

Applications of Cayley Graphs

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Abstract: In 1736, the famous Swiss mathematician Euler proposed graph theory. Graph theory was originally developed to solve the difficult Königsberg Bridge problem in eastern Germany. Twenty years later, Arthur Cayley (1821-1895) also used the concept of trees to describe the chemical problem of hydrocarbons (Heri Sukarno). Nowadays, graph theory is used in geography, physics, electronics, information processing, architectural design, and other fields. Recently, the atomic track and the Hamiltonian path have been particularly prominent in applications.

Keywords: Atom tracking, Hamiltonian path, Structure of alkane.

1. Introduction

A group is an ordered pair $(Z, *)$ where Z is a set and $*$ is a binary operation on Z satisfying the following axioms:

- (i) $(p * q) * r = p * (q * r)$, for all $a, b, c \in Z$
- (ii) all $e \in Z$ such that for all $p \in Z$ we have $p * e = e * p = p$
- (iii) for each $p \in Z$, $p^{-1} \in Z$ such that $p * p^{-1} = p^{-1} * p = e$

Given a group Z of Z and a subset S of Z , the Cayley graph $\text{Cay}(Z, S)$ is an undirected graph where the set of vertices Z and the set of edges contain an edge from Z to sz and an edge from Z to $s^{-1}z$. When $z \in Z$ and $s \in S$, the edges from $Z \rightarrow sz$ and $S \rightarrow s^{-1}z$ are the same if $|z| = 2$, that gives us an edge. An undirected, linked, acyclic graph is called a tree. In Z , every pair of vertices has a different path. $E(Z) = V(Z) - 1$ represents the $(N-1)$ edges that make up a tree with N vertices [1-3].

Group actions are shown geometrically in Cayley graphs. We will review the essential basic knowledge of group and graph theory to investigate this fully. Although Cayley graphs are commonly employed to depict the abstract structure of a group in graph form, we will mainly concentrate on Cayley graphs rather than Cayley digraphs with directed edges. A Cayley graph is an illustration of a group that is created with a collection of generators that specify the composition and functions of the group. Using these generators illustrates how the group's members interact. Cayley graphs show the group structure and the relationships between the members under group operations. The Cayley type of graphic is the source of Cayley graphs. Cayley color diagrams, first introduced by Arthur Cayley in 1878, are the source of Cayley graphs. Its formulation is based on the Cayley theorem, which states that every group G is isomorphic to a subgroup of the symmetric group acting on Z , $\text{Sym}(Z)$. Finds a directed graph, also known as a Cayley graph, for each finite group G and generating set

Φ . In essence, the generator set selection determines its structure. The Cayley graph is a key tool for fusing group theory and graph theory because it can turn abstract groups into visible graphs. They visually capture the essence of a group by mapping its structure and relationships based on its generators. Cayley graphs are a powerful tool for understanding and analyzing group properties in various mathematical and scientific contexts. Take into consideration the Z_6 group of integers under addition, modulo 6. The elements of this group are $\{0,1,2,3,4,5\}$. The Cayley graph for Z_6 would have 6 vertices, each labeled by these integers. An edge between vertices g and h would be labeled by $h^{-g} \bmod 6$ [4-6].

2. Symmetry and regularity of graphs

Let Γ be a simple finite graph (V, E) . If each vertex of a graph Γ has a degree of k , it is considered a k -regular graph. Otherwise, it is considered a regular graph of degree k . When a regular graph has degree 3, it is called a cubic graph. The automorphism expressed by σ is a permutation of the set of vertices of the graph Γ , such that if and only if $\{\sigma(u), \sigma(v)\}$ is an edge of Γ , then $\{u, v\}$ is an edge of Γ . If an automorphism $\sigma(u) = v$ exists for any two vertices u and v of Γ , the graph Γ is marked as a vertex-transitive graph. Each vertex-transitive graph is a regular graph. However, it is important to note the distinction between regular and transitive graphs. As Figure 1 shows, Frucht graphs, for example, are not transitive. An automorphism $\sigma(\Gamma)$ mapping x to y occurs for any pair of edges x and y of Γ . In this case, Γ is a transitive edge graph. The two qualities are not interchangeable because these symmetry properties show that every vertex and edge on the Γ graph looks the same. As the edges $\{u, v\}$ and $\{u', v'\}$ are not automorphic, Γ in Figure 2 is transitive instead of transitive. An example of a non-vertex-transitive edge graph is a complete bipartite graph $K_{p,q}$, where $p \neq q$. [5,7-10].

