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ON REALIZABILITY OF A SET OF INTEGERS AS DEGREES OF THE VERTICES OF A LINEAR GRAPH. I*

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Abstract. This paper is mainly concerned with the realizability of a set of n integers as the degrees of vertices of an n-vertex linear graph. Other related problems, such as when a set of integers is realizable as a connected graph, connected graph without "parallel" elements, separable graph, and nonseparable graph, are considered. The relationship between this problem and the problem of isomers in the organic chemistry is described. A similar problem in weighted graphs is also studied.

1. Introduction. Let G be a linear graph with n vertices (nodes) [1, 2, 3]. Let the degree of a vertex in G be the number of elements (arcs) connected to (incident at) that vertex. Suppose we are given a set of positive integers $d_1, d_2, \cdots, d_n$, $(d_i \leqq d_{i+1}, 1 \leqq i \leqq n-1)$. How can we tell whether or not there exists a graph G whose vertices $v_1, v_2, \cdots, v_n$ have degrees $d_1, d_2, \cdots, d_n$? If such a graph exists, we say that the set of integers is realizable, or the graph realizes the set of integers. Other questions, such as whether or not the set of integers is realizable as a connected graph, separable graph, and nonseparable graph[1] are considered.

Suppose a positive number is attached to every element of a linear graph. Such a graph, represented here by G_w, is called a weighted graph. Let w_i represent the sum of the weights of the elements incident at vertex v_i of G_w. Then, given a set of positive numbers $w_1, w_2, \cdots, w_n$, the necessary and sufficient condition for this set of numbers to be realizable as the "degrees" of the vertices of a weighted graph are found.

We shall make use of many concepts in linear graph theory. Definitions of some of the terms used in this paper are found in the Appendix.

2. The basic theorem.

Theorem 1. *The necessary and sufficient conditions for positive integers*[2] $d_1, d_2, \cdots, d_n$ *to be realizable* (*as the degrees of the vertices of a linear graph*) *are*:

(i) $\sum_{i=1}^{n} d_i = 2e$, *where e is an integer*,

(ii) $\sum_{i=1}^{n-1} d_i \geqq d_n$.

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[1] Since the realization, in general, is not unique, it is possible that a set of integers is realizable as a separable and as a non-separable graph simultaneously. The question of uniqueness is a complex one and is considered in the companion paper.

[2] Throughout this paper every *given* set of integers is assumed to contain only positive integers and to be in a nondecreasing order.

Proof. The necessity of (i) is proved by noting that $\sum_{i=1}^{n} d_i = 2e$ where e is the number of elements in a graph G. To prove the necessity of (ii), assume otherwise, that is, there exists a graph G in which $\sum_{i=1}^{n-1} d_i < d_n$. Let the vertex v_n in G correspond to the integer d_n. Then, the inequality $\sum_{i=1}^{n-1} d_i < d_n$ implies that there exists in G at least one element incident at v_n which is not incident at any other vertex. This is impossible, hence $\sum_{i=1}^{n-1} d_i \geqq d_n$.

The sufficiency is proved by induction. If $n = 2$, then (ii) implies that $d_1 = d_2$. Such a pair of integers is realized as a graph with two vertices between which $d_1 = d_2$ elements are connected. For $n = 3$, we have positive integers d_1, d_2, d_3 which satisfy (i) and (ii), and we must find a three-vertex graph realizing these integers.

Consider a graph with three vertices. Let $n_{ij} = n_{ji}$ represent the number of elements connected between vertices v_i and v_j, $(i, j = 1, 2, 3, i \neq j)$. Then, we have

$$d_1 = n_{12} + n_{13},$$

$$d_2 = n_{23} + n_{21} = n_{32} + n_{12},$$

$$d_3 = n_{32} + n_{31} = n_{23} + n_{13}.$$

Solving the above linear equations for n_{12}, n_{13}, and n_{23}, we obtain

$$n_{12} = \frac{(d_1 + d_2 + d_3) - 2d_3}{2},$$

$$n_{13} = \frac{(d_1 + d_2 + d_3) - 2d_2}{2},$$

$$n_{23} = \frac{(d_1 + d_2 + d_3) - 2d_1}{2}.$$

The existence of the desired graph is established, if we show that the numbers n_{12}, n_{13}, and n_{23} are all nonnegative integers. Condition (ii) implies that the sum of any $n - 1$ integers is no less than the remaining one, therefore, n_{12}, n_{13}, and n_{23} are all nonnegative. Condition (i) implies that $\sum_{i=1}^{n} d_i - 2d_j$, $(1 \leqq j \leqq n)$ is an even number, hence n_{12}, n_{13} and n_{23} are integers.

