Chinese Systematic Naming Saturated Chain Hydrocarbon (SCH) by Graph Algorithms

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MonkeyHouse.Info

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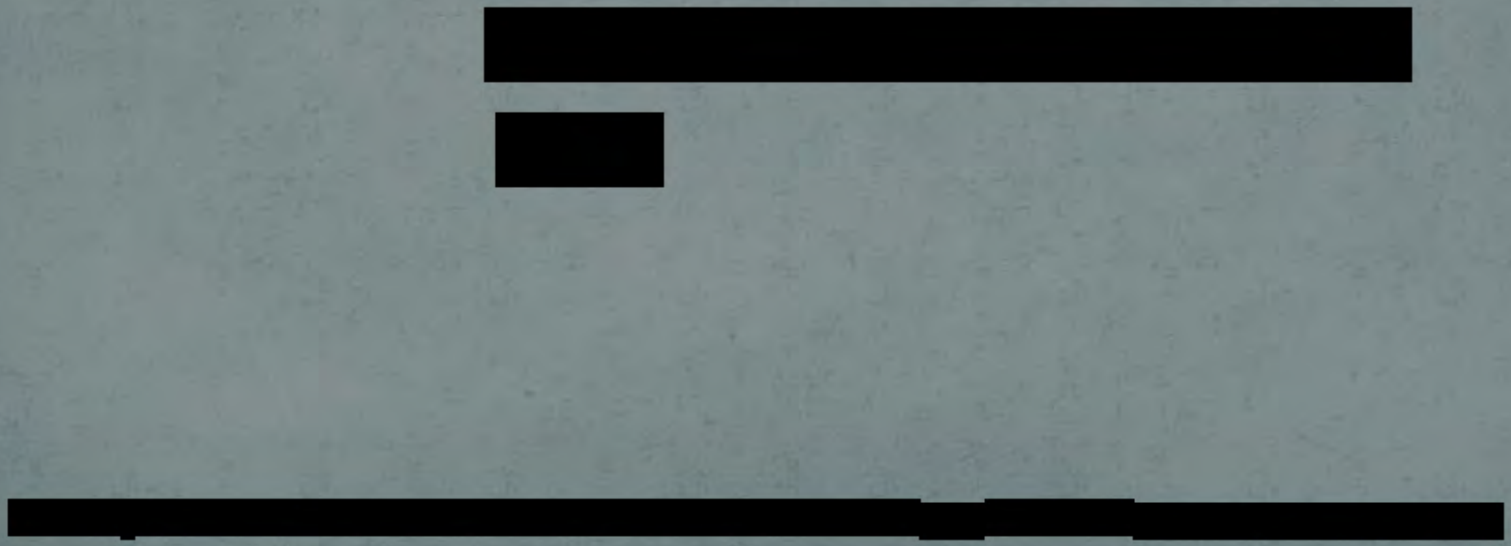
Outline

- Overview
- Transformation
- Algorithms and its Optimizing
- Conclusions and Future Work

