Journal of Education and Science (ISSN 1812-125X)

www.edusj.uomosul.edu.iq

Application of Partition Theory to Calculate the Chemical Displacement of the Nuclei of the Carbon 13 Atom of Cyclohexane Derivatives II

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Article information

Article history:
Received: January 19, 2025
Accepted: March 04, 2025
Available online: April 01, 2025

Keywords:
Partition Theory
e-abacus diagram
Cyclohexane Derivatives

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Abstract

This research is a generalization of the first part, which has the same title, which was a question from one of the evaluators: How can we develop this part? Thus, how can we, in the event of development, exploit partition theory, specifically the *e*-abacus diagram, to solve this generalization? Especially since it is the first time that the idea of what is more than (two things) used primarily in the *e*-abacus diagram is used. A proposal was made to use the two- stories *e*-abacus diagram for the first time under very specific and specific conditions, which is completely useful later to become multi-story. The method that will be presented will be suitable for any chemical model that can use LCAO and contains numerical variables that start from zero and are not negative, because it will be, according to our belief and according to what we will present, a completely suitable method for its application through the abacus diagram.

DOI: 10.33899/edusj.2025.156766.1530,

1. Introduction

Altaie, Mahmood and Alhyali [1] presented an exclusive study on the relationship between cyclohexane, *e*-abacus diagram and the results were in one direction, which is to find a value for the partition for each type according to the rule (the two things are the knot and the space or possible one and zero). Here the study will focus on the cyclohexene compound and link physical chemistry to the partition theory in a new way based on the rule (LCAO to calculate the number of carbon atoms) where we will number the carbon atoms and the methyl groups added from the closed sticky branching as in Figure 1:

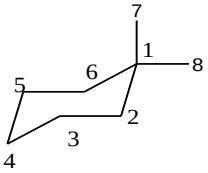


Figure 1

Through applying the linear combination of Atomic orbitals to calculate the number of Carbon Atoms (**LCAO No. of Carbon**) [2]. It depends on the concept of creating a matrix whose capacity is the number of vertices of the compound. We symbolize the rows with the symbol C_r, where (r) represents the head number, and as for the columns (which represent the number of carbon atoms), we will symbolize the column primary with the number one(that is the carbon atomC_r is bonded to a single carbon

atom), symbolize the secondary column with the number two (that is theC_r is bonded to a double linked carbon atom), the same applies to the tertiary column, which we refer to as three etc. (LCAO No. of Carbon) for Figure (1) will be as follows:

	1	2	3	4	5	6	7	8
C_1	2	2	0	0	0	0	0	0
C_2	0	1	0	1	0	0	0	0
C_3	0	2	0	0	0	0	0	0
C_4	0	2	0	0	0	0	0	0
C_5	0	2	0	0	0	0	0	0
C_6	0	1	0	1	0	0	0	0
C_7	0	0	0	1	0	0	0	0
C_8	0	0	0	1	0	0	0	0

Figure 2. LCAO No. of Carbon about Figure 1

2. *e*. Abacus Diagram

In this section, we will delve into mathematics. Let t be a positive integer number the sequence $\mu = (\mu_1, \mu_2, \dots, \mu_n)$ is called a partition of t if $(|\mu| = \sum_{j=1}^{n} \mu_j = t)$ & $(\mu_j = \mu_{j+1}, \forall j \geq 1)$. Now defining $\beta_i = \mu_i + b - i, 1 \leq i \leq b$. The set $\{\beta_1, \beta_2, \dots, \beta_b\}$ is said to be the set of β – numbers for μ. Let e be a positive integer number greater than or equal to 2, we can represent β – numbers by (main diagram or e -abacus diagram) see [3-4] (Table 3). Where every β will be represented by (●) and else that by (-).

Table 1. e -Abacus Diagram

Runner 1	**Runner 2**	**……**	**Runner e**
0	**1**	**……**	**$e-1$**
e	**$e+1$**	**……**	**$2e-1$**
2e	**$2e+1$**	**……**	**$3e-1$**
:	**:**	**:**	**:**

For example, if $\mu = (4, 3, 2, 2, 1)$ and $b = 5$ the β – numbers at e = 2, 3, 4 it will be as follows:

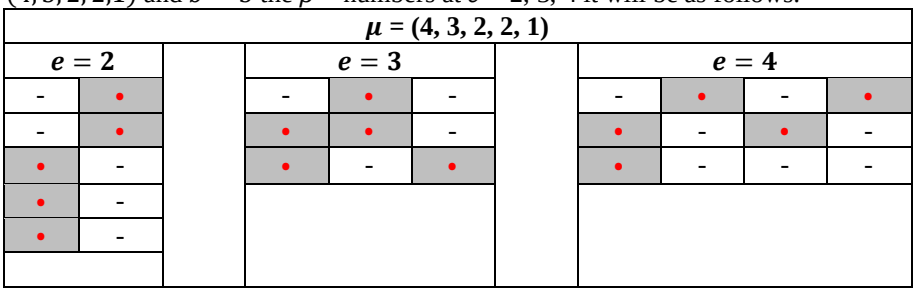


Figure 3. e-abacus diagram of μ = (4, 3, 2, 2, 1)

