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On the M−Polynomial of Planar Chemical Graphs

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ABSTRACT

Let G be a graph and let $m_{i,j}(G)$, $i,j \geq 1$, be the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i,j\}$. The M-polynomial of G is $M(G;x,y) = \sum_{i\leq j} m_{i,j}(G)x^i y^j$. With $M(G;x,y)$ in hands, numerous degree-based topological indices of G can be routinely computed. In this note a formula for the M-polynomial of planar (chemical) graphs which have only vertices of degrees 2 and 3 is given that involves only invariants related to the degree 2 vertices and the number of faces. The approach is applied on several families of chemical graphs. In one of these families an error from the literature is corrected.

1. INTRODUCTION

Let $G = (V(G), E(G))$ be a graph. The degree of a vertex $v \in V(G)$ will be denoted by $d_v(G)$. If $m_{i,j}(G)$, $i,j \geq 1$, denotes the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i,j\}$, then the *M-polynomial* of G is defined as

$$M(G;x,y) = \sum_{i\leq j} m_{i,j}(G)x^i y^j .$$

This two-variable counting polynomial has been introduced in [5] with the main message that by using elementary calculus, numerous degree-based topological indices of G can be routinely calculated from $M(G;x,y)$. The technical details of the calculations using elementary calculus can be found in [5,6] and will not be repeated here.

Among the degree-based topological indices one finds BID (bond incident degree) index, first Zagreb index, second Zagreb index, second modified Zagreb index, (general)

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Randić index, symmetric division index, harmonic index, inverse sum index, augmented Zagreb index, and more. We refer to [9] for a general treatment of degree-based topological indices and to [7] for the investigation of their structure-sensitivity which is important in chemistry. See also [16, 17, 21] for recent investigations of extremal values of degree-based topological indices and [1] for more on the symmetric division index. Due to the wide applicability of the M-polynomial, it is not surprising that this polynomial has been used in many papers to derive formulas for different degree-based topological indices. The papers [2, 3, 13, 14, 15, 18, 20] represent a small selection of such investigations.

The main purpose of this note is to propose an approach how to determine the M-polynomial of planar, (chemical) graphs in which $d_G(v) \in \{2,3\}$ for each vertex v of G. More precisely, we prove a formula for the M-polynomial of such graphs that involves only invariants related to the degree 2 vertices and the number of faces. We believe that such a formula is very convenient since in many cases, especially for chemical graphs, the degree 2 vertices can be easily treated. Moreover, many important families of chemical graphs such as benzenoid graphs, phenylenes, fluoranthenes, and fullerenes have only vertices of degrees 2 and 3. We demonstrate the approach on several families of chemical graphs where we obtain the M-polynomial as straightforward consequences of our main result. One of these consequences also corrects an error from the literature.

If $G = (V(G), E(G))$ is a graph, then we will use the notation $n(G) = |V(G)|$ and $m(G) = |E(G)|$. If G is planar, then the number of faces in its plane embedding will be denoted by $f(G)$.

2. PLANAR GRAPHS WITH VERTICES OF DEGREES 2 AND 3

Let G be a planar graph which has only vertices of degrees 2 and 3. We denote by $v_j(G)$ the number of vertices of degree j, $j \in \{2,3\}$. In case when G will be clear from the context, we may simplify the notation $v_j(G)$ to v_j. In such cases we may also simplify the notation $m_{i,j}(G)$ to $m_{i,j}$.

The M-polynomial of a planar graph which has only vertices of degrees 2 and 3 can be expressed only in terms of the degree 2 vertices and the number of faces as follows.