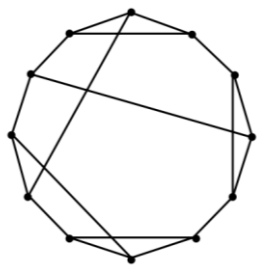


Figure 1: Frucht graph 1

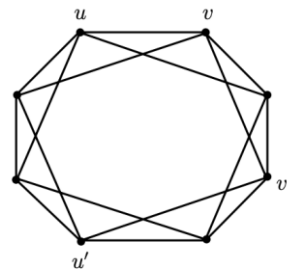


Figure 2: Frucht graph 2

The Frucht graph: A cubic graph with 12 vertices, 18 edges, and no nontrivial symmetries is known as a Frucht graph in graph theory. Frucht graphs are regular but not vertex-transitive; A graph Γ in which vertices pass but not edges [11].

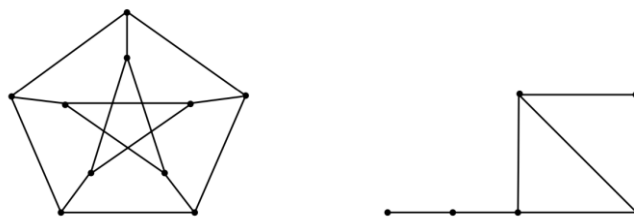


Figure 3: The Petersen graph

An undirected graph with ten vertices and fifteen edges is known as a Petersen graph in graph theory. The graph Γ for passing neither vertices nor edges and the Petersen graph for passing both vertices and edges are depicted in Figure 3 [8].

3. Atom tracking using cayley graphs

Cayley graphs can represent molecules where vertices correspond to atoms and edges represent bonds between them. By analyzing these graphs, one can track how atoms are connected and how these connections change in various chemical reactions or structural transformations.

Directed and undirected graphs can have labels on either vertices or edges. From a chemical perspective, referring to undirected labeled graphs as molecules is often more intuitive. In this case, the vertex represents the atom and the label represents the atom type. Edges represent keys, and labels distinguish single, double, triple, and aromatic keys. Despite this chemical framework, using standard graph terminology in mathematical descriptions is more accurate.

The structure of molecules can be likened to undirected labeled graphs, which allows us to view chemical reactions as transformations of these graphs. This approach involves transforming a set of initial graphics (educts) into a new set of graphs (products) using the double pushout (DPO) method. To fully understand the DPO approach and its variations. In this case, the DPO will specifically outline how chemical reactions can be modeled as rules within the framework of the DPO. This involves considering a rule, expressed as p , which describes the transformation of graph Z to graph H , expressed as $Z \xRightarrow{p} H$. In our setup, p represents the chemical mechanism, $Z \xRightarrow{p} H$ represents the reaction, and G and H linking components represent the molecules that are converted from reactants to products in the reaction. The number of atoms in the starting material (educt) and the reaction product must be the same. This means that the number of vertices in the graph representing the starting material (Z) must be the same as the number of vertices in the graph representing the product (H), expressed as $|V(Z)| = |V(H)|$. We can create a one-to-one mapping or bijection, denoted $\phi: V(Z) \rightarrow V(H)$, to show where the vertices of Z can be found in H after a graph transformation $Z \xRightarrow{p} H$. It is important to note that only vertices with the same label can map to each other. The mapping ϕ is not unique, and there can be several different mappings for a given graph transformation. We use $tr(Z \xRightarrow{p} H)$ to represent all such mappings. Each edge (e^+, e^-) is a pair of subsets of vertices in a directed hypergraph. We represent it by letting $Y_e = e^+ \cup e^-$, which is the set of vertices contained in the starting vertex e^+ and the ending vertex e^- of the edge e . A chemical network (CN) is a hypergraph where each vertex represents a molecule, and each super edge represents a chemical reaction. In this case, each hyperedge e of CN corresponds to a set of direct transformations that convert the input vertices of the hyperedge to the output vertices. For a given set of sides E of CN, D is the set of all direct Sp derivatives obtained by E . Then, $tr(E) = \bigcup_{Z \xRightarrow{p} H \in D} tr(Z \xRightarrow{p} H)$ and $tr(CN) = tr(E(CN))$ [7,12,13]

