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ON DISSECTION OF ACYCLIC GRAPHS

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Abstract

A decomposition of graphs into components which are either isolated vertices or isolated edges is suggested. One arrives at these ultimate components by a successive elimination of a vertex and all incident edges, one at a time, and repeating the process until a fragment for dissection no longer remains. Application of the procedure raises the question of reconstruction of a graph from the data of a dissection. It appears that in some instances such a reconstruction is possible. It is of interest that isospectral graphs examined have a different dissection, hence the potential use of the dissection in graph isomorphism problem should be examined. The analysis leads to a pair of numbers (A,B) which signify the number of isolated atoms (A) and the number of isolated bonds (B) which molecular graph contains when dissected by a successive elimination of the vertices in various fragments generated by the process.

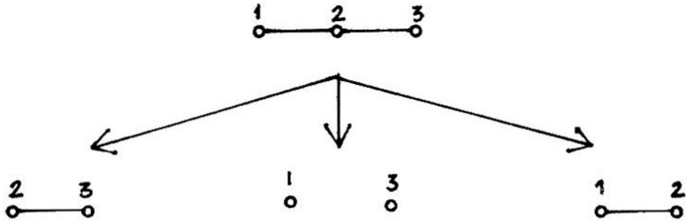
Introduction

In graph theory and its applications, particularly in chemistry, we are concerned with manipulations with structures, rather than in manipulations with numbers as the basic quantities. We assume here structure to be a system built according to particular rules from smaller units. Molecular structure is an example of a system built from atoms, the rules being the axioms of quantum mechanics. We are not necessarily concerned with the rules as such, but are primarily interested in consequences of those rules as manifested in the connectivity of the system. It is useful to divorce the mathematical (abstract) aspects from the chemical (applicative) aspects in such studies. While the latter frequently may stimulate initiation of a particular study, the former are more general and apply to other branches of science. Among the mathematical topics one may include problems of recognition of graphs,[1] their characterization, and classification. Related problems include comparison of graphs and their ordering,[2] most commonly in a sequence. These problems may require a practical scheme for construction of graphs,[3] and here it may be of use to have lists of fragments and use these in composing larger structure. A test for isomorphism is essential in order to avoid duplication and maintain high efficiency in solving the problem in question. In some problems it will be essential to include all structures of prescribed type, hence one has to watch for omissions. Enumeration of all graphs of the considered type is here of interest.[4]

Different problems may call for different fragments, hence different decompositions are of interest in different applications. For instance, in the construction of a characteristic polynomial one is interested in isolated edges and isolated rings,[5] while a construction of Kekulé valence forms can be viewed as a search for a set of isolated edges which span molecular graph.[6] In this contribution we will be concerned with graph decomposition and will introduce the concept of graph dissection. By dissection or total graph decomposition we understand here arriving at fragments which are either isolated vertices or isolated edges which are considered in this exposition as ultimate fragments. One arrives at these fragments by a recurrent application of removal of a single vertex and all incident edges. Generally, in such a process one or more fragments are produced at first, and the number of fragments increases as one continues the dissection. In the process all vertices are considered at each stage, only isolated vertices and isolated edges already created are eliminated from further decomposition. The first step in the process corresponds to construction of Ulam's subgraphs.[7] Since we wish to keep open the possibility for graph reconstruction, it is essential to stop the dissection once one arrives at isolated edges, since graph K_2 , an isolated edge, cannot be reconstructed (i.e. is not distinguished from subgraphs of two isolated vertices).

Acyclic Graphs

We will limit our considerations to acyclic graphs and will discuss polycyclic graphs in a separate contribution. The simplest graph then is a skeleton of a triatomic molecule. It gives rise to three subgraphs, each resulating by a removal of one of the three vertices:



Since, as a result, we obtained in each case either isolated vertices (atoms) or isolated edge (bond) the process of dissection is terminated. We can summarize the dissection by the expression: (2 a + 2 b) , where a and b refer to atoms and bonds, respectively. Observe, however, that the summation as an operation may result in a reduction of the available information. Before the summation we knew which fragments constituted each subgraph, after the summation we know that the above fragments appear, but in what combination, partitioned to give original subgraphs, needs to be investigated. If such investigations can recover the proper partitioning, there was no loss of information involved, otherwise the summation of the fragmentation products introduces a loss of the content of information on the system. Generally, whenever one has data reduction, a possibility for a loss of information arises. The problem of recovery or reconstruction is concerned with finding conditions and circumstances when contraction of data does not lead to a loss of the information content. Suprising as it may appear, there is not yet available a general mathematical theory of reconstruction.[8] A special problem of great interest in graph theory is Ulam's conjecture or the problem of graph reconstruction from a set of subgraphs derived by erasure of a single vertex and all incident edges, one vertex at a time. The process that we consider is closely related, the difference being that we repeat the process of vertex erasure for all derived subgraphs, and then for subgraphs of subgraphs and so on until no fragment longer remains. During the performance of the dissection, whenever an isolated vertex or an isolated edge is found, they are registered and removed from further examination. Ulam's conjecture is known to be valid for acyclic graphs as well as for disconnected graphs.[7] From this one can expect that a graph may also be reconstructed from the smaller fragments, and ultimately from the set of isolated edges and isolated vertices.