Theorem 2.1. *If G is a planar graph with vertices only of degrees 2 and 3, then*

$$M(G;x,y) = m_{2,2}x^2y^2 + 2(v_2 - m_{2,2})x^2y^3 + (3f(G) - v_2 + m_{2,2} - 6)x^3y^3 .$$

Proof. Note first that $2m_{2,2} + m_{2,3} = 2v_2$ and $m_{2,3} + 2m_{3,3} = 3v_3$, so that

$$3v_3 - 2m_{3,3} = 2v_2 - 2m_{2,2} . \quad (1)$$

Set $f = f(G)$. Euler's formula gives $v_2 + v_3 + f - m_{2,2} - m_{2,3} - m_{3,3} = 2$. Using $m_{2,3} = 2v_2 - 2m_{2,2}$ we get $v_2 + v_3 + f - m_{2,2} - 2v_2 + 2m_{2,2} - m_{3,3} = 2$, that is,

$$m_{3,3} - v_3 = f + m_{2,2} - v_2 - 2 . \quad (2)$$

Multiplying (2) by 3 and adding it to (1) gives

$$m_{3,3} = 3f + m_{2,2} - v_2 - 6 .$$

Since we already know that $m_{2,3} = 2(v_2 - m_{2,2})$ we have thus derived that $M(G; x, y) = m_{2,2}x^2y^2 + 2(v_2 - m_{2,2})x^2y^3 + (3f - v_2 + m_{2,2} - 6)x^3y^3$. ■

Note that if G is a cubic graph (say a fullerene), then of course $m_{2,2}(G) = v_2(G) = 0$ and Theorem 2.1 reduces to the obvious fact that $M(G; x, y) = (3f(G) - 6)x^3y^3$ which follows directly from Euler's formula $n(G) - m(G) + f(G) = 2$ and the fact that $3n(G) = 2m(G)$.

In a similar manner as Theorem 2.1 is proved, one can derive the following variants of it where the number of faces is replaced with the number of vertices and the number of edges of a graph, respectively.

Theorem 2.2. *If G is a planar graph with vertices only of degrees 2 and 3, then*

$$M(G; x, y) = m_{2,2}x^2y^2 + 2(v_2 - m_{2,2})x^2y^3 + \frac{1}{2}(3n(G) - 5v_2 + 2m_{2,2})x^3y^3 .$$

Theorem 2.3. *If G is a planar graph with vertices only of degrees 2 and 3, then*

$$M(G; x, y) = m_{2,2}x^2y^2 + 2(v_2 - m_{2,2})x^2y^3 + (m(G) + m_{2,2} - 2v_2)x^3y^3 .$$

The reader can thus select one formula from the ones given in Theorems 2.1-2.3. Normally it would be the one from which it is easiest to determine the M-polynomial, that is, depending which of the number of faces, the number of vertices, and the number of edges, is easiest to determine.

Consider now the family of graphs $G(h, q, n)$, where

- h is the number of hexagons in each hexagon segment,
- q is the number of squares connecting any two consecutive hexagon segments, and
- n is the number of hexagon segments.

The graph $G(3,5,4)$ is drawn in Figure 1; the reader can easily deduce the general definition from this example.

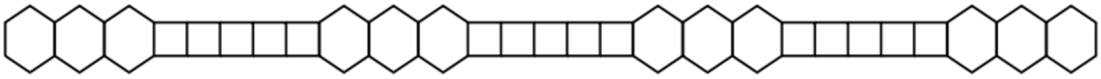

Figure 1. The linear generalized phenylene $G(3,5,4)$.

Before moving on we add that the graphs $G(h,q,n)$ were named linear phenylenes in [8]. However, the term phenylene is usually reserved for chemical graphs that are obtained from catacondensed benzenoid systems by adding a square between all pairs of adjacent hexagons, cf. [4, 19, 22]. Hence a more suitable name for these graphs would be *linear generalized phenylenes*.