4. Hamiltonian path in cayley graphs

A path in Γ that visits each vertex precisely once is called a Hamiltonian path, and a closed Hamiltonian path is called a Hamiltonian cycle. It has been conjectured that every Cayley graph is Hamiltonian. Interest in this and other closely related questions has grown in recent years. Finding Hamiltonian cycles in graphs is a challenging task. We surveyed several results and then found three theories about the specific conditions under which the Cayley graph is Hamiltonian [9].

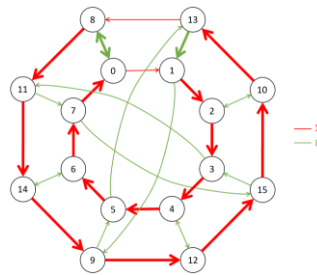


Figure 4: Cayley graph with vertices and directed edges (corresponding to elements of a group and their generators)

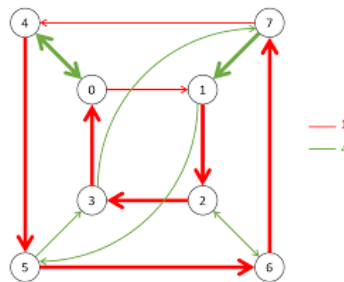


Figure 5: Another example

Figure 4 represents a Cayley graph with vertices and directed edges corresponding to elements of a group and their generators. The red arrows denote one generator (labeled “1”), and the green arrows denote another generator (labeled “8”). This graph illustrates the relationships between group elements when acted on by these generators.

Figure 5 is similar but simpler, with fewer vertices and arrows representing a different group or generating set. Here, the generators appear to be “1” (red) and “4” (green), and it shows how elements of the group are connected through these generators.

4.1. Theorem 1

As Pak and Radoičić mentioned, a Hamiltonian cycle can be found in the appropriate Cayley graph $\Gamma(Z, S)$ for every finite group Z of size $|Z| \geq 3$ if its generating set S has a size of $|S| < \log_2 |Z|$.

The claim that most, if not all, Cayley graphs of finite groups are Hamiltonian graphs cannot be proven. Nevertheless, Theorem 1 establishes the existence of a Hamilton Cayley graph with a generated set of modest dimensions for any finite group G . This demonstration is based on a corollary to the classification of finite simple groups and an explicit combinatorial construction.

For the other results, if Z is allowed to be a finite group and S to be a symmetrical generating set, a Cayley graph $\gamma = \gamma(Z, S)$ is defined as a graph with vertices $z \in Z$, and edges $(Z, zs), (Z, zs^{-1}) \in Z^2$, where $s \in S$. Obviously, γ is d -regular, where $d = |S|$. And then we can only consider Cayley's graphs. For a finite group G , let $n(Z)$ be the number of constituent factors of G . $h(Z)$ and $k(Z)$ represent, respectively, the number of Abelian and non-abelian constituent factors. Obviously, $n(Z) = h(Z) + k(Z)$ [8,14-17].

4.2. Theorem 2

According to Pak and Radoičić, in the finite group Z , $n(Z)$, and $l(Z)$, as defined above, there exists a generator set S , $|S| \leq n(Z) + 2l(Z)$. The set S corresponds to a Cayley graph $\Gamma(Z, S)$ containing a Hamiltonian path.

We label ∂X as the set of vertices $v \in Z - X$ connected to X by an edge, for any subset of vertices $X \subset Z$. If the total number of vertices in a subset X is half or less of the total number of vertices in Z , then the graph is considered an ε -expander. We have the property that for some fixed $\varepsilon > 0$ the magnitude of the boundary of X (denoted by $|\partial X|$) is greater than ε times the magnitude of X (denoted by $|X|$).

