J Math Chem (2008) 44:913–916
DOI 10.1007/s10910-008-9437-9

ORIGINAL PAPER

Resonance structure counts in parallelogram-like benzenoids with holes

Sasan Karimi · Anthony Delgado · Marty Lewinter

Received: 10 March 2008 / Accepted: 15 June 2008 / Published online: 7 August 2008

Abstract If a hexacyclic graph G represents a benzenoid, a perfect matching corresponds to a configuration of π-bonds. We present an algorithm for counting the number of configurations of π-bonds for parallelogram-like benzenoids with parallelogram-like holes by counting descending paths in a corresponding rectangular mesh with rectangular holes.

Keywords Parallelogram-like benzenoid · Holes · Mesh

Coronafusene, as described by Balaban [1], is a corona-condensed polycyclic system which belongs to a class of fused benzenoid hydrocarbons with a cavity. The nomenclature and topological centric coding of these types of *polyhexes* [2–4], as well as the extra stability (superaromaticity) associated with the configuration of π-bonds in these super-ring structures are well documented [5]. The resonance structure counts in primitive coronoid hydrocarbons are also well established [6–8]. In several articles, we presented a special type of coronafusene which we term *cyclofusene* [9–14]. The graphs described in this article do not require the same restrictions as the ones imposed on the geometry of the holes in cyclofusene [9–13].

The *rectangular mesh* $M(a, b)$ is defined as follows [15]. The vertices are the labeled points (x, y) such that x and y are integers satisfying $1 \leq x \leq a$ and $1 \leq y \leq b$.(x, y) and (x', y') are adjacent if either $x = x'$ and $|y - y'| = 1$, or $y = y'$

S. Karimi (✉)
Chemistry Department, Queensborough Community College, Bayside, NY 11364, USA
e-mail: skarimi@qcc.cuny.edu

A. Delgado
Purchase College, Purchase, NY 10577, USA

M. Lewinter
Math Department, Purchase College, Purchase, NY 10577, USA

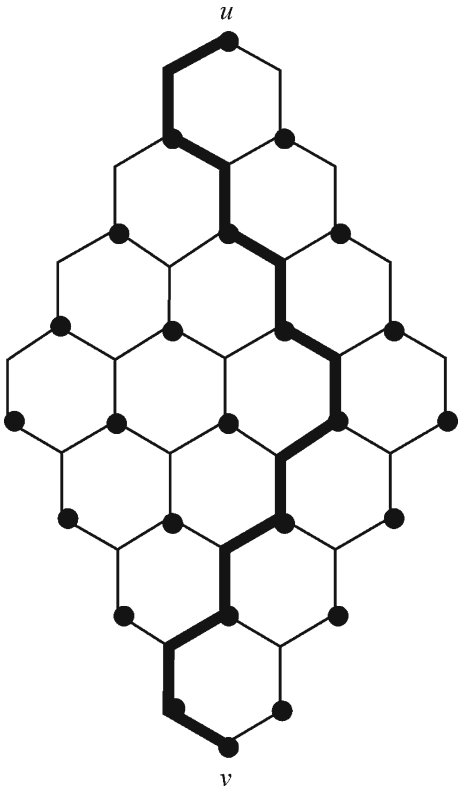

Fig. 1 A parallelogram-like benzenoid G with a descending $u - v$ path

and $|x - x'| = 1$. The four vertices (1, 1), $(a, 1)$, $(1, b)$ and (a, b) of degree two are called *corner* vertices. The number of shortest paths from a corner vertex of the mesh $M(a, b)$ to the opposite corner is the *combinatorial number* $\binom{a+b-2}{a-1}$.

We have previously shown an algorithm for counting perfect matchings in benzenoids such as the parallelogram-like graph G in Fig. 1 by counting descending $u - v$ paths in the corresponding rectangular mesh H of Fig. 2 [14]. This algorithm is valid because a perfect matching in G corresponds to a configuration (in G) of π-bonds [16–22]. The perfect matching is the set of "slanting" edges on the descending path and the vertical edges not on the descending path. This method was extended to *diminished* meshes obtained by deleting one or more submeshes that include corner vertices of the given mesh [14].

