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TRANSIT ISOMORPHISM AND ITS STUDY ON OCTANE ISOMERS

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Abstract: Having defined and studied, the transit index and transit decomposition of a connected graph, we introduce the concept of transit isomorphism. In this paper we discuss the transit isomorphism between certain graphs and its line graphs. Construction of transit isomorphic graphs is also dealt with. Finally we discuss how transit isomorphism relates to chemical properties of octane isomers.

Keywords and Phrases: Transit index, Transit decomposition, Majorized Shortest Paths, Transit Isomorphism.

2020 Mathematics Subject Classification: 05.

1. Introduction

In mathematical chemistry, a molecule's properties are predicted based on its structure. Molecules are modeled as graphs, and their properties are studied using graph invariants. A graph invariant can be a polynomial, a set of values or a single value. A single value characterising the topology of a molecular graph has been termed a topological index by Hosoya. In the literature we come across many such topological indices.

In paper [3], a novel index called the transit index of a graph was introduced. This index has an effect on both the degree and the distance of the graph. The transit index of the molecular graph displayed a strong negative correlation with the MON of octane isomers. Hence some theoretical study of this index was carried out.

The study of graphs with similar properties has attracted the attention of graph theorists forever. Graph isomorphism is one such concept. It is a phenomenon in which the same graph appears in more than one form. A graph of this type is called an isomorphic graph. In this paper, the concept of transit isomorphism is introduced. Relevance of transit isomorphism in octane isomers was investigated.

Throughout this paper G denotes a simple, connected, finite, undirected graph with vertex set V and edge set E. For undefined terms we refer [1].

2. Preliminaries

Definition 2.1. [3] *Let $G(V, E)$ be a graph with vertex set V and edge set E. For $v \in V$, the transit of v denoted by $T(v)$ is defined as "the sum of the lengths of all shortest path with v as an internal vertex" and the transit index of G denoted by $TI(G)$ is*

$$TI(G) = \sum_{v \in V} T(v)$$

Lemma 2.2. [3] *In $G(V, E)$, $T(v) = 0$ iff $\langle N[v] \rangle$ is a clique.*

Theorem 2.3. [3] *For a path P_n, Transit index is*

$$TI(P_n) = \frac{n(n+1)(n^2 - 3n + 2)}{12}$$

Theorem 2.4. [4] *For a cycle, the transit index*

i) $TI(C_n) = \frac{n^2(n^2-4)}{24}$, *n even.*

ii) $TI(C_n) = \frac{n(n^2-1)(n-3)}{24}$, *n odd*

Definition 2.5. [5] *Let $G(V, E)$ be a graph. A path M through $v \in V$ is called a majorized shortest path of v, abbreviated as msp(v) or normally msp, if it satisfies the following conditions.*

1. M is a shortest path in G with v as an internal vertex.

2. There exist no path M' such that, M' is a shortest path in G with v as an internal vertex and M as a sub-path of it.

We denote the collection of all msp(v) by $\mathcal{M}_v$ and $\bigcup_{v \in V} \mathcal{M}_v$ by $\mathcal{M}_G$.

Proposition 2.6. [5] *In a tree* T, $Msp(v)$ *connects pendant vertices of* $T, \forall v \in V$. *Conversely every path connecting two pendant vertex is a msp for every internal vertex of it.*

Definition 2.7. [2] *A decomposition of a graph* G *into a collection of subgraphs* $\tau = \{T_1, T_2, \ldots, T_r\}$, *where each* T_i *is either an induced cycle of* G *with atleast two of its subpath in* $\mathcal{M}_G$ *or a majorized shortest path of* G *such that,* $TI(G) = \sum_i TI(T_i) - \sum_{i \neq j} TI(T_i \cap T_j) + \ldots + (-1)^{r+1} \sum TI(T_1 \cap T_2 \cap \ldots \cap T_r)$ *is called a Transit Decomposition of* G. *We denote a transit decomposition of minimum cardinality by* τ_{min}.
For a graph G, *the transit decomposition need not be unique. Of these we choose the one with minimum cardinality and such that the msp/induced cycles in it are of least length. Such a transit decomposition will be unique for a graph* G *and we denote it by* τ_{min}.

