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# Application of concepts of graph theory to determine the difference between some cyclic organic chemical compounds.

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**A R T I C L E I N F O**

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**A B S T R A C T**

In this paper, we use the concept of paths in graph theory in order to distinguish some cyclic aliphatic organic chemical compounds (13 compounds) and determine the difference among them. By increasing the length of the path from ($p_0$) to $p_4$ ($p_0 \rightarrow p_4$) divided into four cases, we which to study the nature of internal structural of the compound according to the length of each case and identify the complete structural spectrum (CSS) for each compound. Then we find the index of complexity of these compounds to find the number of classes for the set of compounds, where the increase in the number of classes leads to increase the accuracy of distinguish, which we got in the fourth case because the number of classes equals the number of elements of the set of compounds so that for each compound in this case, the properties differ from other compounds. Thus, increasing the length of the path means an increase in the description of the nature of the internal structural of the compound and we also wish to determine additional properties for each compound from which to distinguish it compared with the rest of the compounds.

**Introduction:**

As is well known applied mathematics, there is the possibility of finding some of the properties that can be used in various applications in the branches of other sciences and in view of the necessity of these applications, the paper comes in touch with a series of researchs presented in this filed to study the possibility of these applications and diligent in developed by find mathematical properties. This has been talked in previous studies [4], [5], [6] that talked the discrimination mechanism some of graphs where we can study discrimination using several properties and each property has results and applications.

In the field of chemistry, there are chemical and physical properties of the compounds as possible on this basis classification or distinction of these compounds as required for specific study in addition to the possibility of finding mathematical properties enables us to distinguish these compounds and determine the difference between them where indicated a lot of studies in this filed about the possibility of the application of concepts of graph theory to diagnose and distinguish some chemical compounds as there are a lot of books and papers that called under the headings apply mathematical concepts in chemistry, for example application of graph theory in chemistry [4] and a series of chemical mathematics [7] as well as mathematical concepts in organic chemistry [8] and other books and literature, which contributed much to the advancement of research chemistry and for the purpose to enrich the knowledge base in this area, we study method of distinguish of graphs which are used to distinguish chemical compounds depending on the nature of the internal structure of these compounds and the possibility of identifying complete structural spectrum(CSS) these

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compounds according to what is selected from the concepts of graph theory.

**Distinguish of graphs:**

There are a lot of properties in the theory of graphs used to distinguish the graphs and for each property results and the accuracy in distinguishing different from other properties. For example, we can distinguish the graphs on the basis of the number of vertices for each graph, but this property become ineffective if equal the number of vertices of all graphs as well as for a number of edges and degrees of vertices and other properties so it was necessary to look for other properties to help more effectively in distinguish of graphs and depending on the nature of the internal structure of the graph and the possibility of identifying complete structural spectrum(CSS) of graph by defined concept, for example, determine the complete structural spectrum of graph if these concepts are chains or paths with different lengths so that each graph have set of properties help to distinguish compared with other graphs and the possibility of finding number of the classes to a set of graphs and each class contains some graphs have the same properties [5].

**Chemical compounds to be indistinguishable:**

We chose a set of cyclic aliphatic organic compounds (tetradecahydrophenanthrene), consisting of 23 carbon atoms and 25 bond among these atoms and denominations as shown below in Fig. 1.