In Table 1 we illustrate the decomposition of small acyclic graphs (butane and pentane isomers). The first step, which gives Ulam's subgraphs, is pictorially represented. In deriving the enumeration of dissected vertices and edges for larger graphs one uses the already available results for smaller graphs. In Table 2 we show the dissection for hexane isomers, while in Table 3 and Table 4 the final results for heptane and octane isomers are given, respectively.

Properties of the Dissection

Each molecular graph is characterized by a pair of integers (A,B). Some regularities in the magnitudes of A and B are immediately evident. We see that n-alkanes (path graphs) have always A = B, while in all

Table 1 : The Dissection of Butane and Pentane Isomers

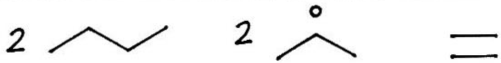
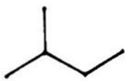
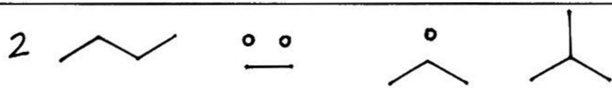
	 2 (2a + 2b) + 2 (a + b)	6a + 6b
	 3 (2a + 2b) + 3a	9a + 6b
	 2 (6a + 6b) + 2a + 2 (2a + 2b) + 2b	18a + 18b
	 2 (6a + 6b) + 2a + b + 2a + 2 (2a + 2b) + (9a + 6b)	26a + 21b
	 4 (9a + 6b) + 4a	40a + 24b

Table 2 : The Dissection of Hexane Isomers

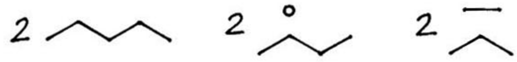
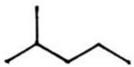
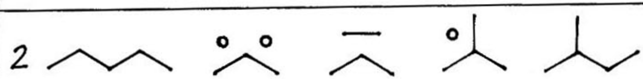
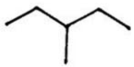
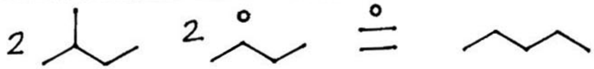
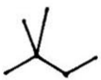
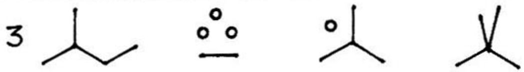
	 2 (18a + 18b) + 2a + 2 (6a + 6b) + 2b + 2 (2a + 2b)	54a + 54b
	 2(18a + 18b) + 2a + (2a + 2b) + b + a + (9a + 6b) + (26a + 21b + (2a + 2b)	78a + 68b
	 2 (26a + 21b) + 2a + 2(6a + 6b) + a + 2b + (18a + 18b)	85a + 74b
	 4 (26a + 21b) + 2a + 2 (2a + 2b)	110a + 74b
	 3 (26a + 21b) + 3a + b + a + (9a + 6b) + (40a + 24b)	131a + 89b

Table 3

The Dissection of Heptane Isomers

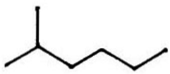
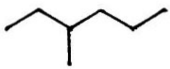
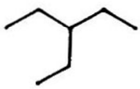
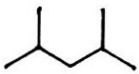
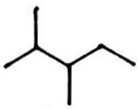
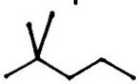
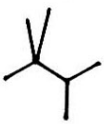
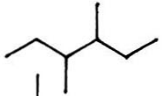
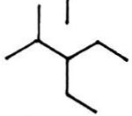
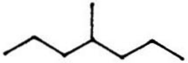
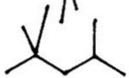
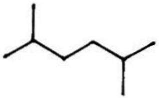
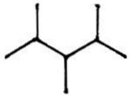
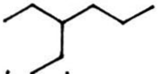
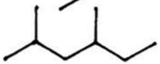
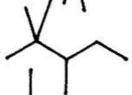
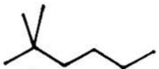
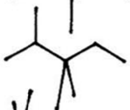
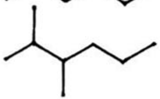
		(A, B)
	162 a + 162 b	(162, 162)
	234 a + 214 b	(234, 214)
	272 a + 245 b	(272, 245)
	312 a + 279 b	(312, 279)
	338 a + 288 b	(338, 288)
	396 a + 334 b	(396, 334)
	420 a + 326 b	(420, 326)
	488 a + 370 b	(488, 370)
	608 a + 450 b	(608, 450)