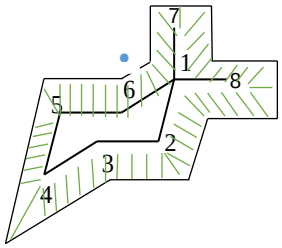
From the diagram, we notice that we only have ● and -, so we consider that every (1 is •) and (0 is -) [5], we also need the first position to always be (-) [6], it is quite clear that any LCAO No. of carbon would be quite easy to form as an e-abacus diagram but the opposite is not true because the possibility of it forming a scientific chemical form or basically it does not actually exist on the ground. In order to provide a solution to the dilemma we are facing, we suggest that we have a (hotel) and there is definitely an external courtyard (we will give it a green color, and we will be replaced by 0 with the number C_r , [1]) and we add the main door to the hotel entrance (let it be blue), and now we will see the problems that we will face, which are:

1. In the e -Abacus diagram we have ● and – only while in (LCAO NO. of Carbon) we have 0, 1 and 2. How will be dealt with 2?
2. We have different directions. When methyl groups are added to the Cyclohexane compound, these groups may have two different directions and in the same location, so how will they be treated?

It was suggested that every (room) occupied on the ground floor is matched by (1) and the unoccupied rooms are matched by (0) and then the room that was originally occupied on the ground floor exclusively (possibly) is occupied on the first floor and here also this room will be matched by (we indicate the occupied rooms on both floors as Ï and in e -abacus

diagram we color the entire cell yellow), and in this way we can completely solve the problem of the existence of the number (2) in our case that is studied within the model in Figure 1. To solve the second problem, we will draw a red arrow in the location to indicate the direction of the methyl group. In Figure (1), we will draw an arrow in the location (C_1,1) in the proposed ground floor plan its direction is to the top and in the proposed first floor plan its direction is to the right. Thus, the (LCAO* No. of Carbon) according to the method proposed for Figure 1, will be:

1,1- Di methyl Cyclohexane



LCAO* No. of Carbon

	0	0	0	0	0	0	0	0	0
c_1	0	2	2	0	0	0	0	0	0
c_2	0	0	1	0	1	0	0	0	0
c_3	0	0	2	0	0	0	0	0	0
c_4	0	0	2	0	0	0	0	0	0
c_5	0	0	2	0	0	0	0	0	0
c_6	0	0	1	0	1	0	0	0	0
c_7	0	0	0	0	1	0	0	0	0
c_8	0	0	0	0	1	0	0	0	0

Proposed ground floor plan

0	0	0	0	0	0	0	0	0
0	1↑	1	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0

Proposed first floor plan

0	0	0	0	0	0	0	0	0
0	1→	1	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0

Merging the two floors

0	0	0	0	0	0	0	0	0
0	1̈	1̈	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0
0	0	1̈	0	0	0	0	0	0
0	0	1̈	0	0	0	0	0	0
0	0	1̈	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0
0	0	0	0	1	0	0	0	0

***e* -Abacus Diagram**

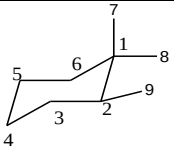
(66, 58, 50, 49, 4̈1, 3̈3, 2̈5, 19, 18, 1̈0, 1̈0 ↑→)

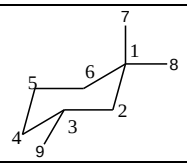
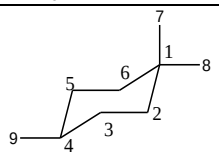
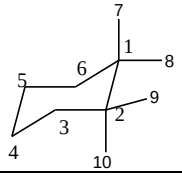
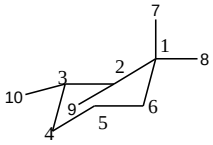
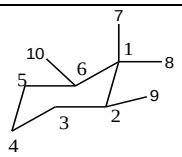
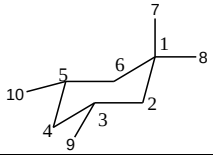
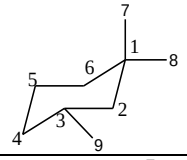
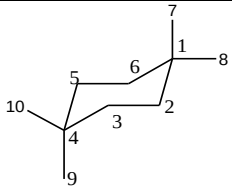
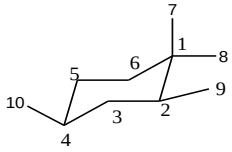
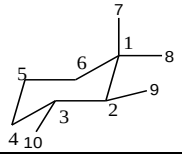
-	-	-	-	-	-	-	-	-
-	•↑→	•	-	-	-	-	-	-
-	-	•	-	•	-	-	-	-
-	-	•	-	-	-	-	-	-
-	-	•	-	-	-	-	-	-
-	-	•	-	-	-	-	-	-
-	-	•	-	•	-	-	-	-
-	-	-	-	•	-	-	-	-
-	-	-	-	•	-	-	-	-