3. Transit Isomorphism

Definition 3.1. *Let* G_1 *and* G_2 *be two graphs. We say that* G_1 *is transit isomorphic to* G_2, *if there exists a bijection, say* Ψ *from* $\tau_{min}(G_1) = \{H_i,\ i = 1, 2, \ldots, k\}$ *to* $\tau_{min}(G_2) = \{H'_i\ , i = 1, 2, \ldots, k\}$ *such that* $\Psi(H_i) = \Psi(H'_i),\ i = 1, 2, \ldots, k$ *whenever* $H_i \simeq H'_i$. *We write* $G_1 \simeq_T G_2$.

Remark 3.2. *The graphs may be transit isomorphic without being isomorphic. Consider the graphs in Figure 1. Clearly they are non isomorphic.*
Here $\tau_{min}(G_1) = \{T_1, T_2, T_3\}$, *where* $T_1 = 1234, T_2 = 1265, T_3 = 234562$

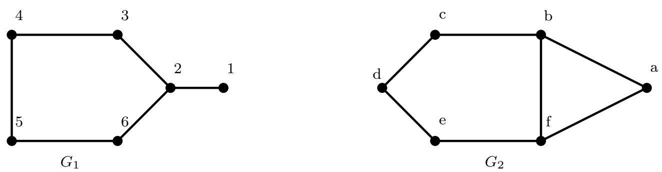

Figure 1: Non isomorphic graphs that are transit isomorphic.

$\tau_{min}(G_2) = \{H_1, H_2, H_3\}$, *where* $H_1 = abcd, H_2 = afed, H_3 = bcdefb$
Define $\Psi : \tau_{min}(G_1) \to \tau_{min}(G_2)$ *by* $\Psi(T_i) = H_i, i = 1, 2, 3$. *Then* Ψ *is a transit isomorphism.*

Remark 3.3. *The graphs* G_1 *and* G_2 *are transit isomorphic need not imply that* $TI(G_1)$ *and* $TI(G_2)$ *are equal.*

Consider the graphs in Figure 2. They are transit isomorphic, but their transit indices differ. For the graph G_1, $\tau_{min}(G_1) = \{T_1, T_2, T_3\}$, *where* $T_1 = 123457, T_2 = 123657, T_3 = 34563$
And for the graph G_2, $\tau_{min}(G_2) = \{H_1, H_2, H_3\}$, *where* $H_1 = abcegh, H_2 = abdfgh, H_3 = cdfec$
Define $\Psi : \tau_{min}(G_1) \to \tau_{min}(G_2)$ *by* $\Psi(T_i) = H_i, i = 1, 2, 3$. *Then* Ψ *is a transit isomorphism. But,* $TI(G_1) = 142$ *and* $TI(G_2) = 148$

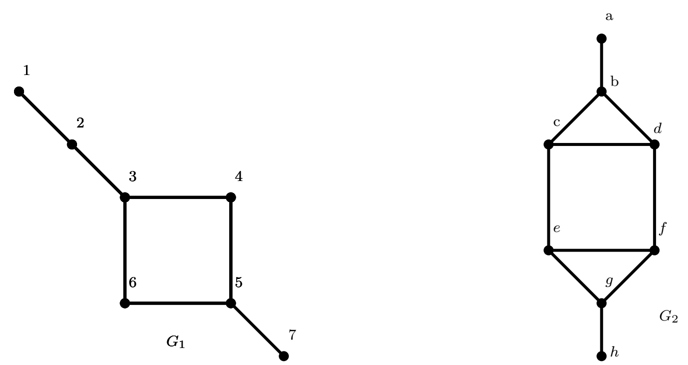

Figure 2: Transit isomorphic graphs with different transit index

4. Graphs G that are Transit Isomorphic to $L(G)$

In trees transit isomorphism and isomorphism are the same. Hence the study of transit isomorphism will be fruitful if the graph contains atleast one cycle. In this section we investigate the occurrence of transit isomorphism between a graph and its line graph.

Theorem 4.1. *Let* G *be a unicyclic graph formed by identifying the center vertex of a star graph* S_p *with one of the vertices of the odd cycle* C_r. *Then* G *and* $L(G)$ *are transit isomorphic.*

Proof. We know that the line graph of a star is a complete graph and that of a cycle is isomorphic to itself. In the case of the graph G under our consideration $L(G)$ can be viewed as the graph got by identifying an edge of the complete graph K_{p+1} with any one of the edges of C_r. Let τ_1 and τ_2 denote the transit decompositions of G and $L(G)$ of minimum cardinality. Clearly, there is only one induced cycle in τ_1 and τ_2 and it is isomorphic to C_r, when $r > 3$. (When r=3, no cycles are there in τ_1 and τ_2). Let it be T_1 and H_1 respectively.