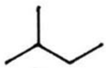
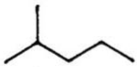
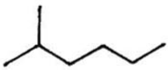
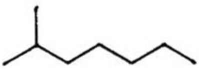
Table 4 : The Dissection of Octane Isomers

	(486, 486)		(1522, 1320)
	(702, 662)		(1596, 1384)
	(853, 786)		(1693, 1368)
	(905, 830)		(1919, 1554)
	(1014, 914)		(1981, 1670)
	(1072, 974)		(2032, 1614)
	(1241, 1096)		(2367, 1880)
	(1314, 1096)		(2519, 1970)
	(1336, 1170)		(3669, 2712)

other cases A is greater than B. In cyclic graphs, except K_3, again A = B, but for polycyclic systems (without pendant bonds) one finds A to be smaller than B. Moreover, for n-alkanes the magnitude of A is simply related to the size of the system:

$$A_n = 2\ (\ 3\ )^{n-3}$$

where n is the number of the vertices in the graph. Branching of the skeleton introduces complications in the expressions for A or B, but even here, if one consider a family of structurally related graphs, regularities in the values of A and B become apparent. Consider for instance homologous series shown below:

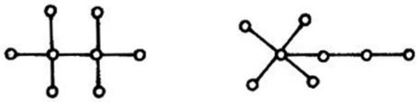
	(A, B)	Difference
	(26, 21)	5
	(78, 68)	10
	(234, 214)	20
	(702, 662)	40

We see that the difference A - B doubles for each vertex added. Each such family of graphs which has a simple regularity for magnitudes of A and B indicates graphs for which reconstruction is possible, at least within the so qualified class of graphs. For a reconstruction to be absolute we would need guarantees that no other graph with the same pair of parameters A, B is possible.

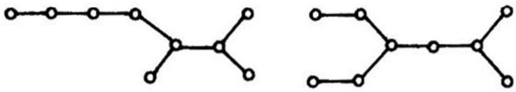
From Table 1 - 4 we see that for graphs of the same size A (and B, which parallels A) generally increases as the number of branching vertices increase or as their valency increases. This suggests a possibility of using the parameters A, B for ordering graphs with an expectation that the sequence may parallel some properties of branched skeletons. The possibility for ordering of graphs and reconstruction of some suggests that isospectral graphs[9] are discriminated. We illustrate in Table 5 the dissection for isospectral graphs having eight and nine vertices. It remains to be investigated how generally the above will hold. However, in view of the exponential growth of the number of components with the size of a dissected graph, even if the dissection is to be shown to be unique, the approach nevertheless may find only a limited application for graph isomorphism test.

Table 5

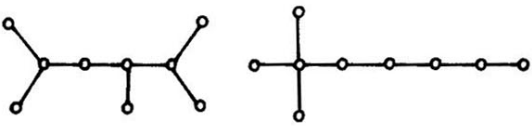
Dissection of Selected Isospectral Graphs



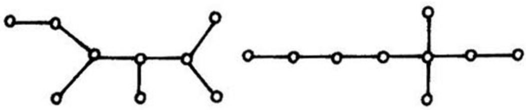
(3669, 2712)
(1338, 920)



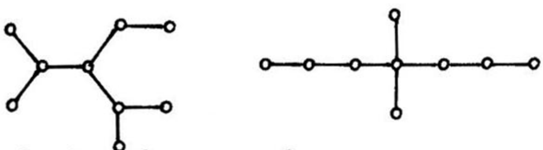
(4340, 3912)
(3971, 3574)



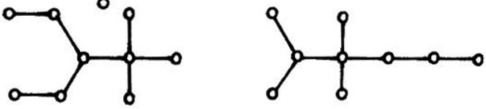
(6400, 5633)
(4117, 3610)



(8122, 7014)
(5604, 4740)



(8866, 7635)
(6200, 5190)