Figure 4. All cases (hotel)

In exactly the same way we were able to find everything related to this as follows:

Table 2. Partition of Methyl Cyclohexane Substitutions

Name of Type	Symbol	*e* -Abacus Diagram
1, 1, 2- Tri Methyl Cyclohexane		(79, 71, 62, 53, 52, 4̈3, 3̈4, 26, 26, 19, 18, 18↗, 11, 11, 1̈1 ↑→)

1, 1, 3- Tri Methyl Cyclohexane		(80, 72, 63, 54, 53, 44, 36, 36, 27, 27 , 21, 21, 11,11 ↑→)
1, 1, 4- Tri Methyl Cyclohexane		(79, 71, 62, 53, 52, 44, 44, 35, 35←, 28, 28, 21, 20, 11, 11 ↑→)
1, 1, 2, 2- Tetra Methyl Cyclohexane		(99, 89, 79, 69, 59, 58, 48, 38, 30, 29, 21, 20, 20 ↓↗, 13, 12, 12 ↑→)
1, 1, 2- Trans- 3- Tetra Methyl Cyclohexane		(96, 86, 77, 67, 57, 56, 46, 37, 37, 28, 28, 28↙, 21, 21, 20↙, 12, 12, 12 ↑→)
1, 1, 2- Cis- 6- Tetra Methyl Cyclohexane		(97, 87, 78, 68, 58, 57, 57↖, 49, 49, 39, 30, 30, 22, 21, 21↗, 13, 12 ↑→)
1, 1, 3- Cis- 5- Tetra Methyl Cyclohexane		(99, 89, 80, 70, 60, 60, 49, 49↙, 41, 30, 30↙, 23, 23, 12, 12 ↑→)
1, 1, 3- Tri Methyl Cyclohexane		(80, 72, 63, 54, 53, 44, 36, 36, 27, 27↘ , 21, 21, 11,11 ↑→)
1, 1, 4, 4- Tetra Methyl Cyclohexane		(99, 89, 79, 69, 59, 58, 50, 49, 39, 39 ↓↖ , 32, 31, 23, 22, 12, 12 ↑→)
1, 1, 2- Cis- 4- Tetra Methyl Cyclohexane		(97, 87, 78, 68, 58, 57, 48, 48, 38 , 38↖ , 30, 21, 20, 20↗,12, 12, 12 ↑→)
1, 1, 2- Trans- 3- Tetra Methyl Cyclohexane		(96, 86, 77, 67, 57, 56, 46, 37, 37, 28, 28, 28↙, 21, 21, 20↗,12, 12, 12 ↑→)

3. Delete Unoccupied Columns

In the (LCAO No. of Carbon) matrix, we noticed that there are columns whose cells are all zeros (starting from column 5 to the end), meaning that they are not occupied, and these zeros have a significant impact when reading, so we deleted these zeros (after making sure that they will not affect the chemical compounds), and it appears to us a completely different new reading.

Table 3. Partition of Methyl Cyclohexane Substitutions by Delete Unoccupied Columns