Let's consider a prime number p , which has the property of being congruent to 1 modulo 4. We have a finite field, denoted as F_p , which contains p elements. In this field, an element 'a' exists such that $a^2 = -1$.

We can look at the group $SL(2, p)$, which consists of 2×2 matrices over F_p with determinant equal to 1. Additionally, we have the quotient group denoted as $PSL(2, p)$, obtained by dividing $SL(2, p)$ by the subgroup of diagonal matrices $\{\pm 1\}$. For the elements α, β, γ in $PSL(2, p)$, we can represent them

using matrices: $\alpha = \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix}, \beta = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \gamma = \begin{pmatrix} a & 0 \\ a & -a \end{pmatrix}$

These elements form group Z : $PSL(2, p) = \langle \alpha, \beta, \gamma \rangle$. We can verify that $\alpha^2 = \beta^2 = \gamma^2 = 1$. Now consider the Cayley graph $\Gamma_p = \Gamma(PSL(2, p), \{\alpha, \beta, \gamma\})$ [8,14,15].

4.3. Theorem 3

As Pak and Radoičić (2009) said, the diagram of Cayleys Γ_p is an ε -expander for $\varepsilon > 0$, and by definition, it has a Hamiltonian cycle, regardless of the prime $p \equiv 1 \pmod{4}$ [14].

4.4. Proof of theorem 1

Assuming that G is a complicated series, let $n = n(Z)$ and $l = l(Z)$. Make use of K_r, L_1 , and... The Abelian and non-Abelian parts of G are represented by L_m . Observe that $|L_j| \geq 60 > 4$. We've got: $2^{n+2l} = 2^n 4^l \leq \prod_{i=1}^n |K_i| \cdot \prod_{j=1}^l |L_j| = |Z|$. Therefore, $n(Z) + 2l(Z) \leq \log_2 |Z|$, only when. In the case of n greater than or equal to 2, a simple inductive argument can help us find the Hamiltonian cycle. In other cases, the construct set can have an extra group element that joins the Hamiltonian path's ends. The proof is finished with this addition, which supplies the necessary Hamiltonian cycle.

4.5. Proof of theorem 2

The property that arises from categorizing finite simple groups is that two components, at least one of which is involutory, can construct any non-abelian finite simple group. For any simple non-abelian finite group for the Cayley graph corresponding to a Hamiltonian cycle, a set of S generation is created. In the case where group G is cyclical ($Z = Z_p$), a generator suffices. The subsequent fundamental reduction is necessary [15].

4.6. Proof of theorem 3

For matrices A and B belonging to $SL(2, p)$, we denote $A = \pm B$ to represent that these elements map to the same elements in $PSL(2, p)$. For matrices α, β , and γ , note the following:

$$\alpha^2 = \gamma^2 = \begin{pmatrix} a^2 & 0 \\ 0 & a^2 \end{pmatrix} = \pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \beta^2 = \pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\alpha \beta = \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}, \quad \beta \alpha = \begin{pmatrix} 0 & -a \\ -a & 0 \end{pmatrix} = \pm \alpha \beta,$$

$$\gamma \alpha = \begin{pmatrix} a^2 & 0 \\ a^2 & a^2 \end{pmatrix} = \pm \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad \beta \gamma \alpha \beta = \pm \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}.$$

The initial line indicates that in $\text{PSL}(2, p)$, α , β , and γ are directed downwards. The second line demonstrates how $\text{PSL}(2, p)$ modifies α and β . Therefore, lemma 1 implies that the Cayley graph $\Gamma_p = \Gamma(\text{PSL}(2, p), \{\alpha, \beta, \gamma\})$ contains a Hamiltonian cycle. Finally, the third line suggests a basic transition.

$$E = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \quad E^{-1} = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}, \quad F = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad F^{-1} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$$

You can get words of up to 4 lengths in α , β , γ . It is shown that $\Gamma_{ep} = \Gamma$ in the Cayley diagram [14,15,18].