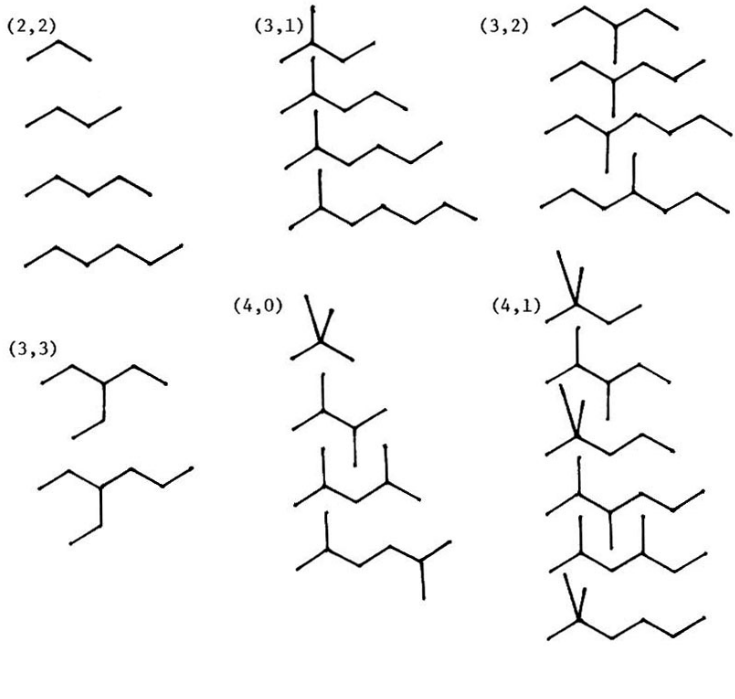
(10394, 8590)
(9382, 7657)

Classification of Acyclic Graphs

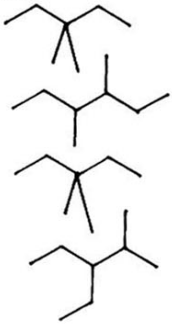
We will now describe a classification of acyclic graphs which follows from the first step in the dissection: a construction of Ulam's subgraphs. We define a residual R of a graph as the collection of the isolated vertices and isolated edges obtained when deriving Ulam's subgraphs. We find that structurally related graphs have identical residuals, as illustrated in Table 6:

Table 6

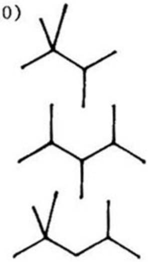
Grouping of skeletons of alkanes in families with the same residual



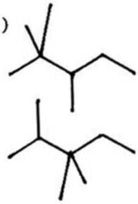
(4,2)



(5,0)



(5,1)



The number of isolated vertices and edges is given as an ordered pair (A', B'). In some instances, two or three homologous series will be characterized by the same residual. In these situations it is not difficult to recognize certain structural operations which relate different members in the class. For instance, the class (4,0) shows that we can imagine a process of augmenting a graph by creating a new edge between two "halves" of a vertex. The opposite process, that of contraction of an edge until eventually the end points fuse into a single vertex, is perhaps easier to recognize. The derived classification merely provides a subdivision of a relatively large body of acyclic graphs in a number of smaller groupings. A' represents the number of terminal vertices, while B' represents the number of bonds (1,2), where 1 and 2 stand for the valency of the involved vertices.[10] We see that the rule for augmentation of a graph permits "splitting" of any vertex if that does not creates new (1,2) - bond types. The parameter A' characterize the number of branches, while B' characterize the relative sizes of the branches present.

The outlined concept of dissection of a graph, which can be viewed as a generalization of Ulam's procedure for deriving subgraphs by deleting a single vertex at a time, reflects some structural differences among acyclic graphs. To what extent such an approach will be of interest in applications remains to be seen. An important result is the possibility of considering a two-dimensional ordering of graphs (in contrast to the usual one-dimensional sequencing of structures). One can also consider a further classification of acyclic graphs, or only graphs within selected acyclic families, by considering residuals of Ulam's subgraphs, and iterating the process if necessary several times. A simple visualization of a two-dimensional "ordering" of graphs is achieved by considering the parameters A and B (of Table 1 - 4) as coordinates in a plane. Along the diagonal A = B we have n-alkanes, while the more branched structures approach the horizontal A-axis. As one can see, the range of values of A and B grows fast with the increase in the size of graphs, so it is not suprising that no pair of graphs has yet been found which have the same A, B parameters.

Acknowledgment

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