Name of Type	*e* -Abacus Diagram
1, 1- Di Methyl Cyclohexane	(34, 30, 26, 25, $\ddot{2}\dot{1}$, $\ddot{1}\dot{7}$, $\ddot{1}\dot{3}$, 11, 10, 6, $\ddot{6}$ ↑→)
1, 1, 2- Tri Methyl Cyclohexane	(34, 31, 27, 23, 22, $\ddot{1}\dot{8}$, $\ddot{1}\dot{4}$, 11, 11, 9, 8, 8↗, 6, 6, $\ddot{6}$ ↑→)
1, 1, 3- Tri Methyl Cyclohexane	(35, 32, 28, 24, 23, $\ddot{1}\dot{9}$, 16, 16, $\ddot{1}\dot{2}$, 12↙, 11, 11, $\ddot{6}$, $\ddot{6}$ ↑→)
1, 1, 4- Tri Methyl Cyclohexane	(34, 31, 27, 23, 22, 19, 19, $\ddot{1}\ddot{5}$, 15←, 13, 13, 11, 10, $\ddot{6}$, $\ddot{6}$ ↑→)
1, 1, 2, 2- Tetra Methyl Cyclohexane	(39, 35, 31, 27, 23, 22, $\ddot{1}\ddot{8}$, $\ddot{1}\ddot{4}$, 12, 11, 9, 8, $\ddot{8}$ ↓↗ ,7, 6, $\ddot{6}$ ↑→)
1, 1, 2- Trans- 3- Tetra Methyl Cyclohexane	(36, 32, 29, 25, 21, 20, $\ddot{1}\ddot{6}$, 13, 13, 10, 10, 10↙, 9, 9, 8↙, 6, 6, $\ddot{6}$ ↑→)
1, 1, 2- Cis- 6- Tetra Methyl Cyclohexane	(37, 33, 30, 26, 22, 21, 21↖, 19, 19, $\ddot{1}\ddot{5}$, 12, 12, 10, 9, 9↗, $\ddot{7}$, $\ddot{6}$ ↑→)
1, 1, 3- Cis- 5- Tetra Methyl Cyclohexane	(39, 35, 32, 28, 24, 24, $\ddot{1}\dot{9}$, 19↙, $\ddot{1}\dot{7}$, $\ddot{1}\dot{2}$, 12↙, 11, 11, $\ddot{6}$, $\ddot{6}$ ↑→)
1, 1, 3- Tri Methyl Cyclohexane	(35, 32, 28, 24, 23, $\ddot{1}\dot{9}$, 16, 16, $\ddot{1}\dot{2}$, 12↘, 11, 11, $\ddot{6}$, $\ddot{6}$ ↑→)
1, 1, 4, 4- Tetra Methyl Cyclohexane	(39, 35, 31, 27, 23, 22, 20, 19, $\ddot{1}\ddot{5}$, $\ddot{1}\ddot{5}$ ↓↖ ,14, 13, 11, 10, $\ddot{6}$, $\ddot{6}$ ↑→)
1, 1, 2- Cis- 4- Tetra Methyl Cyclohexane	(37, 33, 30, 26, 22, 21, 18, 18, $\ddot{1}\ddot{4}$, 14↖, $\ddot{1}\ddot{2}$, 9, 8, 8↗, 6, 6, $\ddot{6}$ ↑→)
1, 1, 2- Trans- 3- Tetra Methyl Cyclohexane	(36, 32, 29, 25, 21, 20, $\ddot{1}\ddot{6}$, 13, 13, 10, 10, 10↙, 9, 9, 8↗, 6, 6, $\ddot{6}$ ↑→)

4. Conclusion

i. The idea of (the hotel) solved a complex problem, which is the presence of two in the matrix.
ii. We can generalize this idea and apply it to numbers greater than two.
iii. It is later possible to take any chemical compound consisting of more than two elements.
iv. The possibility of applying part or all of what was mentioned in this research with the ideas in [7-9], especially in the possibility of isolation or division and with the presence of certain movements specific to the diagram.

5. Acknowledgements

When scientific ideas come in the field of scientific cooperation between scientific departments, we extend our gratitude to the deanship of the College of Education for Pure Sciences at the University of Mosul for providing all assistance in completing this research.

6. References

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تطبيق نظرية التجزئة لحساب الإزاحة الكيميائية لنوى ذرة الكربون 13 لمشتقات الهكسان الحلقي II

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الخلاصة:

هذا البحث هو تعميم للجزء الأول والذي يحمل نفس العنوان والذي كان عبارة عن سؤال من أحد المحكمين وهو كيف نستطيع تطوير هذا الجزء وبالتالي كيف نستطيع في حالة التطوير استغلال نظرية التجزئة وتحديدا مخطط المعداد من النمط - e لحل هذا التعميم خاصة وأنها المرة الأولى التي تستخدم فيها فكرة ما هو أكثر من (شيئين) المستخدمة بشكل أساسي في مخطط المعداد من النمط - e. حيث تم تقديم اقتراح تم بموجبه ولاول مرة استخدام المخطط المعداد من النمط – e ذو الطابقين وفق شروط معينة وخاصة جدا وهو ينفع تماما لاحقا ليصبح متعدد الطبقات. ان الطريقة التي ستقدم ستكون قابلة للتنفيذ لاي نموذج كيميائي ممكن ان يستخدم LCAO وفيه من المتغيرات العددية التي تبدا من الصفر ولا تكون سالبة, لانها ستكون حسب اعتقادنا ووفق ما سنقدمه من طريقة مناسبة تماما لتطبيقها من خلال المخطط المعداد. ولأن هذا النموذج الذي تم اقتراحه نجح في تنفيذ فكرتهُ كيميائيا فإننا نعتقد أنه ليس من الصعب تحقيقها مع أي تطبيق علمي.