting the number of configurations of double bonds for various benzenoids.

KEY WORDS: perfect matching, diminished mesh, benzenoid

Planar graphs such that each edge belongs to one or two hexacycles and whose vertices belong to at most three hexacycles are useful in representing benzenoids. Much attention has been devoted to counting perfect matchings in such graphs [1–5]. The *mesh* $M(a, b)$ is defined as follows. The vertices are the points (x, y) such that x and y are integers with $1 \leqslant x \leqslant a$ and $1 \leqslant y \leqslant b$. (x, y) and (x', y') are adjacent if either $x = x'$ and $|y - y'| = 1$, or $y = y'$ and $|x - x'| = 1$. The number of shortest paths from a corner vertex of the mesh $M(a, b)$ to the opposite corner is $\binom{a+b-2}{a-1}$.

We present an algorithm for counting perfect matchings in fused hexacylic systems such as the graph in figure 1. We consider fused hexacylic systems with a unique pair of vertices a and z where a is the highest, and z the lowest vertex (a and z are called “peak” and “valley”, respectively [6]). If two 6-cycles intersect, they have exactly one common edge.

For reasons which will soon become clear, some vertices such as f, g, and h are suppressed in figure 1. Edges such as fi, shall be called *vertical* while edges such as df shall be called *slanting*. Figure 2 depicts a perfect matching for the graph G of figure 1.

We make three observations about any perfect matching M for G. (1) Every row of slanting edges has exactly one edge in M. (2) Every row of vertical edges has all but one edge in M. (3) The slanting edges in M and the vertical edges not in M form a descending a–z path.

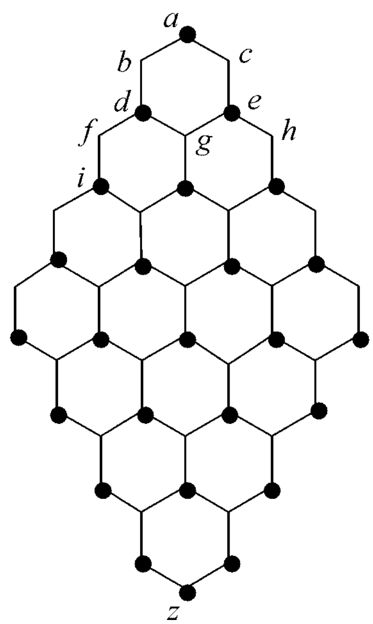

Figure 1. A parallelogram-like fused hexacyclic system G.

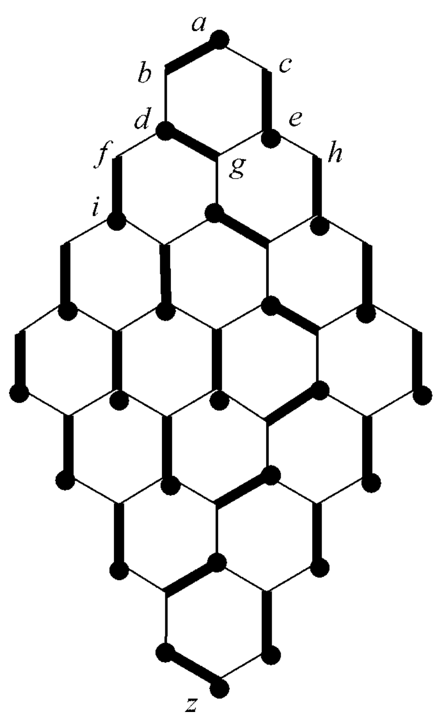

Figure 2. A perfect matching for the graph G of figure 1.

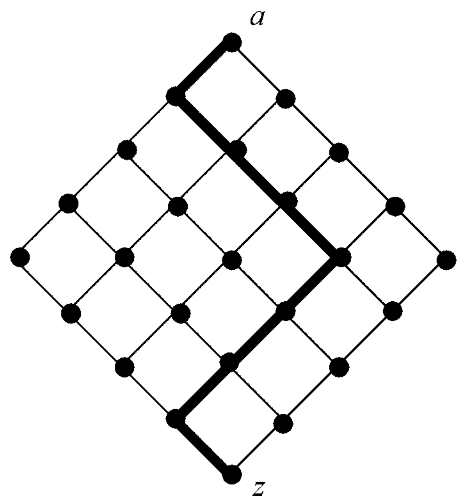

Figure 3. The mesh $H(G)$ with an a–z path corresponding to a perfect matching of G.