Let v be the vertex common to C_r and S_p in G. If e_v and e'_v are the edges of C_r

incident to v in G, then they will form the end vertices of the edge common to K_{p+1} and C_r in $L(G)$. Let u_1 and u_2 be the vertices of C_r at a distance $\lfloor \frac{r}{2} \rfloor$ from v in G. Then $e = u_1u_2$ will be the vertex at a distance $\lfloor \frac{r}{2} \rfloor$ from e_v and e'_v in $L(G)$. Let $e_1 = vw_1, e_2 = vw_2, \ldots, e_{p-1} = vw_{p-1}$ be the pendant edges of G. Then $e_1, e_2, \ldots, e_{p-1}, e_v$ and e'_v will be the vertices of K_{p+1} in $L(G)$.
The majorized shortest paths in τ_1 are those connecting w_i to v_1, say $T_{i,1}$ and those connecting w_i to v_2, say $T_{i,2}$ of length $\lfloor \frac{r}{2} \rfloor + 1$ each and $2p - 2$ in number. When we consider τ_2, the majorized shortest paths are those connecting the vertices $e_1, e_2, \ldots, e_{p-1}$ to e along e_v, say $H_{i,1}$ and along e'_v, say $H_{i,2}$. Again they are also of length $\lfloor \frac{r}{2} \rfloor + 1$ each and $2p - 2$ in number. Also $|\tau_1| = |\tau_2|$
Define $\Psi : \tau_1 \to \tau_2$ by $\Psi(T_1) = H_1, \Psi(T_{i,1}) = H_{i,1}$ and $\Psi(T_{i,2}) = H_{i,2}$ for $i = 1, 2, \ldots, p-1$. Then Ψ is a transit isomorphism.

Remark 4.2. *Note that in Theorem 4.1 when r is even, G and $L(G)$ are not transit isomorphic. The cardinalities of the transit decompositions are equal, but the lengths of majorized shortest paths in τ_1 will be one more than those in τ_2.*

Theorem 4.3. *Let G be the unicyclic graph formed by identifying one of the pendant vertex of the path P_p with a vertex of the odd cycle C_r. Then G and $L(G)$ are transit isomorphic.*

Proof. Consider the given graph G. Let us denote the common vertex of P_p and C_r by v. Name the edges of C_r that are incident to v by e_v and e'_v. Call the edge in P_p incident to v as e. Note that two vertices of C_r are at a distance $\lfloor \frac{r}{2} \rfloor$ from v. Call them u_1 and u_2. Let $e_u = u_1u_2$

In $L(G)$, e_v , e'_v and e forms a copy of C_3. We can view $L(G)$ as the graph got by identifying two of the vertices of this C_3 with two adjacent vertices of C_r and the third vertex with one of the pendant vertex of the path P_{p-1}. Then e_u will be at a distance $\lfloor \frac{r}{2} \rfloor$ from e_v and e'_v.

Let τ_1 and τ_2 denote the transit decompositions of G and $L(G)$ of minimum cardinality. Since both G and $L(G)$ have a copy C_r as an induced cycle, $C_r \in \tau_1, \tau_2$. We name these respectively as T and H. The majorized shortest paths in τ_1 are the two paths T_1, T_2 connecting u_1 and u_2 respectively to the pendant vertex of G. They are of length $\lfloor \frac{r}{2} \rfloor + p - 1$. When we consider the majorized paths in τ_2, they are the ones connecting the pendant vertex (if $p \neq 2$) to e_u via e_v and e'_v respectively. They also have length $\lfloor \frac{r}{2} \rfloor + 1 + p - 2$. Call them H_1 and H_2.
Define $\Psi : \tau_1 \to \tau_2$ by $\Psi(T_1) = H_1$, $\Psi(T_2) = H_2$ and $\Psi(T) = H$. Then Ψ is a transit isomorphism.