We generalize this approach here by permitting the deletion of *internal* submeshes (holes). In order to facilitate parallelogram-like benzenoids with parallelogram-like holes, we begin by counting descending $u-v$ paths in the rectangular mesh with square holes of Fig. 3, and then state an algorithm for the general case. In what follows, we denote the number of descending paths from x to y by $D(x, y)$. This is easily evaluated using the combinatorial coefficients as explained above [14]. Note that x and y must be the upper and lower corners, respectively, of a submesh in order to evaluate $D(x, y)$.

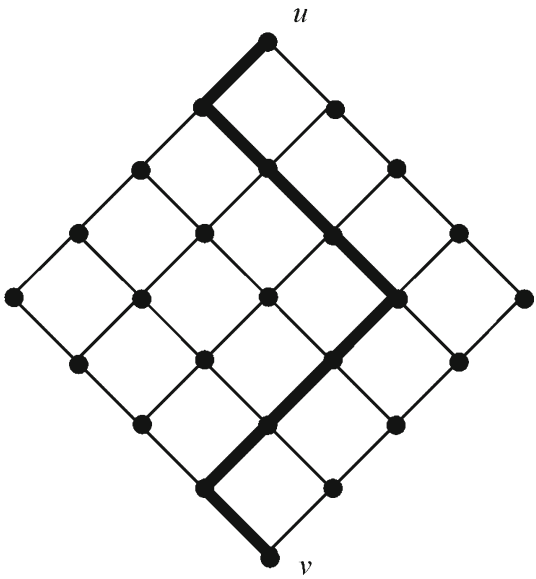

Fig. 2 The corresponding rectangular mesh H with the corresponding descending $u - v$ path

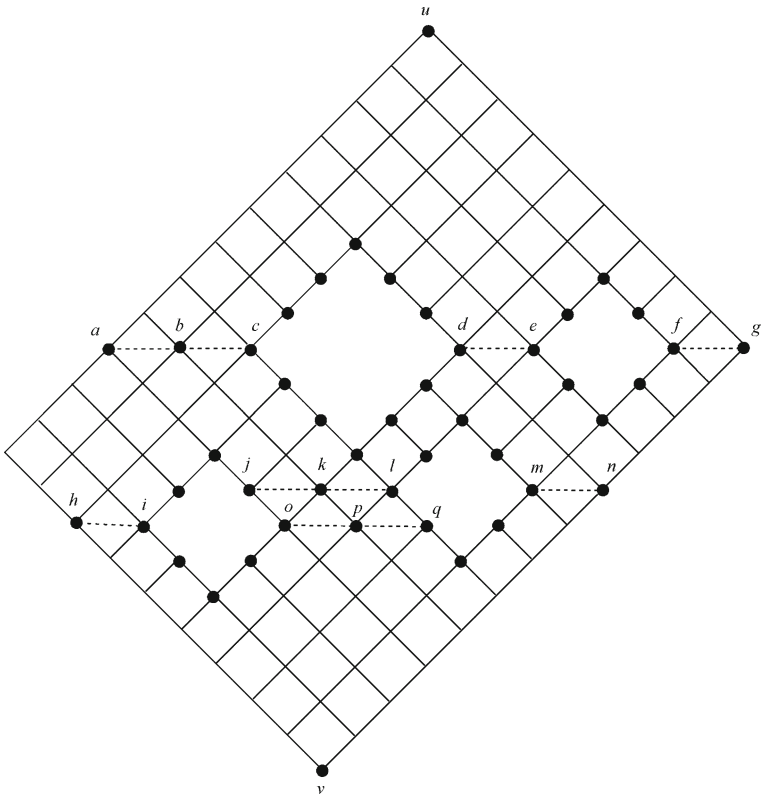

Fig. 3 A rectangular mesh with square holes

Now any descending $u - v$ path in Fig. 3 must contain exactly one of the vertices of the set $\{a, b, c, d, e, f, g\}$. Furthermore, the decision trees for the remainder of these paths necessitate the inclusion of some of the remaining set of labeled vertices $\{h, i, \ldots, p, q\}$. Note, for example, that a descending $u - v$ path containing d must also include exactly one of the vertices below d that are reachable, namely, k, l, m, and n. The number of descending $u - v$ paths for the mesh of Fig. 3 that contain a is

