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COMMENT ON THE PAPER: CYCLE DECOMPOSITION OF LINEAR BENZENE CHAINS

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An error in the paper by Farrell and Grell [1] is pointed out.

The purpose of the present note is to point out an error in the paper "Cycle decomposition of linear benzene chains" by E.J. Farrell and J.C.Grell [1]. Namely, their Lemma 4 is false, as a result of a misunderstanding in the definition of the μ-polynomial.

Farrell and Grell [1] define their circuit polynomial $C(G;\underline{w})$ as the sum of the weights of all cycle covers of the respective graph G. Then they say: "In this paper, we will assign the weight w_n to the cycle with n nodes. Therefore $\underline{w}$ will be of the form $(w_1, w_2, \ldots, w_p)$, where p is the number of nodes in G."

Consequently, all cycles in G, having the same size are associated with the same weight.

Bearing this in mind, Lemma 4 in [1] states that the μ-polynomial is a special case of the circuit polynomial when the weight $-2\ t_1$ is associated to all three-membered cycles, the weight $-2\ t_2$ is associated to all four-membered cycles etc. This, however, is in contradiction with the original definition of the μ-polynomial [2].

The μ-polynomial is obtained by associating a distinct variable weight to each particular cycle of the graph G [2]. The actual relation between the μ-polynomial and the circuit polynomial has been elaborated by Farrell (!) and the present author [3]. The definition of the circuit polynomial in [3] is different (namely more general) than the definition used in [1]. Therefore Lemma 4 in [1] cannot be simply "taken" from [3] because Theorem 1 in [3] applies to a different circuit polynomial than Lemma 4 in [1]*

The error in Lemma 4 becomes particulary evident if one examines the number of variables in the respective polynomials. Farrell-Grell's μ-polynomial of naphthalene has two different (non--zero) weights whereas the true μ-polynomial has three such weights. In the case of anthracene, Farrell-Grell's polynomial depends on three variable parameters, whereas in the reality the number of distinct parameters in the μ-polynomial is six. In general: the μ-polynomial of the h-cyclic linear benzene chain (i.e. polyacene) has a total of $h(h+1)/2$ distinct weights. According to Lemma 4 of [1] the number of these weights would be only h.

REFERENCES

[1] E.J.Farrell and J.C.Grell, Match 21, 325 (1986)
[2] I.Gutman and O.E.Polansky, Theoret.Chim.Acta 60, 203 (1981).
[3] E.J.Farrell and I.Gutman, Match 18, 55 (1985).

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*Theorem 1 in [3] has indeed to be corrected by setting $-t_i$ instead of t_i , $i = 1,2,\dots,r$.