5. Derivative process of structure of alkane

To demonstrate that a molecule with the structure C_nH_{2n+2} (alkane) can be represented as a tree, we can use the following approach:

The number of vertices in a C_nH_{2n+2} molecule is given by $n + (2n+2)$, which simplifies to $3n+2$. For alkanes, where each carbon atom has 4 bonds and each hydrogen atom forms 1 bond, we can consider a graph G to represent the alkane molecule. This graph, G , will have $3n + 2$ vertices and $3n + 1$ edges.

$$\begin{aligned} V(Z) &= 3n+2 \\ E(Z) &= \frac{1}{2} \sum n(V_i) \\ &= \frac{1}{2} (n(C) + n(H)) \\ &= \frac{1}{2} (n \cdot 4 + (2n+2) \cdot 1) \\ &= (4n + 2n + 2)/2 \\ &= 3n + 1 \end{aligned}$$

Thus, $V(Z) - 1 = E(Z)$. In graph theory, trees can be used to depict the structure of the alkane C_nH_{2n+2} . Chemical parameters can be disregarded for determining the number of isomers since they have no bearing on the outcome. Chemical problems can be successfully solved using graph theory, particularly tree theory, which is particularly useful for identifying the isomers of alkanes. Compounds with distinct structures but the same molecular formula are known as isomers. As only structural factors are taken into account in graph theory, counting the number of alkane isomers is made simpler. It's not easy to describe or simulate chemicals, particularly alkanes [19,20].

6. Examples of representation

In addition, table 1 shows the representation of the term in the graph and the chemical terms.

Table 1: The representation of chemical into graph

Chemical Term	The term in Graph
Atom	Vertex
Isomers	Isomorphic
Structural formula	Graph
Acyclic structure	Tree
Chemical bond	Edge

Figure 6 and Figure 7 are examples of representations of graphs in butane (C_4H_{10}), in which Figure 6 shows the centered tree graph and Figure 7 shows the bi-centered tree graph.

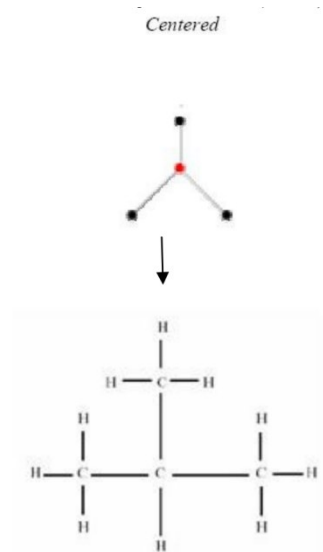


Figure 6: Centered tree of C_4H_{10}

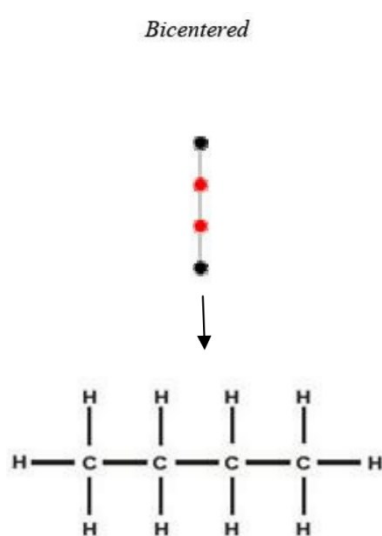


Figure 7: Bi-centered tree of C_4H_{10}

Figure 8, Figure 9, and Figure 10 are examples of representations of the graph in pentane (C_5H_{12}); Figure 8 and Figure 9 show the 2 possible centered tree graphs, and Figure 10 shows the bi-centered tree graph [4].