To complete the induction, we assume that the assertion is true for $n < k$, $(k > 3)$, we will then show that it is also true for $n = k$. Let $d_1, d_2, \cdots, d_k$ be k positive integers satisfying (i) and (ii). Consider the set of nonnegative integers $d_2, d_3 \cdots, d_{k-1}, d_k - d_1$. For the moment let us assume $d_k - d_1 \neq 0$. We would like to establish that this new set of integers satisfies (i) and (ii). The sum of these integers is equal to $\sum_{i=1}^{k} d_i - 2d_1$ which is an even number, for $\sum_{i=1}^{k} d_i$ is an even number, hence (i) is satisfied. It remains to be shown that this new set of integers also satisfies (ii). However, we have $\sum_{i=1}^{k-1} d_i \geqq d_k$ which implies $\sum_{i=2}^{k-1} d_i \geqq d_k - d_1$. If $d_k - d_1$, is the largest integer in the set of integers $d_2, d_3, \cdots, d_{k-1}, d_k - d_1$, (ii) is satisfied. If not, then d_{k-1} is the largest, and we must show that $d_2 + d_3 + \cdots + d_{k-2} + (d_k - d_1) \geqq d_{k-1}$. The, above inequality is satisfied for $k > 3$, because $d_k \geqq d_{k-1}$ and $d_2 \geqq d_1$.

According to the hypothesis any set of $n < k$ integers satisfying (i) and (ii) is realizable, therefore, there exists a graph G_1 which realizes integers $d_2, d_3, \cdots, d_{k-1}, d_k - d_1$, as the degrees of its vertices. To the graph G_1 we add a vertex called v_1 and we connect d_1 elements between vertex v_1 and the vertex in G_1 corresponding to the integer $d_k - d_1$. The graph thus constructed realizes the original set of integers. If[3] $d_k - d_1 = 0$, then the new set of integers will be $d_2, d_3, \cdots, d_{k-1}$, which also satisfies (i) and (ii), and hence, is realizable as a graph G_1. However, we must now add two vertices to G_1, and connect $d_1 = d_k$ elements between these vertices. This ends the proof of the theorem. As a direct consequence of the proof of this theorem, we can state the following corollary.

COROLLARY. *For any set of realizable three integers d_1, d_2, d_3, there exists only one graph whose vertices have degrees d_1, d_2, d_3.*

Suppose we are given the set of integers 1, 1, 1, 1. This set of integers satisfies conditions (i) and (ii). However, the graph realizing these integers is not connected. A *connected* graph is a graph in which there exists a path between every pair of vertices. In the next section we shall give necessary and sufficient conditions for a set of integers to be realizable as a connected graph.

3. Realizability as a connected graph and d-invariant transformation. Suppose a graph G realizes integers $d_1, d_2, \cdots, d_n$. Consider a pair of elements $e(v_i, v_j)$ and $e(v_k, v_0)$ in G which are connected between vertices v_i and v_j, v_k and v_0 respectively. Assume that vertices v_i, v_j, v_k, and v_0 are all distinct. Suppose we transform graph G into a graph G_1 by removing elements $e(v_i, v_j)$ and $e(v_k, v_0)$ from G and either adding (1) elements $e(v_i, v_k)$ and $e(v_j, v_0)$ between vertices v_i and v_k, v_j and v_0, or adding (2) elements $e(v_i, v_0)$ and $e(v_j, v_k)$ between vertices v_i and v_0, v_j and v_k. We should notice that in this transformation of graphs the degrees of the vertices remain unchanged. Such a transformation is called an elementary d-invariant transformation. The class of all graphs realizing the same set of integers is called a class of d-invariant graphs. It will be shown (in the companion paper) that the class of all invariant graphs can be found by a finite number of elementary d-invariant transformations.

