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ON THE RELATION BETWEEN CHARACTERISTIC GRAPHS AND GEOMETRIC DUALS: AN UNEQUIVOCAL DEFINITION OF GEOMETRIC DUALS

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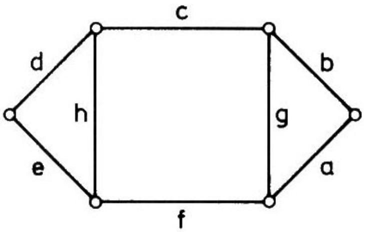
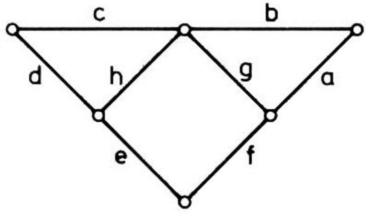
The structural C-graphs A of condensed aromatic systems are connected graphs consisting of a number n of cycles of length 6. Every cycle has an edge in common with at least one other cycle. Recently Balaban and Harary [1] proposed the representation of condensed aromatic systems by their characteristic graphs C. In the construction of these graphs C a vertex is associated with each cycle; two vertices are connected by an edge only if the two corresponding cycles have an edge in common. Obviously the graph C is obtained from the geometric dual A^* of A by excising the vertex representing the outer region and all edges incident with this vertex.

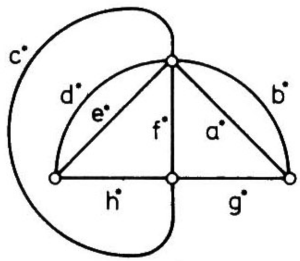
Originally duals were introduced into graph theory by Whitney [2] for the purpose of discussing planarity. As he recognized, duals of inequivalent graphs may be isomorphic (see Fig. 1). This is without particular significance in the discussion of planarity, but in the representation of structures by truncated duals it becomes of crucial importance. To achieve a one-to-one relation between a planar graph and its geometrical dual we propose to define both the graph G and its geometrical dual G^* not only by their respective sets of vertices V and V^* and edges E and E^* but by their sets of faces F and F^* too. In symbols we thus have:



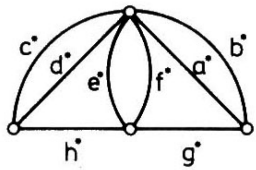
$\mathcal{G}_1$



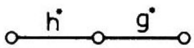
$\mathcal{G}_2$



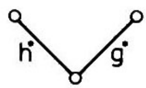
$\mathcal{G}_1^*$



$\mathcal{G}_2^*$



$\bar{\mathcal{G}}_1^*$



$\bar{\mathcal{G}}_2^*$

$$G = [V,\ E,\ F]; \qquad G^{*} = [V^{*},\ E^{*},\ F^{*}]. \tag{1}$$

The property of duality defined in [2] is expressed by the bijective mapping

$$V \Longleftrightarrow F^{*}, \quad E \Longleftrightarrow E^{*}, \quad F \Longleftrightarrow V^{*}. \tag{2}$$

Following this definition in the case of the graphs G_1 and G_2 in Figure 1 the face sets are given by

$$F_1 = \{\{a,b,g\},\ \{c,h,f,g\},\ \{d,e,h\},\ \{a,b,c,d,e,f\}\}$$
$$F_2 = \{\{a,b,g\},\ \{e,f,g,h\},\ \{c,d,h\},\ \{a,b,c,d,e,f\}\}. \tag{3}$$

From the definition (1) it follows that graphs are isomorphic if and only if their respective sets of vertices, edges and faces can be mapped bijectively on to one another.

As a result of the truncation mentioned above it may happen that no cycle of the original dual is preserved. To retain an unequivocal meaning of the graph produced by the truncation of the dual we propose to restore the face set of the dual by a set of angles Θ. These angles are those between pairs of incident edges of the dual. The convention we adopt is that the angles between all pairs of incident edges must be multiples of $2\pi/g$, where g denotes the degree of the vertex concerned in the dual. Let be e_1, $e_2 \in G$ and e_1^{*}, $e_2^{*} \in G^{*}$ with the relations $e_1 \Longleftrightarrow e_1^{*}$ and $e_2 \Longleftrightarrow e_2^{*}$. If e_1 and e_2 are separated by s intervening vertices ($s \geq 1$) the edge angle $\theta(e_1^{*}, e_2^{*})$ will be equal to $2s\pi/g$. The application of this convention to the truncated duals $\bar{G}_1^{*}$ and $\bar{G}_2^{*}$ is shown in Figure 1.

Apart from that vertex which is excised in the course of the truncation, all the other vertices of the dual

A^* have degree 6. Hence the edge angles in the characteristic graphs, $C = \bar{A}^*$, should be multiples of $\pi/3$. In this way isomers such as anthracene (edge angle: $3\pi/3$) and phenanthrene (edge angle: $2\pi/3$) can be represent by readily distinguishable characteristic graphs.

It should be mentioned that if the graphs G_1 and G_2 and their duals are drawn on a sphere as suggested by Whitney [2], the edges c^*, $f^* \in G_1^*$ may be placed on one of the meridians though this is impossible with the edges e^*, $f^* \in G_2^*$.

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References:

[1] A.T. Balaban and F. Harary, Tetrahedron 24, 2505 (1968).

[2] H. Whitney, Amer. J. Math. 54, 150 (1932); Trans. Amer. Math. Soc. 34, 339 (1932); Fund. Math. 21, 73 (1933).