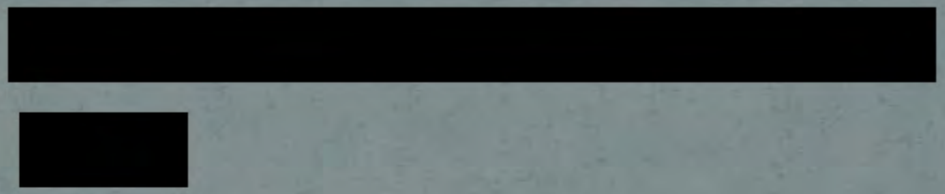
1. Overview

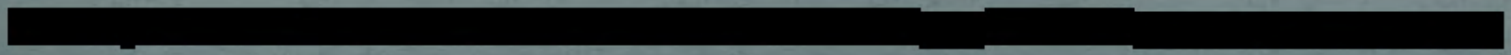
- Problems came from Learning



1. Overview

- Problems came from Learning
- Naming Manually
  - Tedious
  - Low Efficient



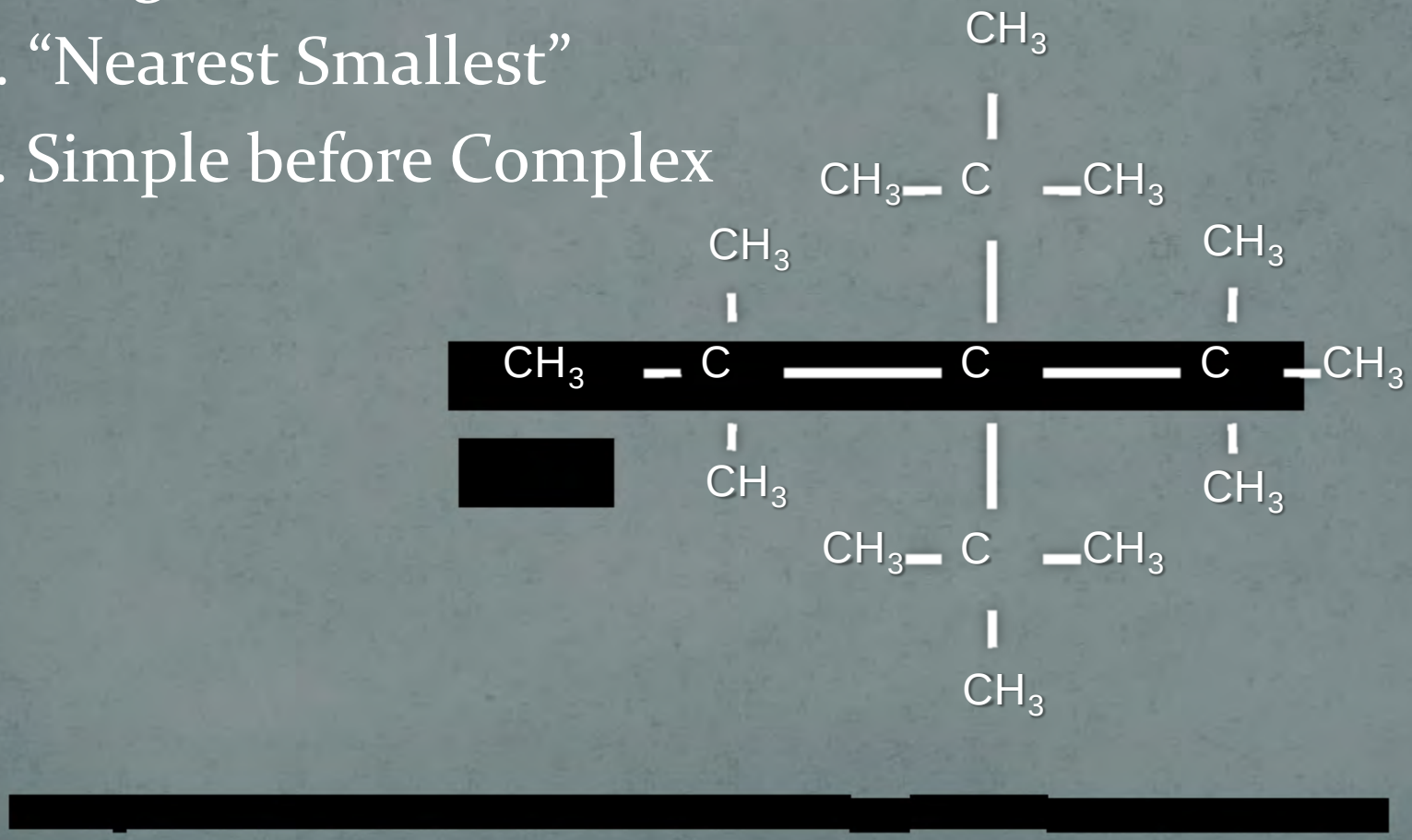


1. Overview

- Problems came from Learning
- Naming Manually
  - Tedious
  - Low Efficient
- Abstracting of Organic Compounds
  - SCH becomes Tree Network
  - Chemistry Problem goes into Graph