Consider a graph G. The subgraphs $g_1, g_2, \cdots, g_r$, $(r > 1)$, of G are called the maximally connected subgraphs[3] (or components) of G if (1)

[3] It must be noted that if $d_1 = d_k$, then $d_1 = d_2 = \cdots = d_k$.

every element of G is in only one of the subgraphs $g_1, g_2, \cdots, g_r$, i.e., the "union" $g_1 \cup g_2 \cup \cdots \cup g_r = G$, and the "intersection" $g_i \cap g_j = 0$, $i \neq j$; and (2) there exist no paths from a vertex in g_i to a vertex in g_j, $i \neq j$. A circuitless graph is a graph which contains no circuits.

LEMMA 1. *Let $g_1, g_2, \cdots, g_r$, $(r > 1)$, be the maximally connected subgraphs of G not all of which are circuitless. Then, there exists a graph G_1 which is d-invariant from G, with $r - 1$ maximally connected subgraphs.*

Proof. Let g_i be a maximally connected subgraph of G containing a circuit. Let e_{i_1} in g_i be an element which is a circuit in g_i. Take an arbitrary element e_{j_1} in g_j, $i \neq j$. By an elementary d-invariant transformation involving e_{i_1} and e_{j_1}, we obtain a graph G_1 in which subgraph g_i and g_j are combined into a connected subgraph, which reduces the number of maximally connected subgraphs by one.

It should be noted that we can keep on reducing the number of maximally connected subgraphs as long as there are circuit elements in any of the maximally connected subgraphs.

THEOREM 2. *The necessary and sufficient conditions for a set of integers $d_1, d_2, \cdots, d_n$ to be realizable as a connected graph are:*

(i) *the set $d_1, d_2, \cdots, d_n$ is realizable, i.e., it satisfies the conditions of Theorem* 1.

(ii) $\sum_{i=1}^{n} d_i \geqq 2(n - 10)$.

Proof. The necessity of condition (i) is already established. To establish the necessity of (ii), consider a connected graph G. In a connected graph of n vertices the number of elements e is at least equal to $n - 1$ [3]. We know $\sum_{i=1}^{n} d_i = 2e$; therefore, $\sum_{i=1}^{n} d_i \geqq 2(n - 1)$.

To prove the sufficiency, we assume a given set of integers $d_1, d_2, \cdots, d_n$ satisfy (i) and (ii), and then prove that among the class of d-invariant graphs realizing $d_1, d_2, \cdots, d_n$, there exists one which is connected. Since the set $d_1, d_2, \cdots, d_n$ satisfy (i), there exists a graph G realizing $d_1, d_2, \cdots, d_n$. If G is connected, there is no problem; therefore, let us assume G is not connected. Let the maximally connected parts of G be $g_1, g_2, \cdots, g_r$, $(r > 1)$. Suppose $g_1, g_2, \cdots, g_r$ are all circuitless subgraphs, for if there is a subgraph g_i which contains a circuit, as suggested by Lemma 1, we can combine this subgraph with another subgraph g_j, hence reducing the number of maximally connected parts. We can continue this operation until all subgraphs are circuitless. If $g_1, g_2, \cdots, g_r$ are all circuitless, then the number of elements in G is equal to $n - r$ [3]. This implies that $\sum_{i=1}^{n} d_i = 2(n - r)$, which contradicts (ii), hence the theorem.

The following corollaries can be easily established as a consequence of the previous theorem:

COROLLARY 1. *The set of integers $d_1, d_2, \cdots, d_n$ is realizable as a circuitless but connected graph if and only if,*

(i) $\sum_{i=1}^{n} d_i = 2(n - 1)$.

COROLLARY 2. *The set of integers* $d_1, d_2, \cdots, d_n$ *is realizable as a connected graph if,*

(i) *the set* $d_1, d_2, \cdots, d_n$ *is realizable,*

(ii) $d_4 \neq 1$.

4. Realizability as separable and nonseparable graphs. A graph G is *nonseparable* if every subgraph g of G has at least two vertices in common with its complement. All other graphs are *separable* [2, 3]. If G is a connected but separable graph, then there exists a subgraph g in G which has only one vertex v_c in common with its complement; v_c is called a *cut vertex* of G [3].

