Bounds for the Hosoya Index

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Some inequalities for Hosoya's topological index are deduced, revealing its dependence on the structure of the carbon-atom sekeleton of a hydrocarbon molecule.

The quantity Z, introduced in 1971 by Hosoya [1], belongs among the best investigated topological indices [2]. It is defined in the following manner. If G is the molecular graph of a saturated hydrocarbon [3] and $m(G, k)$ is the number of k-matchings of G, then

$$Z = Z(G) = \sum_{k=0}^{p} m(G, k) . \tag{1}$$

The summation ranges over all non-zero $m(G, k)$ numbers. Recall that a k-matching of a graph G is a selection of k mutually nonadjacent edges in G [3, 4]. By definition, $m(G, 0) = 1$ for all graphs G. Furthermore, if m denotes the number of edges of G, then $m(G, 1) = m$.

In (1) the parameter p is the size of a maximal matching in G. In other words, $m(G, p) \neq 0$ whereas $m(G, p+1) = 0$.

There exists an extensive literature on the applications of Z to various chemical problems, especially in chemical thermodynamics [3, 5–11]. The dependence of Z on the structure of the molecular graph G is less investigated and the present paper will provide some of the first mathematical findings, relating $Z(G)$ with simple invariants of G.

Our main result are the inequalities

$$\begin{aligned} Z &\leqq [1 + m/p + (p-1)^{1/2}\, T] \\ &\quad \cdot [1 + m/p - (p-1)^{-1/2}\, T]^{p-1} \\ &\leqq (1 + m/p)^p , \end{aligned} \tag{2}$$

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where

$$T = (p\, d - m^2 - p\, m)^{1/2} p^{-1} \tag{3}$$

and d is the sum of the squares of the degrees of the vertices of the molecular graph G. The formulas (2) hold for $p \geqq 1$.

If $p > 2$, then both inequalities in (2) are strict. If $p = 2$, then the l.h.s. relation becomes an equality. If $p = 1$, then both relations reduce to the identity $Z = 1 + m$.

The method used for deducing (2) is to a great extent analogous to the recently employed variational technique, by which an upper bound for total π-electron energy has been obtained [12]. Our starting point is the identity

$$\ln Z = \sum_{i=1}^{p} \ln(1 + y_i^2) , \tag{4}$$

where $y_1, y_2, \ldots, y_n$ ($y_1 \geqq y_2 \geqq \cdots \geqq y_p > 0 \geqq y_{p+1} \geqq \cdots \geqq y_n$) are the zeros of the matching polynomial [4] of the graph G:

$$\alpha(G, x) = \sum_{k=0}^{p} (-1)^k m(G, k)\, x^{n-2k} . \tag{5}$$

Bearing in mind that [4, 13]

$$\sum_{i=1}^{p} y_i^2 = m \tag{6}$$

and

$$\sum_{i=1}^{p} y_i^4 = d - m \tag{7}$$

we may consider the expression

$$\sum_{i=1}^{p} \ln(1 + x_i^2) \tag{8}$$

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and seek for its extremes, provided the conditions

$$\sum_{i=1}^{p} x_i^4 = d - m \tag{9}$$

and/or

$$\sum_{i=1}^{p} x_i^2 = m \tag{10}$$

are obeyed. Since the relations (9) and (10) are chosen so to fully match (7) and (6), respectively, the maximal value of (8) will be an upper bound of $\ln Z$ in (4). In (8)−(10) the quantities x_i are positive variational functions which must be distinguished from the zeros y_i of the matching polynomial (5).

We first determine the maximum of (8) under the constraint (10). According to the standard variational procedure we set

$$L = \sum_{i=1}^{p} \ln(1 + x_i^2) + \lambda \sum_{i=1}^{p} x_i^2$$

and require that

$$\frac{\partial L}{\partial x_j} = 0 \quad \text{for} \quad j = 1, 2, \ldots, p .$$

This yields

$$2 x_j (1 + x_j^2)^{-1} + 2 \lambda x_j = 0 ,$$

i.e.

$$x_j = \sqrt{-1 - 1/\lambda} .$$

Combining this latter result with the condition (10) we find that

$$x_1 = x_2 = \cdots = x_p = \sqrt{m/p} . \tag{11}$$

Therefore the maximum of (8) is equal to $p \ln(1 + m/p)$, which immediately gives the r.h.s. expression in (2).