Rules of Chinese Systematic Naming

1. Longest Main Chain (MC)
2. “Nearest Smallest”
3. Simple before Complex



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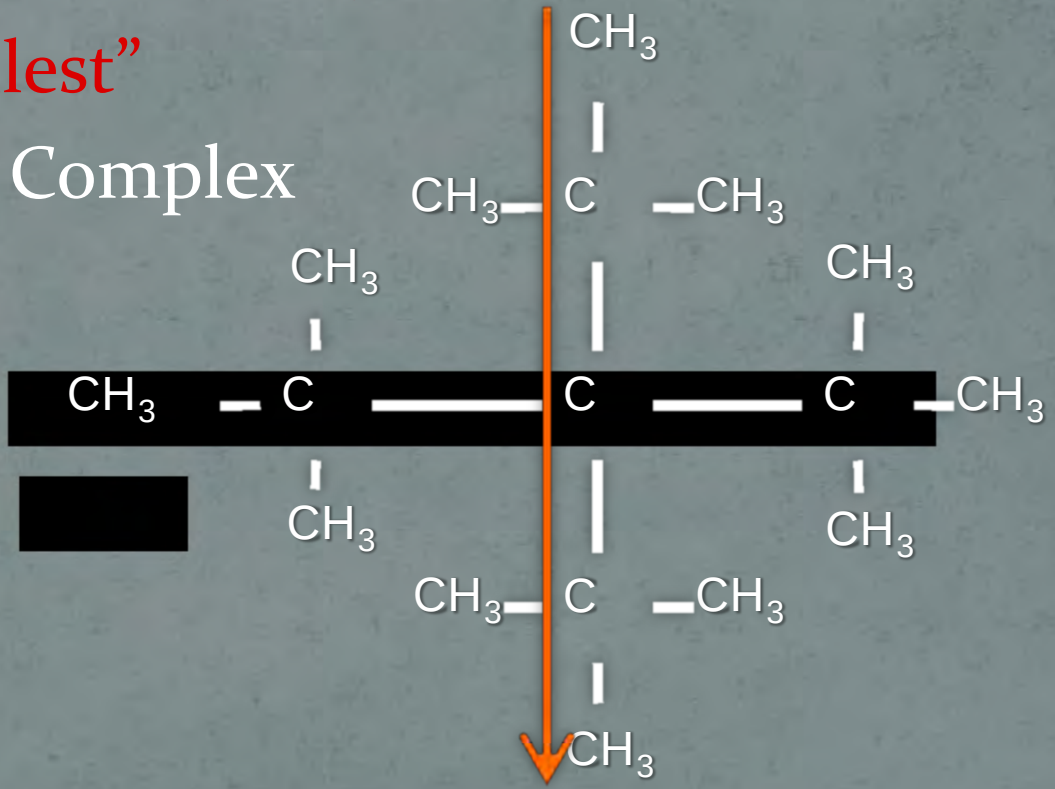

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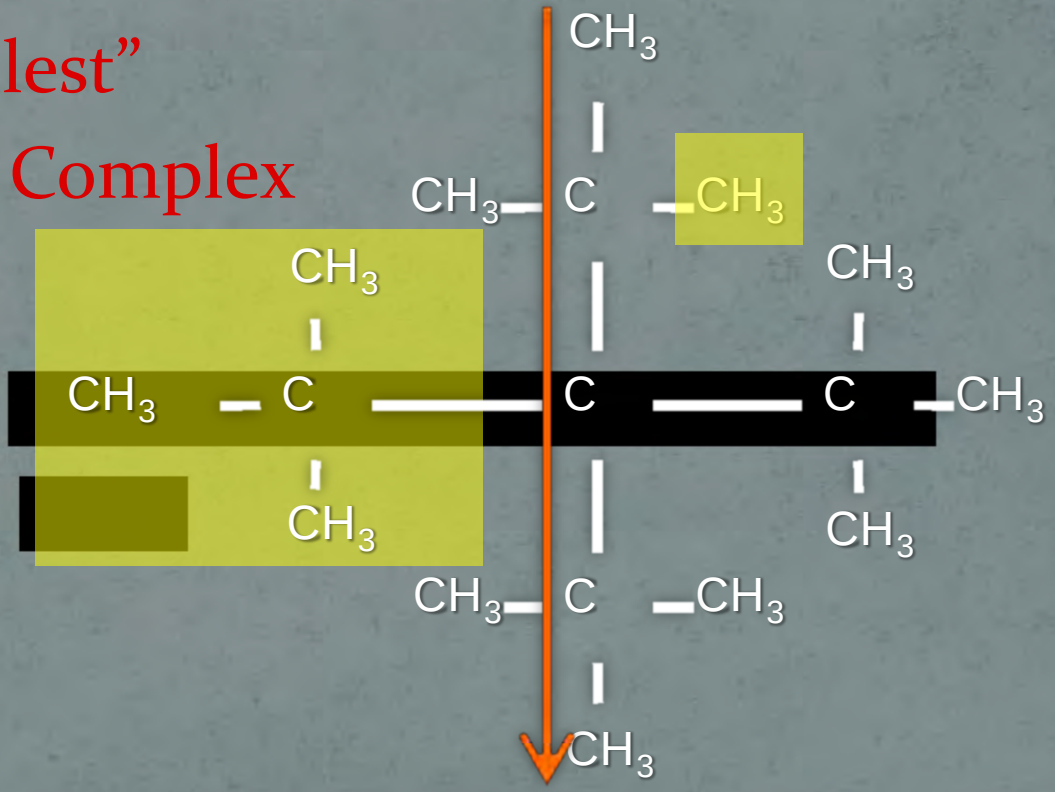

