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COVERING PROJECTIONS OF CHEMICAL REACTION GRAPHS

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Abstract

Graphs have been used to depict the paths of interconvertibility in various stereoisomerization processes and other complex chemical systems. A need has now arisen to go a stage deeper and use suitable graph theory to show how relationships between graphs aid the study of the relationships between the chemical systems which they represent. In this paper, products and quotient structures of graphs are presented as a means of describing explicitly the relationships between some recently studied reaction graphs, and as a systematic means of exploring new examples.

1. Introduction

Several recent papers in the chemical literature (see for example [2], [3], [13], [19]) involve chemical reaction graphs which portray the pattern of interconvertibility in some complex chemical systems. In particular, Desargues' graph (see Fig. 1) has been shown to be of great importance in the description of various isomerization processes. Balaban, Fǎrcaşiu and Bǎnicǎ ([3]) have used it as the first reaction graph in the study of problems involving 1,2-shifts of carbonium ions, considering the independent paths permitting interconversions. Balaban and Rouvray ([1], [2], [12], [13], [20]) have reviewed various applications of this graph. The same graph, sometimes called the Desargues-Levi graph, was also found to depict isomerizations of trigonal bipyramidal systems with five distinct ligands (see [7] and [18] and their references).

As a second example, Petersen's graph (see Fig. 2) has also been used to codify the alternative reaction-paths amongst a set of stereoisomers ([3], [7], [8], [9], [11], [13]).

Chemical reactions, and hence the graphs which portray them, tend to have a high degree of symmetry. Randić ([7] - [11]) studied this symmetry for both Desargues' graph and Petersen's graph.

Our main object in this paper is to draw attention to the ways in which two or more reaction graphs may be inter-related. Having used graphs to portray some chemical reactions, it is natural to go a stage deeper and use the theory of graphs to explore the pattern of inter-relationship between the different graphs.

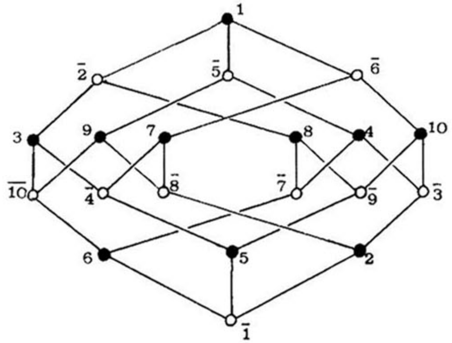

Fig.1. Desargues' graph, the Kronecker double cover of Petersen's graph.

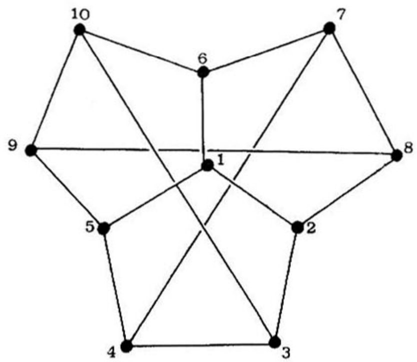

Fig.2. Petersen's graph.

2. The Kronecker Product of Graphs

We shall now present the fundamentals of the appropriate algebraic graph theory for discussing relationships between such graphs, and then return to Desargues' graph and Petersen's graph to make explicit the relationship between them, and show how other examples can be similarly dealt with.

We denote by VG the vertex-set of the graph G. There is an edge $[v,w]$ if the vertices v and w are adjacent, denoted $v \sim_G w$. A homomorphism (or morphism of graphs) $f : G \to H$ is a set-function $f : VG \to VH$ which preserves adjacency:

$$v \sim_G w \text{ implies } f(v) \sim_H f(w).$$

Thus f maps vertices to vertices and edges to edges:

$$[v,w] \mapsto [f(v),f(w)],$$

and never collapses an edge to a vertex.

There are many product-concepts in graph theory, but the one we need here is the unique 'correct' one in the sense of category theory, called the Kronecker product, [6]:

By definition, the Kronecker product $G_1 \wedge G_2$ of the graphs G_1 and G_2 has vertex-set $V(G_1 \wedge G_2) = VG_1 \times VG_2$ (the cartesian product of sets), with adjacency defined by

$$(v_1,v_2) \sim (w_1,w_2) \text{ if and only if } v_1 \sim_{G_1} w_1 \text{ and } v_2 \sim_{G_2} w_2.$$

There are natural projection homomorphisms $p_i : G_1 \wedge G_2 \to G_i$, defined by $p_i(v_1,v_2) = v_i$, $(i = 1,2)$.