If, now, both the constraints (9) and (10) are taken into account, we arrive at

$$2 x_j (1 + x_j^2)^{-1} + 2 \lambda x_j + 4 \mu x_j^3 = 0 ,$$

i.e.

$$2 \mu x_j^4 + (2 \mu + \lambda) x_j^2 + (\lambda + 1) = 0 . \tag{12}$$

Suppose the roots of (12) are real, and denote the positive roots of (12) by a and b, $a > b > 0$. The case $a = b$ must not occur since then we would have the case (11), which evidently violates the condition (9).

Then the solution of our variational problem can be written as

$$x_1 = x_2 = \cdots x_t = a , \tag{13 a}$$

$$x_{t+1} = \cdots = x_p = b , \tag{13 b}$$

where t, $1 \leqq t < p$, remains still to be determined. Substituting (13) back into (9) and (10) we obtain the equations

$$t a^2 + (p - t) b^2 = m , \tag{14}$$

$$t a^4 + (p - t) b^4 = d - m , \tag{15}$$

which are fully analogous to (21) and (22) of [12]. The stationary points of (8) are evidently given by

$$t \ln(1 + a^2) + (p - t) \ln(1 + b^2) , \tag{16}$$

which we shall denote by $\ln Z(t)$, that is

$$Z(t) = (1 + a^2)^t (1 + b^2)^{p-t} . \tag{17}$$

Straightforward calculation gives

$$a = a(t) = [m/p + (p - t)^{1/2} t^{-1/2} T]^{1/2} , \tag{18 a}$$

$$b = b(t) = [m/p - t^{1/2} (p - t)^{-1/2} T]^{1/2} , \tag{18 b}$$

and it is easy to show that $a(t)$ is real for all t, $1 \leqq t < p$, whereas $b(t)$ is real for

$$1 \leqq t \leqq [m^2/(d - m)] .$$

The parameter T in (3) is necessarily real. In order to see this, notice that, since the mean value of the squares is never smaller than the square of the mean value,

$$\frac{1}{p} \sum_{i=1}^{p} x_i^4 \geqq \left(\frac{1}{p} \sum_{i=1}^{p} x_i^2 \right)^2 .$$

Bearing in mind (9) and (10) we get

$$(d - m)/p \geqq (m/p)^2$$

from which

$$p d - m^2 - p m \geqq 0 .$$

Therefore the r.h.s. of (3) must be real.

The above analysis justifies the previous assumption that the roots of (12) are real numbers.

We now demonstrate that $Z(t)$ is a monotonously decreasing function of t. In order to do this we differentiate (14), (15) and (16) with respect to t and (in full analogy to (29) of [12]) obtain for the first derivative of $\ln Z(t)$:

$$[\ln Z(t)]' = f(x_0)\,; \quad x_0 = (1+a^2)/(1+b^2)\,,$$

where

$$f(x) = \ln x - x/2 + (2x)^{-1}\,.$$

It is evident that for $x = 1$, $f(x) = 0$. On the other hand, $f'(x) = -(x-1)^2(2x^2)^{-1}$, from which follows that $f(x)$ is monotonously decreasing. Therefore $f(x)$ is negative for all $x > 1$. Since $(a^2+1)/(b^2+1)$ is necessarily greater than unity, $f(x_0)$ must be negative. Hence, $[\ln Z(t)]'$ is negative. This means that $\ln Z(t)$ and therefore also $Z(t)$ monotonically decrease with increasing t,

$$1 \leqq t \leqq [m^2/(d-m)]\,.$$

As a consequence of the above result, $Z(t)$, $t = 1$ is an upper bound for the Hosoya index. Taking into account (17) and (18) we arrive at the first inequality in (2).

It remains to prove that $Z(1)$ is not greater than $(1+m/p)^p$. This can be done by considering $Z(1)$, namely

$$Z(1) = [1 + m/p + (p-1)^{1/2}\,T] \cdot [1 + m/p - (p-1)^{-1/2}\,T]^{p-1} \qquad (19)$$

as a function of T. Setting formally $T = 0$, the r.h.s. of (19) reduces to $(1+m/p)^p$. On the other hand,

$$\frac{\partial \ln Z(1)}{\partial T} = (p-1)^{1/2}\,[1 + m/p + (p-1)^{1/2}\,T]^{-1} - (p-1)^{1/2}\,[1 + m/p - (p-1)^{-1/2}\,T]^{-1}$$

which is clearly negative for $T > 0$. Therefore, whenever $T > 0$, $Z(1)$ is smaller than $(1+m/p)^p$.

This completes the proof of the inequalities (2).

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