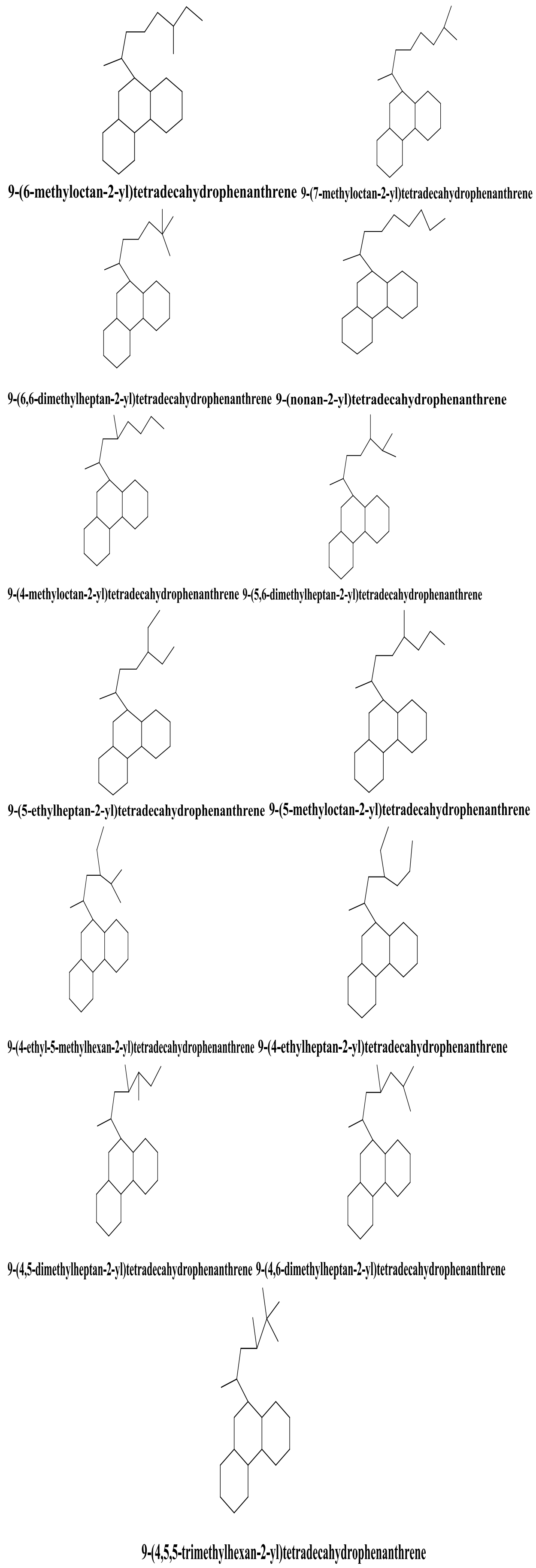



**Fig. 1 : (cyclic organic compounds)**

**9-(nonan-2-yl)tetradecahydrophenanthrene**
**9-(5-methyloctan-2-yl)tetradecahydrophenanthrene**
**9-(4-methyloctan-2-yl)tetradecahydrophenanthrene**
**9-(4-ethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(6,6-dimethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(6-methyloctan-2-yl)tetradecahydrophenanthrene**
**9-(4,5-dimethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(5,6-dimethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(4,5,5-trimethylhexan-2-yl)tetradecahydrophenanthrene**
**9-(5-ethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(4-ethyl-5-methylhexan-2-yl)tetradecahydrophenanthrene**
**9-(4,6-dimethylheptan-2-yl)tetradecahydrophenanthrene**
**9-(7-methyloctan-2-yl)tetradecahydrophenanthrene**

**Representation of compounds:**

Before studying these compounds we wish to represent them in the form of graphs, each graph consists of 23 vertices and 25 edges as shown in Fig. 2 below.

A={$G_1$,$G_2$,…,$G_{13}$} set of all graphs

$G_i$=($V_i$,$E_i$)