THEOREM 3. *The necessary and sufficient conditions for a set of integers* $d_1, d_2, \cdots, d_n$ *to be realizable as a nonseparable graph are:*

(i) $\sum_{i=1}^{n} d_i = 2e$, *where* e *is an integer,*

(ii) $d_i \neq 1$ *for all* i,

(iii) $\sum_{i=1}^{n-1} d_i \geqq d_n + 2(n-2)$.

Proof. Necessity of (i) is already established. The necessity of (ii) is self-explanatory. To prove that condition (iii) is also necessary, suppose there exists a graph G in which

$$\sum_{i=1}^{n-1} d_i < d_n + 2(n-2).$$

We will show that G is separable and the cut vertex is vertex v_n corresponding to the integer d_n. To prove this we will show that deleting all elements incident at v_n from G results in a graph G_1 which is not connected. Let the degrees of the vertices in G_1 be $d_1', d_2', \cdots, d_{n-1}'$. We know that

$$\sum_{i=1}^{n-1} d_1' < 2(n-2).$$

According to Theorem 2, graph G_1 cannot be connected. This ends the proof of the necessity of these conditions.

To prove sufficiency, we assume we are given a set of integers $d_1, d_2, \cdots, d_n$, which satisfies (i), (ii), and (iii). We construct a new set of nonnegative integers $d_1', d_2', \cdots, d_n'$, where $d_i' = d_i - 2$, $(1 \leqq i \leqq n)$. We now show that the set of integers $d_1', d_2', \cdots, d_n'$ is realizable. To do this, we show that these integers satisfy conditions of Theorem 1. The first condition of Theorem 1 is satisfied, for

$$\sum_{i=1}^{n} d_i' = \sum_{i=1}^{n} d_i - 2n$$

which is an even number, due to condition (i) of the hypothesis. Now, we must show that

$$\sum_{i=1}^{n-1} d_i' \geqq d_n'.$$

From (iii), we have

$$\sum_{i=1}^{n-1} d_i \geqq d_n + 2(n-2),$$

which may be written as

$$\sum_{i=1}^{n-1} d_i - 2(n-1) \geqq d_n - 2,$$

or finally,

$$\sum_{i=1}^{n-1} (d_n - 2) \geqq (d_n - 2)$$

which is what was desired. Let a realization of the set of integers $d_1', d_2', \cdots, d_n'$ be a graph G'. It is possible that some of these integers are zero, in which case we allow the corresponding vertices in G' to be isolated vertices (points) in G'. Suppose we superimpose upon G' a collection of n elements forming a Hamiltonian circuit (a circuit going through all vertices of G). It is clear that G realizes the original set of integers. Since G contains a Hamiltonian circuit, G is also nonseparable.

Since a set of integers may be realizable as a nonseparable graph as well as a separable graph, the following question remains to be answered: Given a set of integers, how do we determine whether or not there exists a separable but connected graph realizing these integers as the degrees of its vertices?

THEOREM 4. *A necessary and sufficient condition for a set of integers which is realizable as a connected graph* (*satisfies conditions of Theorem* 2) *to be realizable as a separable but connected graph is*:

(i) *If* $n = 3$, $d_1 + d_2 = d_3$,

(ii) *If* $n = 4$, *there must exist among the set of integers a* d_i *and a* d_j *such that* $d_i \neq d_j$,

(iii) *If* $n > 4$, *there must exist among the set an integer* $d_i \neq 2$.

Proof. If $n = 3$, the necessity and sufficiency of the condition $d_1 + d_2 = d_3$ is self-evident. The necessity of (ii) is established by showing that there exists no four-vertex separable graph which is connected and in which all vertices are of the same degree. Suppose a separable connected graph G is realizing the set of integers $d_1 = d_2 = d_3 = d_4$. Suppose v_1 is a cut vertex in G. It is clear that one of the separable parts of G must contain two vertices one of which is v_1. This implies that there exist *positive* integers d_{11} and d_{12} such that $d_{11} + d_{12} = d_1$ and integers d_{11} and d_2 is a realizable two-vertex graph. However, integers d_{11} and d_2 are realizable if, and only if, $d_{11} = d_2$. This requires $d_{12} = 0$ which is a contradiction. The necessity of (iii) is proved, by merely observing that a connected graph in which all vertices are of degree two is a circuit [3], which is a nonseparable graph.

