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LETTER TO THE EDITOR

Comment on "Zhang–Zhang polynomials of cyclo-polyphenacenes" by Q. Guo, H. Deng, and D. Chen

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Abstract Explicit formulas for computing the Zhang–Zhang polynomial of cyclo-polyphenacenes, presented by Guo et al. (J. Math. Chem. 46:347, 2009) are found to be erroneous. In the present comment, a corrected version of Theorem 4.2 is given. The new formulation has been extensively tested by comparison with the Zhang–Zhang polynomials computed by brute force using a new, completely automatized computer code.

Keywords Zhang–Zhang polynomial · Clar covering polynomial · Cyclo-polyphenacene

In a recent interesting publication [1], Guo et al. presented a number of compact recurrence expressions applicable for explicit determination of the Zhang–Zhang polynomials of a large class of benzenoid molecules: cyclo-polyphenacenes. However, it seems that the authors made an error in the final step of the proof of Theorem 4.2, which led to an incorrect recurrence formula. The present comment points out the origin of the error and presents correct formulas to be used for the determination of the Zhang–Zhang polynomial $C(r_1, r_2, \ldots, r_t)$ for cyclo-polyphenacenes. The definitions and notations used in this comment are the same as in [1]. The reader should be aware that the notation $C(r_1, r_2, \ldots, r_t)$ is used in [1] in two contexts, once as the symbol for a cyclo-polyphenacene with t linear segments of length $r_1, r_2, \ldots, r_t$, respectively, and once as the symbol for the Zhang–Zhang polynomial corresponding to this structure.

The **Theorem 4.2** in [1] says: *Let* $C(r_1, r_2, \ldots, r_t)$ *be a cyclic hexagonal chains with n hexagons and* $r_t \geq 3$.

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(i) *If $t \geq 2$ is even, then*

$$\begin{aligned} C(r_1, r_2, \ldots, r_t) &= \left[\frac{(r_t-2)w+r_t-3}{r_{t-1}-1}+1\right] L(r_1-1, r_2, \ldots, r_{t-1}) \\ &\quad +\frac{(r_t-2)w+r_t-3}{r_{t-1}-1} L(r_1-1, r_2, \ldots, r_{t-2}) \\ &\quad +\frac{1}{r_{t-1}-1}\left[(r_{t-1}-2) L(r_1, r_2, \ldots, r_{t-1})\right. \\ &\quad \left.+L(r_1, r_2, \ldots, r_{t-2})\right]+2; \end{aligned}$$

(ii) *If $t \geq 2$ is odd, then*

$$\begin{aligned} C(r_1, r_2, \ldots, r_t) &= \left[\frac{(r_t-2)w+r_t-3}{r_{t-1}-1}+1\right] L(r_1-1, r_2, \ldots, r_{t-1}) \\ &\quad +\frac{(r_t-2)w+r_t-3}{r_{t-1}-1} L(r_1-1, r_2, \ldots, r_{t-2}) \\ &\quad +\frac{1}{r_{t-1}-1}\left[(r_{t-1}-2) L(r_1, r_2, \ldots, r_{t-1})\right. \\ &\quad \left.+L(r_1, r_2, \ldots, r_{t-2})\right]. \end{aligned}$$

The resulting formulas of **Theorem 4.2** are verified by determination of the Zhang–Zhang polynomial for the C(3,3,3,3,3,3) coronoid, yielding correctly the well-known result

$$w^6+18w^5+123w^4+408w^3+699w^2+594w+200.$$

However, the agreement happens to be purely accidental; an application of the formulas of **Theorem 4.2** for determination of the Zhang–Zhang polynomial of the C(4,4,4,4,4,4) coronoid yields

$$32w^6+392w^5+1{,}886w^4+4{,}611w^3+\ 6{,}090w^2+\frac{12,436}{3}w+\frac{3{,}431}{3},$$

which evidently is not a valid Zhang–Zhang polynomial due to the presence of fractional coefficients.

The incorrect formula in **Theorem 4.2** in [1] resulted, when authors applied incorrectly Corollary 4.1 (numerator of the first term of Corollary 4.1 is missing in the combined expression).

The correct version of **Theorem 4.2** reads: *Let C $(r_1, r_2, \ldots, r_t)$ be a cyclic hexagonal chains with n hexagons and $r_t \geq 3$.*

(i) *If $t \geq 2$ is even, then*

$$C(r_1, r_2, \ldots, r_t) = \left[\frac{(r_{t-1}-2)[(r_t-2)w + r_t - 3]}{r_{t-1}-1} + 1\right] \times L(r_1 - 1, r_2, \ldots, r_{t-1}) + \frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} L(r_1 - 1, r_2, \ldots, r_{t-2}) + \frac{1}{r_{t-1}-1}\big[(r_{t-1}-2)L(r_1, r_2, \ldots, r_{t-1}) + L(r_1, r_2, \ldots, r_{t-2})\big] + 2;$$

(ii) *If $t \geq 2$ is odd, then*

$$C(r_1, r_2, \ldots, r_t) = \left[\frac{(r_{t-1}-2)[(r_t-2)w + r_t - 3]}{r_{t-1}-1} + 1\right] \times L(r_1 - 1, r_2, \ldots, r_{t-1}) + \frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} L(r_1 - 1, r_2, \ldots, r_{t-2}) + \frac{1}{r_{t-1}-1}\big[(r_{t-1}-2)L(r_1, r_2, \ldots, r_{t-1}) + L(r_1, r_2, \ldots, r_{t-2})\big].$$

The new formulas of the corrected **Theorem 4.2** yield now properly the Zhang–Zhang polynomial of the C(4,4,4,4,4,4) coronoid

$$64w^6 + 672w^5 + 2,868w^4 + 6374w^3 + 7791w^2 + 4{,}974w + 1{,}300,$$

which is consistent with a brute force result obtained by our fully automatized computer code [2,3]. The resulting formulas presented in the corrected version of **Theorem 4.2** were verified by a comparison with the Zhang–Zhang polynomials computed with our fully automatized computer code for a large number of other cyclo-polyphenacenes, always giving perfect agreement.

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