V ($G_i$) = {$v_1$,$v_2$,…,$v_{23}$}, set of vertices

E($G_i$)={$e_1$,$e_2$,$e_3$,…,$e_{25}$ |e={u,v}∋ u,v ϵ V($G_i$)}, set of edges

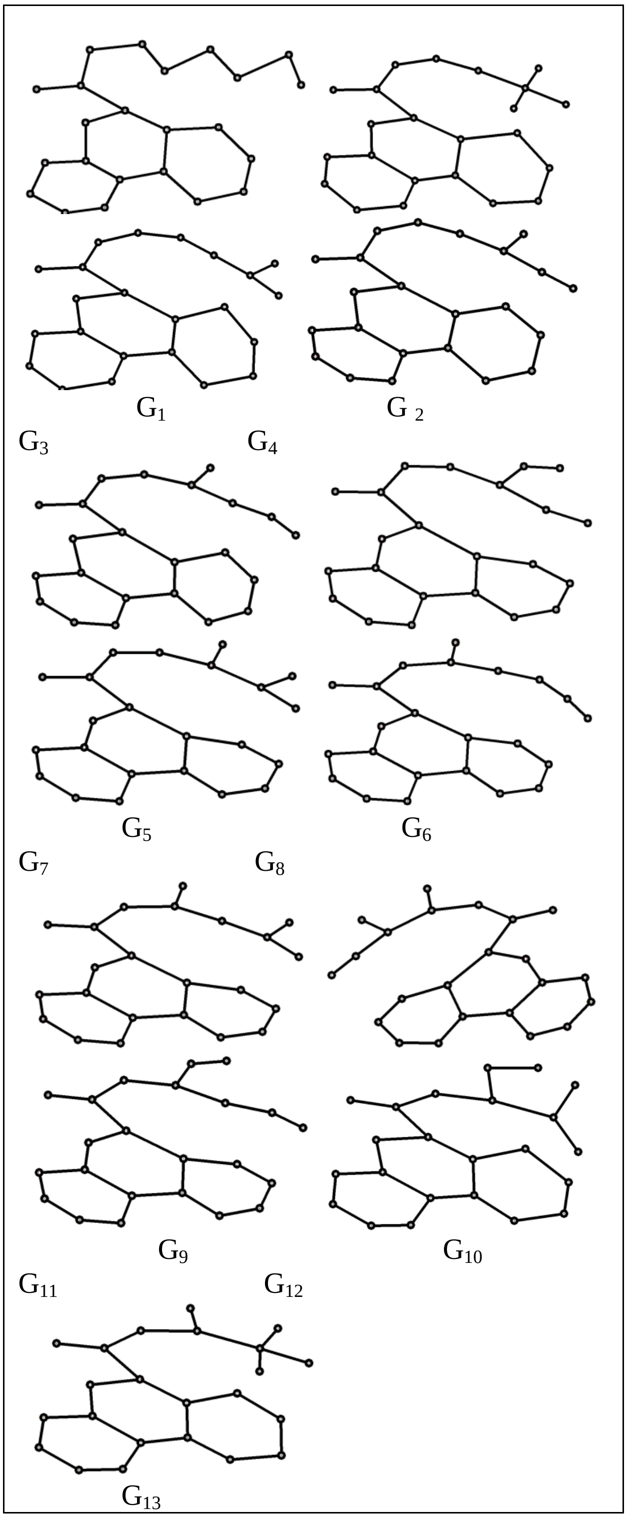



**Fig. 2: (cyclic graphs)**

After representation in the form of graphs using the concept of path(P), we define the complete structural Spectrum(CSS) of these compounds depending on the length of the path($p_0$,$p_1$,$p_2$,…,$p_i$)(i ϵ N). Then we calculate the index of complexity (IC)(According to the eq.(1) below) of these structures and the index of complexity of every compound to be distinguished by the index of complexity where IC(v)=1 and IC(e)=3[9].

For example, choosing the path ($p_0$) means identifying subgraph(f) corresponding to it in the graph and studying the installation of this part within the graph (Determining the shape and parts of this part and the number of every part within the graph) (CSS). Then determine the index of complexity of this part and the index of complexity of the graph where the Increase in the length of the path($p_0$,$p_0 \to p_1$,$p_0 \to p_2$,…) represents an increase of the size of the corresponding subgraph, as shown in figure (3).

$$IC(G_1) = \sum_{i=1}^{n} w_i \cdot IC(f_i) \qquad \dots (1)$$

Where IC ($p_0$) =1 and IC ($p_1$) =3

$f_i$ subgraph

$w_i$, the number of subgraph in G

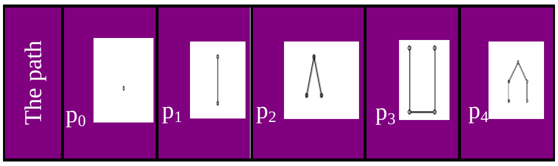



Fig.3: (some lengths of path)

Where $p_0 \to f_1$, $p_1 \to f_2$, $p_2 \to f_3$, …

**Distinguish of compounds:**

Since the distinction of a set of graphs is represented by the number of classes of graphs that we get after a process of distinguish and that the accuracy of distinguish (According to the eq.(2) (below )increases with the increases the number of classes [6],thus the distinguish process of these graphs when the path length is 0( $p_0$) does not give any class except the same set of these graphs because all graphs have the same number of vertices (carbon atoms) also when the path length is 1 ($P_1$), because all of these graphs have the same number of edges (bounds among the carbon atoms), as will explained below, where the first case when the path length is 1 ($P_1$).

$$M/N = £ \qquad \dots(2)$$

Where **N** the number of the classes, **M** the number of compounds.