Let us consider a set of integers $d_1, d_2, \cdots, d_n (n \geqq 4)$ that satisfies conditions (ii) and (iii). We want to show we can find a separable graph realizing these integers. We shall consider two cases. Case 1: $d_1 = d_2 = d_3 \cdots = d_n$, $n > 4$. Suppose d_1 is an even number. Since $d_1 \neq 2$, then $d_1 = 2 + d_{12}$. Consider the following two sets of integers: 2, d_2, d_3 and $d_{12}, d_4, d_5, \cdots, d_n$. Both of these sets of integers satisfy the conditions of Theorem 2; hence they are realizable as connected graphs g_1 and g_2. Superimposing the vertices of the lowest degree in g_1 and g_2, we obtain a separable graph which realizes the original set of integers. If d_1 is an odd number, then n must be an even number. Furthermore, $d_1 \neq 1$, for otherwise the conditions of Theorem 2 are not satisfied. Let $d_1 = 2 + d_{12}$. Consider the two sets of integers 2, d_2, d_3 and d_{12}, d_4, d_5, d_6, $\cdots$, d_n. These two sets of integers satisfy the conditions of Theorem 2, hence they are realizable as connected graphs g_1 and g_2. As before, superimposing the vertices of lowest degree in g_1 and g_2, we obtain a separable and connected graph G which realizes the given set of integers. Case 2: $d_1 \neq d_n$. In this case, we shall consider the following two sets of integers, d_1, d_1 and d_2, d_3, $\cdots$, $d_n - d_1$. The first set is obviously realizable. The proof of the realizability of the set of integers d_2, d_3, $\cdots$, d_{n-1}, $d_n - d_1$ is already given in the proof of Theorem 1. However, we must show that d_2, d_3, $\cdots$, d_{n-1}, $d_n - d_1$ is realizable as a connected graph. To do this, we must show that $d_2 + d_3 + \cdots + d_{n-1} + (d_n - d_1) \geqq 2(n-2)$. The left side of the above inequality is equal to $\sum_{i=1}^n d_i - 2d_1$. If $d_1 = 1$, then

$$\sum_{i=1}^n d_i - 2d_1 \geqq 2(n-1) - 2 = 2(n-2).$$

If $d_1 > 1$, then

$$\sum_{i=1}^n d_i - 2d_1 \geqq nd_1 - 2d_1 = (n-2)d_1 \geqq 2(n-2).$$

This ends the proof of the theorem, for the two sets of integers are realizable as connected graphs g_1 and g_2 and superimposing a vertex of g_1 upon the vertex of g_2 corresponding to the integer $d_n - d_1$, we obtain the desired graph.

5. Realizability as a graph without parallel elements. A graph G has parallel elements if there exist at least two elements in G which are connected between the same vertices. The question we would like to answer is: Under what circumstances may a set of integers be realized as a graph in which there are no parallel elements? We shall make use of the following reduction process.

Let a set of integers d_1, d_2, $\cdots$, d_n be called reducible if $d_n \leqq n - 1$. The set of integers d_{i_1}, d_{i_2}, $\cdots$, $d_{i_{n-1}}$ are obtained from the original set as follows:

$$d_{i_j} = \begin{cases} d_{n-j} - 1 & (1 \leqq j \leqq d_n), \\ d_{n-j} & (j > d_n). \end{cases}$$

Let d_1', d_2', $\cdots$, d_p' $(p \leqq n - 1)$ be positive integers in the set $d_{i_1}, d_{i_2}, \cdots, d_{i_{n-1}}$ arranged in a nondecreasing order. The set of integers d_1', d_2', $\cdots$, d_p' are called a reduced set of integers and the process just described is called a reduction cycle. Starting with d_1', d_2', $\cdots$, d_p', we can go through another reduction cycle and obtain another set of integers, if $d_p' \leqq p - 1$.