In particular, if G_2 is the complete graph K_2 on two vertices then the graph $G_1 \wedge K_2$ has twice as many vertices and twice as many edges as G_1, and $G_1 \wedge K_2$ is called the Kronecker double cover of G_1.

This concept makes precise the relationship between our examples above:

Example 1. Desargues' graph is the Kronecker double cover of Petersen's graph (see [4], [16]).

Example 2. Balaban discusses a 35-vertex graph ([2], Fig.4) whose vertices correspond to choices of three objects from 7, and refers to it as the 'regular halved combination graph' of a certain 70-vertex graph ([2], Fig.3). The larger graph is in fact the Kronecker double cover of the 35-vertex graph (which is also known as the odd graph O_4, [4]).

Such relationships can be clarified if we represent a graph G by its adjacency matrix $A = [a_{ij}]$, where a_{ij} is the number of edges (0 or 1) between the ith and jth vertices. The Kronecker double cover of G is always bipartite, and a suitable labelling of its vertices gives its adjacency matrix as

$$\left[\begin{array}{c:c} 0 & A \\ \hdashline A & 0 \end{array}\right].$$

The problem of enumerating the spanning trees in a graph, which is of considerable chemical interest, [17], can be greatly simplified by such a matrix decomposition (see [6] and [15]).

3. Covering Projections of Graphs

There are other covering graphs of chemical interest, besides Kronecker double covers. A homomorphism $p: G \to H$ is called a k-fold covering projection (of graphs) if

(i) the valency of each vertex v in G is equal to the valency of its image $p(v)$ in H,

and (ii) each vertex in H is the image of exactly k vertices of G.

It follows from the definition that each edge $[v,w]$ of H is the image of exactly k edges between $p^{-1}(v)$ and $p^{-1}(w)$ in G.

Examples of current chemical interest are double covers (i.e. the case $k = 2$). The Kronecker double covers $p_2: G \wedge K_2 \to G$ above have this form. Also the 'Systems analysis' section of Rouvray's article [13] includes the Dodecahedron graph D together with Petersen's graph. Although D has twice as many vertices and edges as Petersen's graph, it cannot be the Kronecker double cover, but it is a double cover of Petersen's graph. The covering projection p is obtained by identification of antipodal pairs of vertices in D, which induces identification of antipodal pairs of edges in D. For details concerning such double covers, see [14] and [16].

Double cover projections can be applied in the search for symmetry in graphs. If $p: D \to G$ is a double cover projection then the homomorphism p can be used to relate the symmetries of D and G by the 'projection' and 'lifting' of some automorphisms of these graphs (see Farzan [5] for details). The homomorphism p enables us to relate the circuit-structure and path-structure of G and D. An n-circuit C_n in G may be covered in D by either the circuit C_{2n} or two disjoint copies of C_n:

$$\begin{tikzcd} C_{2n} \arrow[d, "p"] & \subset & D \arrow[d, "p"] & \supset & C_m \cup C_m \arrow[d, "p"] \\ C_n & \subset & G & \supset & C_m \end{tikzcd}$$

Here the circuit C_n is <u>doubled</u> by p and the circuit C_m is <u>duplicated</u>. One can easily prove the following characterization result, which enables Kronecker double covers to be recognised, and distinguished from all other double covers:

<u>Theorem</u> The double cover projection $p: D \to G$ is Kronecker if and only if

(i) all odd circuits of G are doubled by p,

and (ii) all even circuits of G are duplicated by p.

In contrast with circuits, a <u>path</u> (or <u>tree</u>) in G can only be covered by two isomorphic copies of itself (in <u>any</u> double cover D of G) (see [14] for details).

Finally I should like to mention <u>antipodality</u> in double covering projections. $p: D \to G$ is called <u>antipodal</u> if $p(v) = p(\bar{v})$ if and only if v and $\bar{v}$ are antipodal vertices in D (i.e. their distance apart is equal to the diameter of the graph D). This 'pure mathematical concept' can claim chemical relevance as all three of the examples of double cover projections given above are in fact antipodal ones. These ideas illustrate how products and covering projections provide unification and coordination in algebraic graph theory and its applications.

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