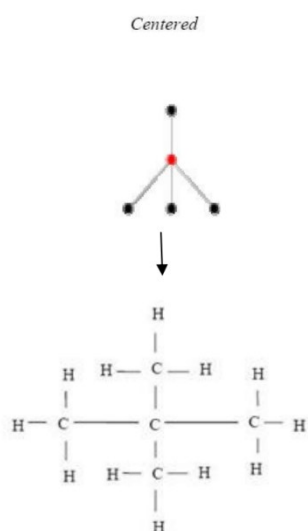


Figure 8: Centered tree of C_5H_{12}

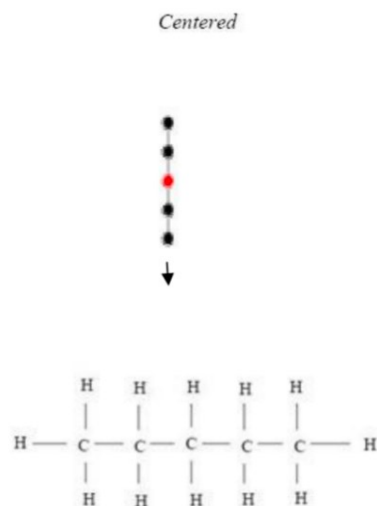


Figure 9: Another centered tree of C_5H_{12}

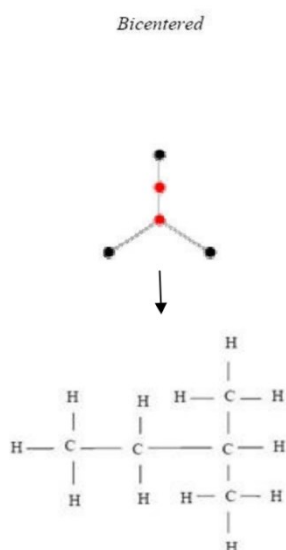


Figure 10: Bi-centered tree of C_5H_{12}

7. Read's contribution

The combination of Liya's theory with the astounding finding by Harary and Norman (1960) to enumerate the stereoisomers and constitutional isomers of alkanes in Read (1976) made Read's study unique. The first result that Read uses is the list of alkanes that have only one carbon atom marked. Read only considers the potential that constitutional isomers, or the radicals connected to the tagged carbon atom, can change through any combination of S_4 in the first step. Next, Pólya's theorem is used with S_4 as the group and $A(x)$ as the figure-counting series. Since the cycle index of the group is $\frac{1}{24}(s_1^4 + 6s_1^2s_2 + 3s_2^2 + 8s_1s_3 + 6s_4)$ [19].

Additionally, our configuration series has the form because we must multiply by x to account for the additional (labeled) carbon atom.

$$P(x) = \sum_{n=1}^{\infty} P_n x^n = x Z(S_4; A(x)) = \frac{1}{24}x \{A^4(x) + 6A^2(x)A(x^2) + 3A^2(x^2) + 8A(x)A(x^3) + 6A(x^4)\}$$

P_n is the number of these compounds that have n carbon atoms.

Listing alkanes with one tagged carbon-carbon valence electron bond—that is, one that can be identified from the others—is the second necessary result. Such labeling is just a means to an end and has no direct bearing on a workable chemical process [19].

8. Conclusion

From the results and comments previously presented, the following conclusions are inferred:

1. A chemical network (CN) is a hypergraph where each hyperedge denotes an application of a rule for a chemical reaction and each vertex is a connected graph that represents a molecule. As thus, every hyperedge of CN maps to a set of direct derivations that convert each hyperedge's entering vertices into its outgoing vertices. Let D be the set of all direct S_p derivations from a given set of edges (E) of CN. Then, $\text{tr}(E) = \bigcup_{Z \xrightarrow{p} H \in D} \text{tr}(Z \xrightarrow{p} H)$ and $\text{tr}(\text{CN}) = \text{tr}(E(\text{CN}))$.

2. Hamiltonian routes exist for Cayley graphs under some conditions. One requirement is that each finite group Z have a small-sized generating set and a Hamiltonian Cayley graph. The second one is a Cayley graph with a generating set that is restricted by composition factors that are both Abelian

and non-Abelian. The third one is the ε -expander Cayley graphs $\Gamma_p = \Gamma(\text{PSL}(2, p), \{\alpha, \beta, \gamma\})$ that have Hamiltonian cycles. [14]

3. Because $E(Z) = V(Z) - 1$, the structure of chemical compounds, particularly alkanes having the formula C_nH_{2n+2} , is a graph tree. Table 2 displays the number of alkane isomers based on the quantity of centered and bi-centered trees [20].

Table 2: Number of alkane isomers

n	Centered	Bicentered	Total
1	1	0	1
2	0	1	1
3	1	0	1
4	1	1	2
5	2	1	3
6	2	3	5
7	6	3	9
8	9	9	18
...	...	...	...

Acknowledgment

Mingzhe Li and Lutong Wang contributed equally to this work and should be considered co-first authors.

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