THEOREM 5. *A set of realizable integers, $d_1, d_2, \cdots, d_n$ is realizable as a graph without parallel elements if, and only if, the set is reducible and every set of integers obtained from this set by successive reduction cycles is reducible.*

Proof. Let G be a graph with no parallel elements. Let the degrees of the vertices of G be $d_1, d_2, \cdots, d_n$. There are at most $n - 1$ elements incident at vertex v_n, hence $d_n \leqq n - 1$. Let G_1 be a graph obtained from G by removing from G the vertex v_n and all elements incident at v_n. Let the degrees of the vertices in G_1 be $d_1^{(1)}, d_2^{(1)}, \cdots, d_{p'}^{(1)}, (d_i^{(1)} \leqq d_{i+1}^{(1)}$ for $1 \leqq i \leqq p' - 1)$. Since G_1 has no parallel elements, $d_{p'}^{(1)} \leqq p' - 1$. Let $d_1', d_2', \cdots, d_p'$ be the set of integers obtained from integers $d_1, d_2, \cdots, d_n$ by a single reduction cycle. It can easily be seen that $d_p' \leqq d_{p'}^{(1)}$ and $p' \leqq p$, which implies that $d_p' \leqq p - 1$. The continuation of this process also establishes the necessity of the reducibility of the sets of integers obtained in the successive reduction cycles.

To prove this condition is also sufficient, we shall outline a procedure that results in a graph without parallel elements. Let us pick n points (vertices) $v_1, v_2, \cdots, v_n$. We now connect an element between each of the following pairs of vertices $v_n - v_{n-1}, v_n - v_{n-2}, \cdots, v_n - v_{n-d_n}$. Since $d_n \leqq n - 1$, this can always be done. There are now exactly d_n elements incident at v_n, none of which are in parallel. To construct the rest of the graph, we note that the degrees of the vertices of the remaining graph must be the reduced set of integers, $d_1', d_2', \cdots, d_p'$. Since $d_p' \leqq p - 1$, we can successively continue on similar cycles and finally obtain a graph which has no parallel elements. However, there remains a question that must be answered. That is, we must show that if $d_1, d_2, \cdots, d_n$ is realizable so is the reduced set of integers $d_1', d_2', \cdots, d_p'$. However, since $\sum_{i=1}^{p} d_i' = \sum_{i=1}^{n} d_i - 2d_n$, the sum of the reduced set of integers is even. Also, since $d_p' \leqq p - 1$, we have $\sum_{i=1}^{p-1} d_i' \geqq d_p'$. This shows that if the original set of integers is realizable and successively reducible, then all of the reduced sets of integers are also realizable. This ends the proof of the theorem.

6. Realizability of a set of positive numbers as the degrees of a weighted graph. The concept of a weighted graph is found to be extremely useful in the applications of graph theory to electrical networks and other physical systems. It is, therefore, natural to extend the result discussed here to the case of weighted graphs.

THEOREM 6. *Given a set of numbers $w_1, w_2, \cdots, w_n, (w_i \leqq w_{i+1})$ a necessary and sufficient condition for this set to be realizable as weighted degrees of the vertices of a linear graph is*

(i) $\sum_{i=1}^{n-1} w_i \geqq w_n$.

Proof. Proof of the necessity is entirely the same as Theorem 1, hence will not be repeated here. As in the case of Theorem 1, we shall prove the sufficiency by induction. For $n = 2$, w_1 must be equal to w_2. An element of weight w_1 connected between a pair of vertices would realize such a pair of numbers. For $n = 3$, we define numbers $n_{ij} = n_{ji}$ $(i, j = 1, 2, 3, i \neq j)$ which is to be the weight of the element connected between vertices v_i and v_j. The unique realization for this case is determined by calculating the values of these weights according to the following equations:

$$n_{12} = \frac{w_1 + w_2 - w_3}{2},$$

$$n_{13} = \frac{w_1 - w_2 + w_3}{2},$$

$$n_{23} = \frac{-w_1 + w_2 + w_3}{2}.$$

Now let us assume the theorem is true for $n < k$; we prove it for $n = k$. Consider a set of numbers $w_1, w_2, \cdots, w_k$. We construct the set of numbers $w_2, w_3, \cdots, w_{k-1}, w_k - w_1$ and prove as in the case of Theorem 1, that this set satisfies the condition (i) of the theorem, and hence is realizable. Let the weighted graph realizing $w_2, w_3, \cdots, w_{k-1}, w_k - w_1$, be G_w'. To this graph we add a vertex v_1, and between v_1 and the vertex in G_w' corresponding to the number $w_k - w_1$ we connect an element whose weight is w_1. Thus, we obtain a graph G_w realizing the given set of numbers as the degrees of the vertices of a weighted graph.