**The first case:**

We take the path $p_1$ ($p_0 \to p_1$) and determine (CSS)(Fig.No.4) of the graphs and find IC by (1) as follows in table.1 :

**For $G_1$**

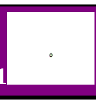
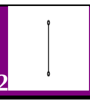
| Complete Structural Spectrum (CSS) | Subgraphs | f1  | f2  |
|---|---|---|---|
| | Number of subgraph in $G_1$ | 23 | 25 |

**Fig.No.4 (CSS of G1 by p1)**

$$IC(G_1) = \sum_{i=1}^{n} w_i \cdot IC(f_i)$$

Where IC ($p_0$) =1 and IC ($p_1$) =3

$IC(G_1) = w_1 \cdot IC(f_1) + w_2 \cdot IC(f_2) = 98$

**For all graphs**

| No. | number of $f_i$ in G | CSS | IC (G) |
|---|---|---|---|
| 1 | 48 | ( 23 25) | 98 |
| 2 | 48 | ( 23 25) | 98 |
| 3 | 48 | ( 23 25) | 98 |
| 4 | 48 | ( 23 25) | 98 |
| 5 | 48 | ( 23 25) | 98 |
| 6 | 48 | ( 23 25) | 98 |
| 7 | 48 | ( 23 25) | 98 |
| 8 | 48 | ( 23 25) | 98 |
| 9 | 48 | ( 23 25) | 98 |
| 10 | 48 | ( 23 25) | 98 |
| 11 | 48 | ( 23 25) | 98 |
| 12 | 48 | ( 23 25) | 98 |
| 13 | 48 | ( 23 25) | 98 |

**Table 1(IC for all graphs by p1)**

Now note that the number of classes is 1 because all the graphs in this case have the same IC and that the accuracy of distinguish are as follows:

£=N/M

=1/13

=0.076

**The Second case:**

Increasing the length of the path to $p_2$ ($p_0 \to p_2$), we will get the following results:

**For G1**

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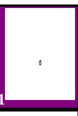
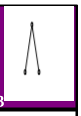
| **Complete Structural Spectrum (CSS)** | **Subgraphs** | $f_1$  | $f_2$  | $f_3$  |
|---|---|---|---|---|
| | **Number of subgraph in G1** | **23** | **25** | **33** |

**Fig.No.5 (CSS by p2)**

**Now we find all subgraphs of f3.**

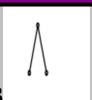
| **subgraph** | **$f_1$** | **$f_2$** |
|---|---|---|
|  **f3** |  |  |
| **Number of subgraph in f3** | **3** | **2** |

**Fig.6: (CSS of f3 by p2)**

Now by (1) we find IC ($G_1$)

$IC(f_3)=w_1 \cdot IC(f_1) + w_2 \cdot IC(f_2) =9$

IC ($G_1$) $=w_1 \cdot IC(f_1) + w_2 \cdot IC(f_2) + w_3 \cdot IC(f_3) =395$

**For all graphs**

| **No.** | **number of $f_i$ in G** | **CSS** | **IC(G)** |
|---|---|---|---|
| **1** | **81** | **( 23 25 33)** | **395** |
| **2** | **84** | **( 23 25 36)** | **422** |
| **3** | **82** | **( 23 25 34)** | **404** |
| **4** | **82** | **( 23 25 34)** | **404** |
| **5** | **82** | **( 23 25 34)** | **404** |
| **6** | **82** | **( 23 25 34)** | **404** |
| **7** | **83** | **( 23 25 35)** | **413** |
| **8** | **82** | **( 23 25 34)** | **404** |
| **9** | **83** | **( 23 25 35)** | **413** |
| **10** | **83** | **( 23 25 35)** | **413** |
| **11** | **82** | **( 23 25 34)** | **404** |
| **12** | **83** | **( 23 25 35)** | **413** |
| **13** | **85** | **( 23 25 37)** | **431** |

**Table .2: (IC for all graphs by p2)**

In this case, we note that the number of classes is 5 and the accuracy of distinguish increases for the first case.