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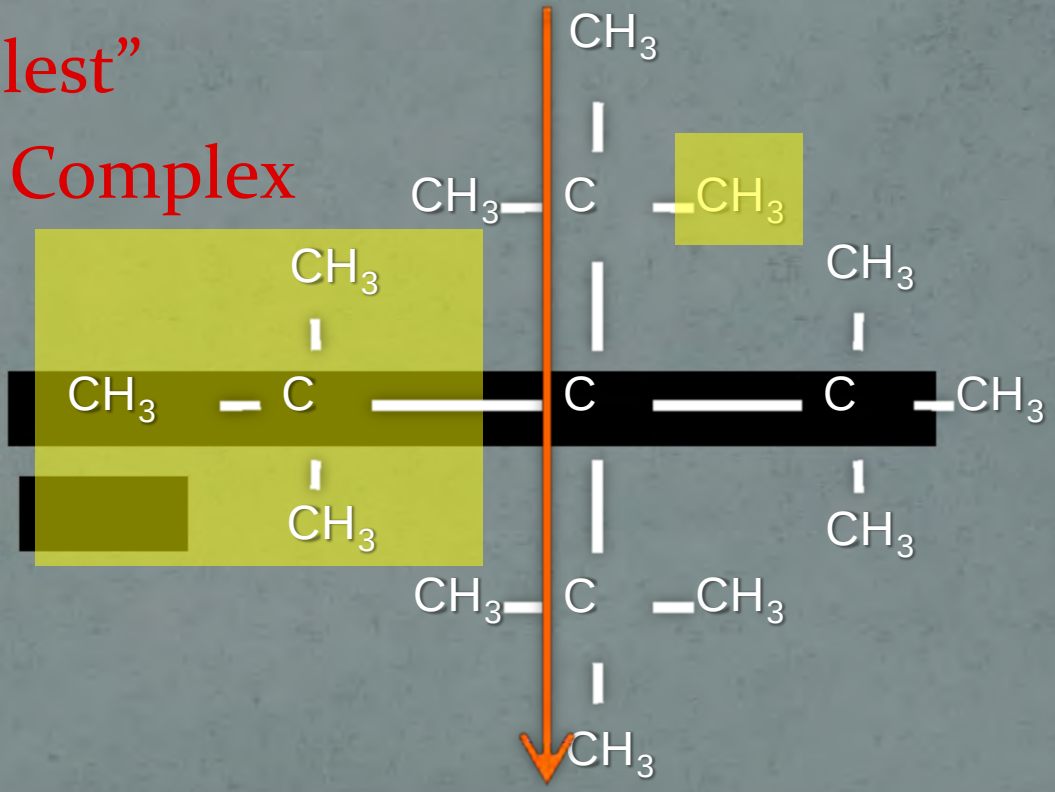
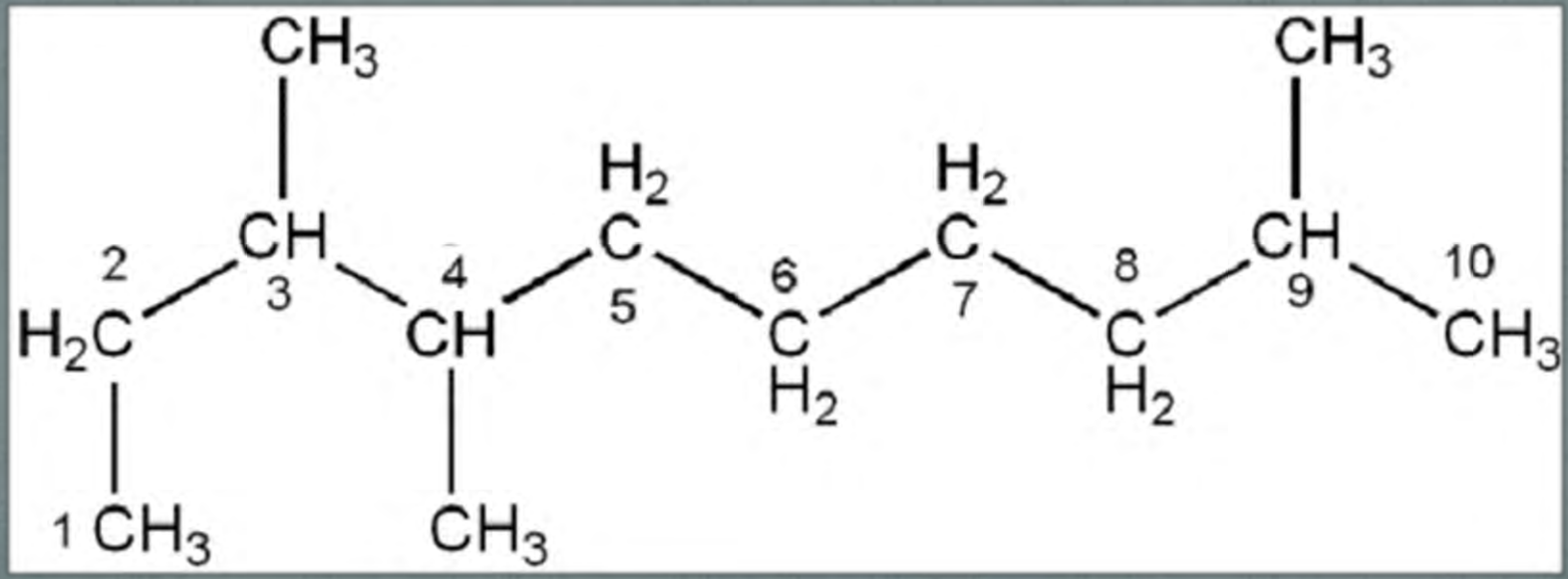