7. Applications and conclusion. Consider the chemical compound N_2O_3. The five structural representations of this compound are shown in Fig. 1a. The corresponding graphs of these structures are shown in Fig. 1b. These five structures are called the isomers of N_2O_3. Apparently, these isomers are also distinguishable from their physical properties.

The common characteristic of the graphs in Fig. 1b is that they are all d-invariant connected graphs realizing the set of integers 2, 2, 2, 3, 3. Therefore, it seems that Theorem 2 enables us to tell whether or not a hypothetical chemical compound could exist. An important, and as yet unsolved problem is to find all isomers of a given chemical compound. This problem essentially boils down to the problem of generating all d-invariant graphs corresponding to a set of integers, for which there is no efficient solution available.

Many theoretical questions remain unanswered, some of which are: Which realization of a set of integers is a graph with a maximum (or mini-

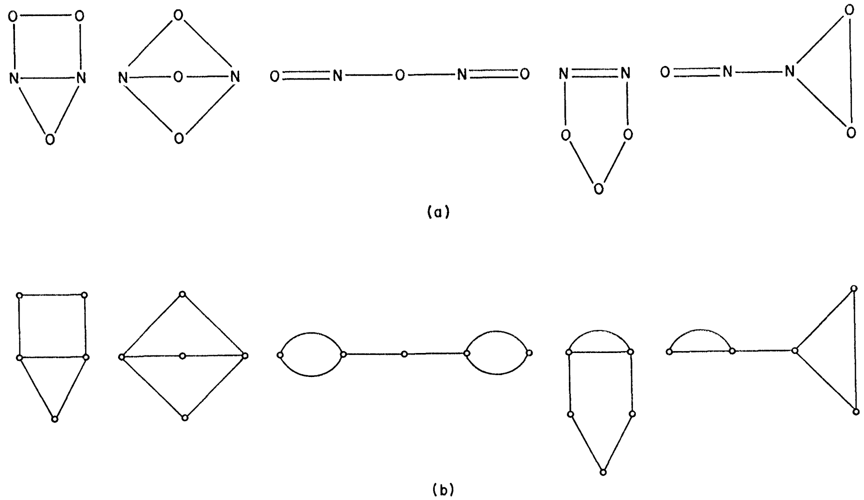

FIG. 1. (a) *The five isomers of N_2O_3.* (b) *Their corresponding graphs.*

mum) number of trees, circuits, or cut sets?[4] Which realization has a maximum (or minimum) number of parallel elements, separable parts, maximally connected parts, or noncircuit elements?

An important question that is answered in the companion paper is: What are the necessary and sufficient conditions for a set of integers to be realizable as a unique and connected graph (i. e., all graphs realizing the set of integers are one-isomorphic)?

APPENDIX

A linear graph is a finite collection of two types of entities, *elements* (arcs) and *vertices* (nodes). Each element $e(v_i, v_j)$ is connected between a pair of distinct vertices v_i and v_j. If a graph g is included in G, then g is said to be a *subgraph* of G. The *complement* of a *subgraph* g is a subgraph $\bar{g}$ which contains all of the elements in G which are not in g, together with every vertex associated with these elements. A *path* in a graph G is a set of elements (a subgraph of G) that can be ordered in the form $e(v_i, v_j), e(v_j, v_k), \cdots, e(v_r, v_t), e(v_t, v_s)$, where the vertices $v_i, v_j, v_k, \cdots, v_r, v_t, v_s$ are distinct. A circuit in a graph G (loop) is a set of elements (a subgraph of G) that can be ordered in the form $e(v_i, v_j), e(v_j, v_k), \cdots, e(v_r, v_t), e(v_t, v_i)$ where the vertices $v_i, v_j, v_k, \cdots, v_r, v_t$ are distinct.

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[4] The number of cut sets and unions of disjoint cut sets in a connected n-vertex graph is $2^{n-1} - 1$; however, the number of cut sets, in general, is a function of the structure of the graph.

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