$Class_1= \{G_1\}$
$Class_2= \{G_2\}$
$Class_3= \{G_3,G_4,G_5,G_6,G_8,G_{11}\}$
$Class_4= \{G_7,G_9,G_{10},G_{12}\}$
$Class_5= \{G_{13}\}$
£=N/M
=5/13
=0.384

**The Third case:**

Increasing the length of the path to $p_3$ ($p_0 \rightarrow p_3$)

**For G1**

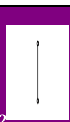
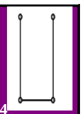
| **Complete Structural Spectrum (CSS)** | **Subgraphs** | $f_1$  | $f_2$  | $f_3$  | $f_4$  |
|---|---|---|---|---|---|
| | **Number of subgraph in $G_1$** | **23** | **25** | **33** | **45** |

**Fig. 7: (CSS of G1 by p3)**

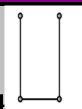
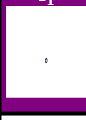
| **subgraph** | **$f_1$** | **$f_2$** | **$f_3$** |
|---|---|---|---|
|  **f4** |  |  |  |
| **Number of subgraph in f4** | **4** | **3** | **2** |

**Fig.8: (CSS of f4 by p3)**

By (1) IC ($G_1$) =1790

**For all graphs**

| **No.** | **number of $f_i$ in G** | **CSS** | **IC(G)** |
|---|---|---|---|
| **1** | **126** | **( 23 25 33 45)** | **1790** |
| **2** | **129** | **( 23 25 36 45)** | **1817** |
| **3** | **127** | **( 23 25 34 45)** | **1799** |
| **4** | **128** | **( 23 25 34 46)** | **1830** |
| **5** | **128** | **( 23 25 34 46)** | **1830** |
| **6** | **129** | **( 23 25 34 47)** | **1861** |
| **7** | **130** | **( 23 25 35 47)** | **1870** |
| **8** | **128** | **( 23 25 34 46)** | **1830** |
| **9** | **129** | **( 23 25 35 46)** | **1839** |
| **10** | **131** | **( 23 25 35 48)** | **1901** |
| **11** | **129** | **( 23 25 34 47)** | **1861** |
| **12** | **131** | **( 23 25 35 48)** | **1901** |
| **13** | **133** | **( 23 25 37 48)** | **1919** |

**Table 3:(IC for all graphs by p3)**

The results above show an increase in the accuracy of discrimination by increasing the number of classes to 9.

$Class_1=\{G_1\}$
$Class_2=\{G_2\}$
$Class_3=\{G_3,\}$
$Class_4=\{G_4,G_5,G_8\}$
$Class_5=\{G_6 ,G_{11}\}$
$Class_6=\{G_7\}$
$Class_7=\{G_9\}$
$Class_8=\{G_{10},G_{12}\}$
$Class_9=\{G_{13}\}$
£=N/M
=9/13
=0.692

We note an increase in distinguishing accuracy because of the different nature of the internal structure of these compounds as the accuracy of distinguish approaching to one up length the path.

**The fourth case:**

Increasing the length of the path to $p_4$ ($p_0 \rightarrow p_4$).

**For G1**

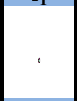
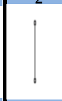
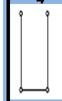
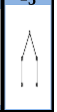
| Complete Structural Spectrum (CSS) | Subgraphs | $f_1$  | $f_2$  | $f_3$  | $f_4$  | $f_5$  |
|---|---|---|---|---|---|---|
| | Number of subgraph in $G_1$ (CSS) | 23 | 25 | 33 | 45 | 61 |

**Fig.9 : (CSS of G1 by p4)**

In the same way as in the third case, we get all the subgraphs of $f_5$.

**For all graphs**

| No. | number of $f_i$ in G | CSS | IC(G) |
|---|---|---|---|
| 1 | 187 | ( 23 25 33 45 61) | 8256 |
| 2 | 190 | ( 23 25 36 45 61) | 8283 |
| 3 | 188 | ( 23 25 34 45 61) | 8265 |
| 4 | 189 | ( 23 25 34 46 61) | 8296 |
| 5 | 190 | ( 23 25 34 46 62) | 8402 |
| 6 | 191 | ( 23 25 34 47 62) | 8433 |
| 7 | 191 | ( 23 25 35 47 61) | 8336 |
| 8 | 191 | ( 23 25 34 46 63) | 8508 |
| 9 | 193 | ( 23 25 35 46 64) | 8623 |
| 10 | 194 | ( 23 25 35 48 63) | 8579 |
| 11 | 193 | ( 23 25 34 47 64) | 8645 |
| 12 | 195 | ( 23 25 35 48 64) | 8685 |
| 13 | 195 | ( 23 25 37 48 62) | 8491 |

**Table.4: (IC for all graphs by p4)**

In this case, the accuracy of distinguishing is equal to one because the number of classes is 13.