Remark 4.4. *The replacement of the odd cycle in Theorem 4.3 by an even cycle makes G and $L(G)$ non transit isomorphic. This leads to transit decompositions* *with same cardinalities, but the lengths of majorized shortest paths in τ_1 will be one more than those in τ_2.*

Theorem 4.5. *Let G be the bicyclic graph got by joining C_m with C_n by a path P_k, $k \geq 1$, where m and n are of different parities. Then $G \simeq_T L(G)$.*
Proof. Without loss of generality, assume m is odd and n is even. Consider two cases.
Case (i) when $k > 1$. Let $P_k : w_1w_2 \dots w_k$, with w_1 a vertex of C_m and w_k that of C_n. Let u_1 and u_2 be the vertices on C_m which are farthest from w_1, with $e_u = u_1u_2$. Let v_1 be the vertex on C_n farthest from w_k, with edges e_v and e'_v incident to v_1. Also denote $e_w = w_1w_2$ and $e_{w'} = w_{k-1}w_k$

Now consider $L(G)$. The edges incident with w_1 and w_k will form C_3 in $L(G)$, which will be connected by a path of length $k-2$ with e_w and $e_{w'}$ as its end vertices. [Note that when $k = 2$, the path will reduce to a vertex, in which case e_w and $e_{w'}$ coincides.] Thus $L(G)$ will be a graph with 4 cycles, isomorphic to C_m, C_3, C_3, C_n. For convenience let us name them C_m, C_3, C_3, C_n, itself. The edge of C_3 non incident to e_w and $e_{w'}$ in each of the C_3 will be part of C_m and C_n respectively.

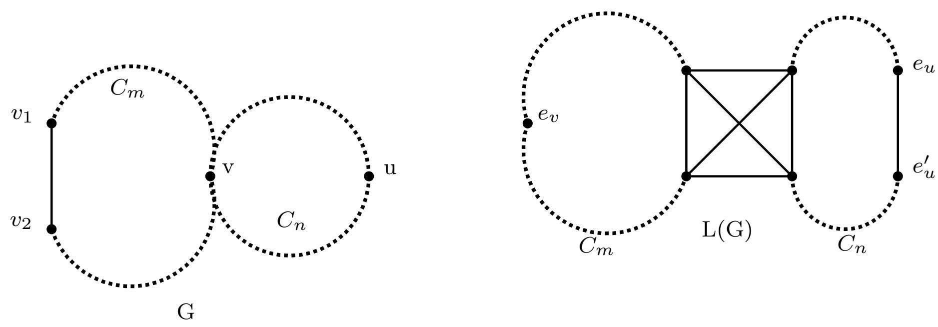

Figure 3: G and $L(G)$

Case(ii) $k = 1$. Here the line graph $L(G)$ of G can be viewed as the graph got by identifying an edge e_1 of K_4 with one of the edges of a copy of C_m and another edge e_2, non adjacent to e_1 with a copy of C_n, as shown in the Figure 3. For convenience, let us denote the copies of C_m and C_n by C_m and C_n itself.

Let τ_1 and τ_2 denote the transit decompositions of G and $L(G)$ of minimum cardinality. If $m \neq 3$, C_m and C_n will be in τ_1 and τ_2. (Otherwise only $C_n \in \tau_1, \tau_2$). The majorized paths in τ_1 are those connecting v_1 to u_1 and v_1 to u_2. There are two shortest paths in each case, each of length $\frac{n}{2} + k - 1 + \lfloor \frac{m}{2} \rfloor$. When we look at $L(G)$

the majorized paths are those connecting e_u to e_v and e_u to e'_v. Altogether they are 4 in number and of lengths $\frac{n}{2}+k-1+\lfloor\frac{m}{2}\rfloor$. Thus we can define a bijection from $\tau_1 \to \tau_2$, which can have the properties of a transit isomorphism. Thus $G \simeq_T L(G)$.

Remark 4.6. *In Theorem 4.5, when n and m are of same parities, it can easily be shown that G and $L(G)$ are not transit isomorphic.*

5. Constructing Transit Isomorphic Graphs

Example 1. Consider Figure 4. Here G and $L(G)$ are not transit isomorphic. But by a suitable manipulation in $L(G)$ we can create a new graph G', which is transit isomorphic to G. Form $L(G)$, then attach a pendant edge to the apex vertex of one of the C_3 to construct G'. Then $G \simeq_T G'$. The idea used here can be carried to a class of graphs, to form transit isomorphic graphs as discussed below.