$$D(u,a)D(a,h)D(h,v) + D(u,a)D(a,i)D(i,v) + D(u,a)D(a,j)D(j,o)D(o,v). \quad (1)$$

Similar expressions must be added for each of the vertices b, c, d, e, f, and g. The algorithm is obvious once a procedure is given for the selection of the vertices that appear in sums such as (1). First include the lateral corners of the holes. In Fig. 3, the lateral corner vertices are c, d, e, f, i, l, m, and o. Once a lateral corner is selected, also include consecutive vertices on its level in the mesh (levels are indicated in Fig. 3 by dashed lines) until reaching a boundary vertex of a hole or of the mesh. Thus the selection of c in Fig. 3 implies the selection of b and a.

It should be noted that the above algorithm extends to diminished meshes with rectangular holes.

References

1. A.T. Balaban, Rev. Roum. Chim. **26**, 407–413 (1981)
2. A.T. Balaban, F. Harary, Tetrahedron **24**, 2505–2516 (1968)
3. A.T. Balaban, Tetrahedron **25**, 2949–2956 (1969)
4. D. Bonchev, A.T. Balaban, J. Chem. Inf. Comput. Sci. **21**, 223–229 (1981)
5. J.I. Aihara, Bull. Chem. Soc. Jpn. **66**, 57–60 (1993)
6. S.J. Cyvin, B.N. Cyvin, J. Brunvoll, H. Hosoya, F. Zhang, D.J. Klein, R. Chen, O.E. Polansky, Monatsh. Chem. **122**, 435–444 (1991)
7. J. Brunvoll, B.N. Cyvin, S.J. Cyvin, J. Chem. Inf. Comput. Sci. **27**, 14–21 (1987)
8. J. Brunvoll, B.N. Cyvin, S.J. Cyvin, I. Gutman, R. Tosic, M. Kovacevic, J. Mol. Struct. (Theochem.) **184**, 165–177 (1989)
9. S. Karimi, M. Lewinter, S. Kalyanswamy, J. Math. Chem. **43**, 892–900 (2008)
10. S. Karimi, M. Lewinter, S. Kalyanswamy, J. Math. Chem. **41**, 59–61 (2007)
11. S. Karimi, M. Lewinter, J. Math. Chem. **39**, 593–596 (2006)
12. S. Karimi, M. Lewinter, J. Math. Chem. **38**, 103–106 (2005)
13. T. Bocchi, S. Karimi, M. Lewinter, J. Math. Chem. **35**, 339–344 (2004)
14. S. Karimi, M. Lewinter, J. Stauffer, J. Math. Chem. **34**, 297–301 (2003)
15. F. Buckley, M. Lewinter, *A Friendly Introduction to Graph Theory*, (Prentice Hall, New Jersey, 2003)
16. F. Rispoli, Math. Mag. **74**, 194–200 (2001)
17. P. Kasteleyn, Graph theory and crystal physics, in *Graph Theory and Theoretical Physics*, ed. by F. Harary (Academic Press, New York, 1967)
18. N. Trinajstic, *Chemical Graph Theory*, 2nd edn. (CRC Press, Boca Raton, FL, 1992)
19. M. Gordon, W.H.T. Davison, J. Chem. Phys. **20**, 428–435 (1952)
20. M. Randic, *Graph Theory, Combinatorics, and Applications,* vol. 2 (Wiley-Interscience, New York, 1991), pp. 1001–1008
21. I. Gutman, S. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons* (Springer-Verlag, Berlin, 1989)
22. H. Sachs, Combinatorica **4**, 89–99 (1984)