£=N/M

=13/13

1

It is possible to represent the results we have obtained for the last case through the following graphical representation which shows the IC and the number of subgraphs of each graph depending on the length of the path chosen for this case.

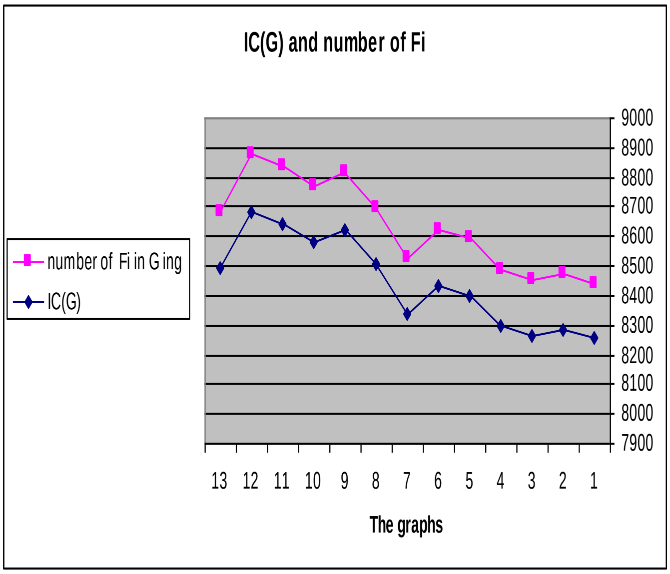



**Fig.10: (Graphical representation of the results of the fourth case)**

**Conclusions:**

It is possible to study these cases through in depth exploration of the nature of the internal structure of the compound by the concept that we choose from the concepts of the graph theory. That is to say, results of distinguish depend on the shape and size of the part and the nature of the internal structure of the compound on the basis of this part chosen in this study. This is what we focus on our study to find other properties and develop methods of compounds distinguish by adding properties that help support scientific studies, which it so clear from the results we have obtained. In the first case, when the path length was ($p_1$), the number of classes was 1 and the accuracy of distinguish (0.076).In the second case, when the length increased to ($p_2$), the number of classes was (5) and the accuracy was (0.384),while In the third case, when the length increased to ($p_3$), the number of classes was (9) and the accuracy was (0.692).In the fourth case, when the length increased to ($p_4$), the number of classes became(13) and the accuracy became (1), i.e. these compounds might completely distinguishable because the number of classes was equal to the number of elements in the set of compounds in such a way that for each compound in this case has properties that differ from other compounds. Thus, increase in the path length means an increase in the description of the internal structure of the compound and the the identification of its additional properties.

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# تطبيق مفاهيم نظرية البيانات لتحديد الاختلاف بين بعض المركبات الكيميائية العضوية الحلقية.

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**الخلاصة :**

تضمن موضوع البحث تمييز لمجموعة من المركبات العضوية الحلقية الالفاتية وعددها 13 مركب حيث استخدمنا مفهوم الدروب في نظرية البيانات لدراسة طبيعة التركيب الداخلي لكل مركب وتحديد طيف تراكيب المركبات الكامل وعلى أربعة مراحل وبأطوال مختلفة للدروب من (1) إلى (4) وتحديد درجة تعقد كل مركب لكل مرحلة محددة يتم من خلالها دراسة طبيعة التركيب الداخلي للمركب حسب الطول الذي تم اختياره ومن ثم تحديد دقة تمييز هذه المركبات على أساس زيادة عدد الصفوف التي نحصل عليها في كل مرحلة وفي المرحلة الأخيرة وبطول (4) كان عدد الصفوف مساويا لعدد المركبات أي تمييز كل مركب عن المركبات الأخرى ، أي إن زيادة طول الدرب تعني زيادة في الوصف لطبيعة التركيب الداخلي للمركب وبالتالي إضافة خصائص إضافية نستطيع من خلالها تمييز كل مركب بالمقارنة مع المركبات الأخرى.