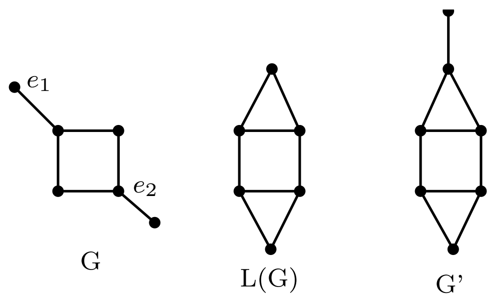

Figure 4: $G \simeq_T G'$

We form G by taking an even cycle and attaching paths P_n and P_m to its diametrically opposite vertices. From this G, form $L(G)$. If n or m is greater than two, $L(G)$ will have atleast one pendant vertex. Attaching an edge to one of these pendant vertex we get G' with $G \simeq_T G'$. If $n = m = 2$, $L(G)$ will have two copies of C_3. In this case attach an edge to the apex vertex of one of the C_3 to form G' transit isomorphic to G.

Example 2. Consider G in the Figure 5. It is formed by joining any two non-adjacent vertices of C_4 and by attaching an edge to a vertex of degree 3. G' is the graph got by attaching two pendant edges to any one of the vertices of C_3. From the figure we understand that $G \simeq_T G'$.

The same construction can be done using any even cycles C_{2n}. Join a vertex of C_{2n} to every non adjacent vertices of it, so that a C_3 is formed in every step. Now attach a pendant edge to the same vertex, thus increasing its degree to $2n$. This forms G. To construct the transit isomorphic graph of G, add as many pendant edges to one of the vertex of C_3, so that its degree is $2n$.

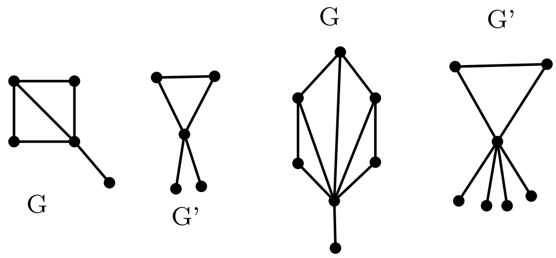

Figure 5: The case when $n = 2, 3$

6. Analysing Octane Isomers

In this section we give a summary of the study done in the structural graphs of octane isomers. As we know there are 18 octane isomers. Obviously, none of them are transit isomorphic. But a few of them shows some similarity in their transit decomposition. This similarity was also reflected in the values of their motor octane number. The significant observations are tabulated in Table 1 and Table 2

Sl.No	Octane Isomer	$\|\tau_i\|$	Paths isomorphic to the majorised shortest paths in τ_i	MON
1	2,2 dimethyl hexane	6	$P_3, P_3, P_6, P_3, P_6, P_6$	77.4
2	2,3 dimethyl hexane	6	$P_3, P_4, P_6, P_4, P_6, P_5$	78.9
3	2 methyl,3 ethyl pentane	6	$P_5, P_5, P_5, P_5, P_5, P_5$	88.1
4	3 methyl,3 ethyl pentane	6	$P_4, P_5, P_6, P_4, P_5, P_4$	88.7
5	2,2,3 trimethyl pentane	10	$P_3, P_3, P_4, P_5, P_3, P_4, P_5, P_4, P_5, P_4$	99.9
6	2,2,4 trimethyl pentane	10	$P_3, P_3, P_5, P_5, P_3, P_5, P_5, P_5, P_5, P_3$	100
7	2,3,3 trimethyl pentane	10	$P_4, P_4, P_5, P_5, P_3, P_4, P_4, P_4, P_4, P_3$	99.4

Table 1: Majorized shortest paths

In table 2 the (i,j)th entry is Y if τ_i and τ_j are of same cardinality and if there is a 1-1 correspondence between majorised shortest paths of them, whenever their length differs at most by one. Observing Table 1 and Table 2 the 7 isomers may be grouped into three. Group A: 1 and 2 ; Group B: 3 and 4 ; Group C: 5,6 and 7 Transit decomposition has the same cardinality in each group. In other words,

↓i,j→	1	2	3	4	5	6	7
1	Y	Y	N	N	N	N	N
2	Y	Y	N	N	N	N	N
3	N	N	Y	Y	N	N	N
4	N	N	Y	Y	N	N	N
5	N	N	N	N	Y	Y	Y
6	N	N	N	N	Y	Y	Y
7	N	N	N	N	Y	Y	Y

Table 2: Majorized shortest paths $\tau_i \longleftrightarrow \tau_j$

there is a bijection. Majorised shortest paths agree in most cases, and when they don't, they differ by at most one edge.

Observing the corresponding values of MON, we can see that this grouping makes sense.

It is easier and simpler to find τ_{min} for a molecular graph than to calculate the transit index for it. Thus, transit isomorphism facilitates a means of classifying chemical isomers according to their motor octane number.

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