It follows that there is a one-to-one correspondence between perfect matchings and descending a–z paths [6,7]. To count the latter, observe that the suppressed vertices play no role in forming a descending path. There are no decisions to be made when we reach them since they are the upper vertices of vertical edges. Then the descending a–z paths in G correspond to the descending a–z paths in a 2-mesh $H(G)$ such as the one depicted in figure 3 whose vertices correspond to those not suppressed in G. The bold a–z path in $H(G)$ corresponds to the one in G corresponding to the perfect matching shown in figure 2.

Since the number of a–z paths in $H(G)$ is $\binom{8}{4}$, it follows that G has 70 perfect matchings and the benzenoid it describes has 70 configurations of pi-bonds (or 70 resonance structures as chemists call them). Rispoli [8], described an alternate approach to solve this problem.

To generalize the algorithm to non-parallelogram-like fused hexacyclic systems, we define a *diminished mesh* as the result of deleting one or more submeshes from a given mesh such that the intersection of these meshes includes boundary vertices of the given mesh. Figure 4 depicts a diminished mesh.

The diminished mesh of figure 4 corresponds to the fused hexacyclic system depicted in figure 5. It is therefore necessary to count a–z paths in the mesh of figure 4. Without loss of generality, given a diminished mesh formed by deleting one submesh, we may enlarge the deleted submesh so that it includes a corner vertex of the given mesh. To count the descending a–z paths in the diminished mesh shown in figure 6, let u and v be the surviving vertices in the row containing the "interior" corner vertex of the deleted submesh. Letting $f(x, y)$ represent the number of descending x–y paths assuming no deletions, the number of descending a–z paths is given by

$$f(a,u)\cdot f(u,z) + f(a,v)\cdot f(v,z) = \binom{5}{2}\binom{3}{1} + \binom{5}{1}\binom{3}{0} = 35.$$

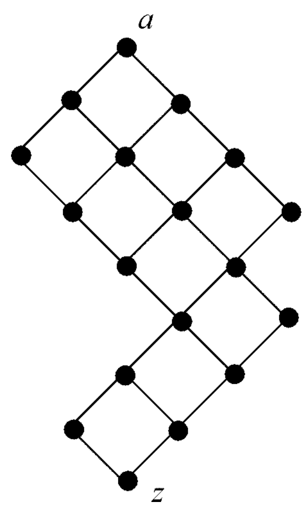

Figure 4. A diminished mesh.

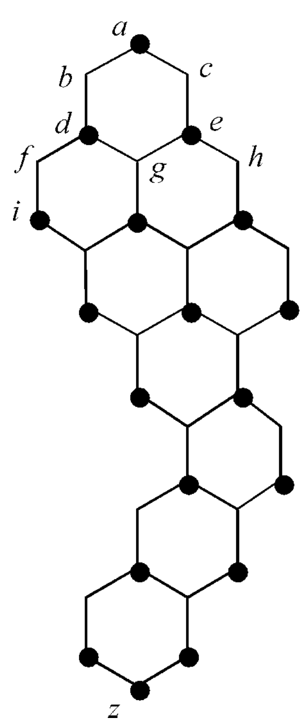

Figure 5. The fused hexacyclic system whose corresponding mesh is the graph of figure 4.

Applying this to the diminished mesh of figure 4, we obtain, after noting that the deleted vertex on the right deletes one a–z path, 34 descending a–z paths. It follows

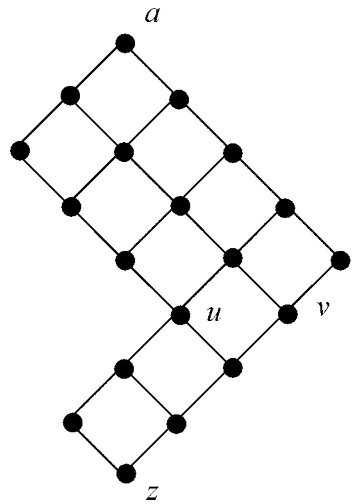

Figure 6. A diminished mesh missing a submesh containing a corner vertex.

that the fused hexacyclic system of figure 5 has 34 configurations of pi-bonds or 34 resonance structures. Note that there are other ways to obtain this answer [3,4,6,7].

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