The M-polynomial of linear generalized phenylenes $G(h,q,n)$ was considered in [8]. It was this study that motivated us for the present note in the first place. Namely, the derivation of $M(G(h,q,n);x,y)$ in [8] appears much complicated and the final result is clearly wrong because it does not depend on the number of squares connecting any two consecutive hexagon segments. Theorem 2.1 enables us to deduce the formula for $M(G(h,q,n);x,y)$ in a straightforward manner. One only needs to observe that for a given $G(h,q,n)$ we have:

$$v_2(G(h,q,n)) = 2hn + 4,$$
$$m_{2,2}(G(h,q,n)) = 6,$$
$$f(G(h,q,n)) = 1 + nh + (n-1)q,$$

from which Theorem 2.1 gives:

Corollary 2.4. *If* $h,q \geq 1$ *and* $n \geq 2$*, then*

$$M(G(h,q,n);x,y) = 6x^2y^2 + 4(hn-1)x^2y^3 + (hn + 3qn - 3q - 1)x^3y^3 .$$

3. TWO MORE EXAMPLES

In this section we give two more examples how our approach can be applied. Consider first networks $BR(p,q)$. These networks and their M-polynomials were investigated in [20]. The general definition of $BR(p,q)$ should be clear from Figure 2, where the network $BR(3,5)$ is drawn.

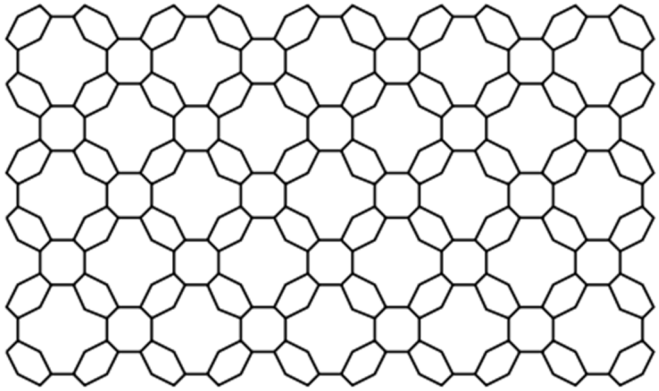

Figure 2. The network $BR(3,5)$.

It is straightforward to see that $v_2(BR(p,q)) = 8pq + 4p + 4q$ and that $m_{2,2}(BR(p,q)) = 4p + 4q$. Moreover, with not much more effort we can deduce that $f(BR(p,q)) = 8pq - 2p - 2q + 2$. Plugging these values into Theorem 2.1 we get the following result proved in [20, Theorem 1].

Corollary 3.1. *If* $p, q \geq 1$*, then*

$$M(BR(p,q);x,y) = 4(p+q)x^2y^2 + 16pqx^2y^3 + 2(8pq - 3p - 3q)x^3y^3 .$$

As the second example consider a family of fluoranthene-type benzenoid hydrocarbons $F(2n)$, see $F(4)$ (here $n = 2$) in Figure 3. The parameter n in general says that there are $2n$ hexagons in the bottom row.

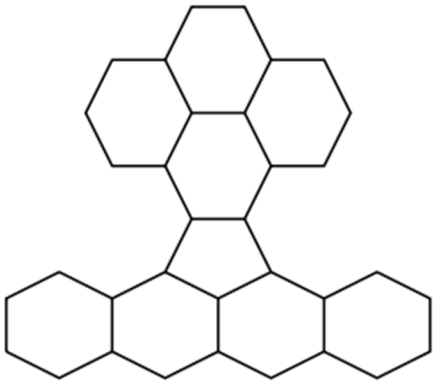

Figure 3. The fluoranthene $F(4)$.

The paper [10] that initiated a graph theoretical study of fluoranthene and its congeners had a great impact; in particular, different topological indices of these chemical

graphs have been studied. Let us just point out the investigation of their degree-based topological indices in [11] and of their augmented Zagreb indices in [12]. By the present example we just wish to point out an alternative simpler way. For $n \geq 2$ we have $v_2(F(2n)) = 4n + 10$ (8 vertices above the 5-gon, 4 vertices on the sides of the bottom row, $2n$ vertices in the bottom row, and $2(n-1)$ vertices on the top of the bottom hexagons), $m_{22}(F(2n)) = 11$, and $f(F(2n)) = 2n + 6$, so that we can immediately state:

Corollary 3.2. *If $n \geq 2$, then*

$$M(F(2n); x, y) = 11x^2y^2 + (8n-2)x^2y^3 + (2n+13)x^3y^3 .$$

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