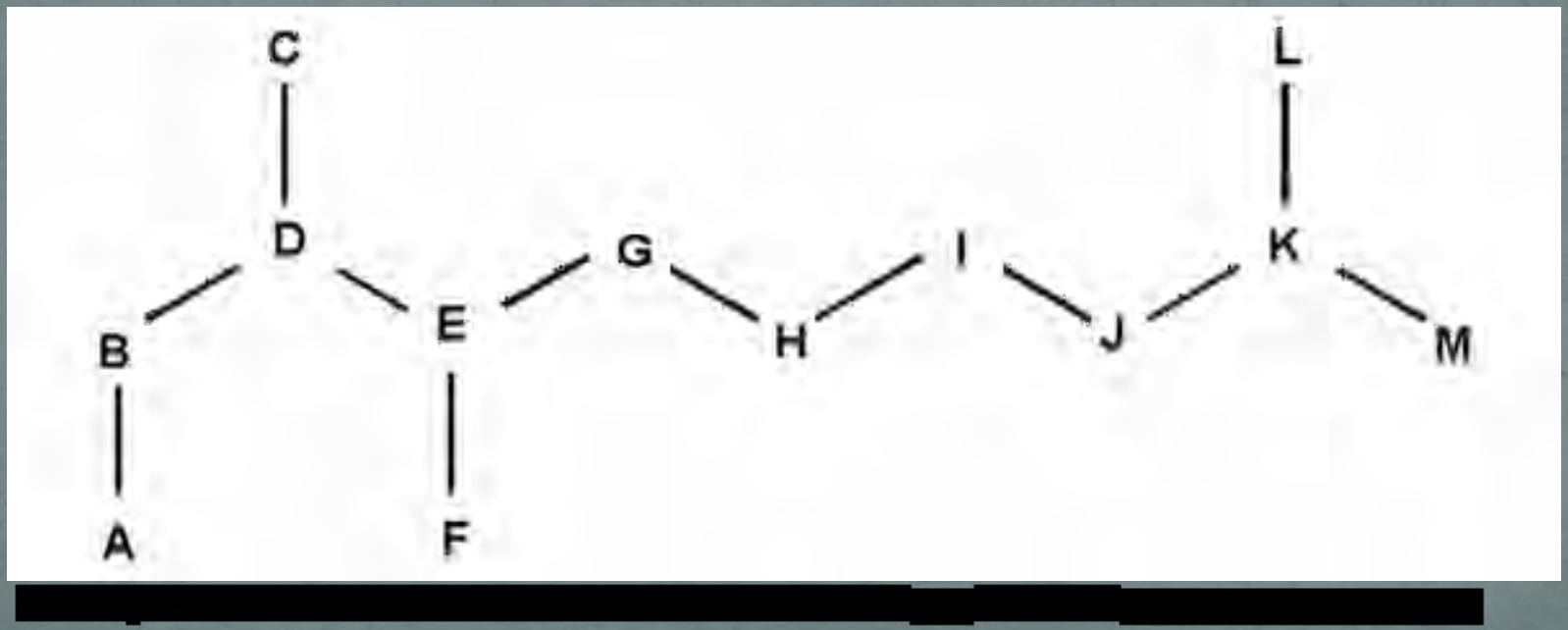
2,2,4,4-四甲基-3,3-二(1,1-二甲基乙基)戊烷

2. Transformation



2. Transformation

- Organic Compounds→Graph



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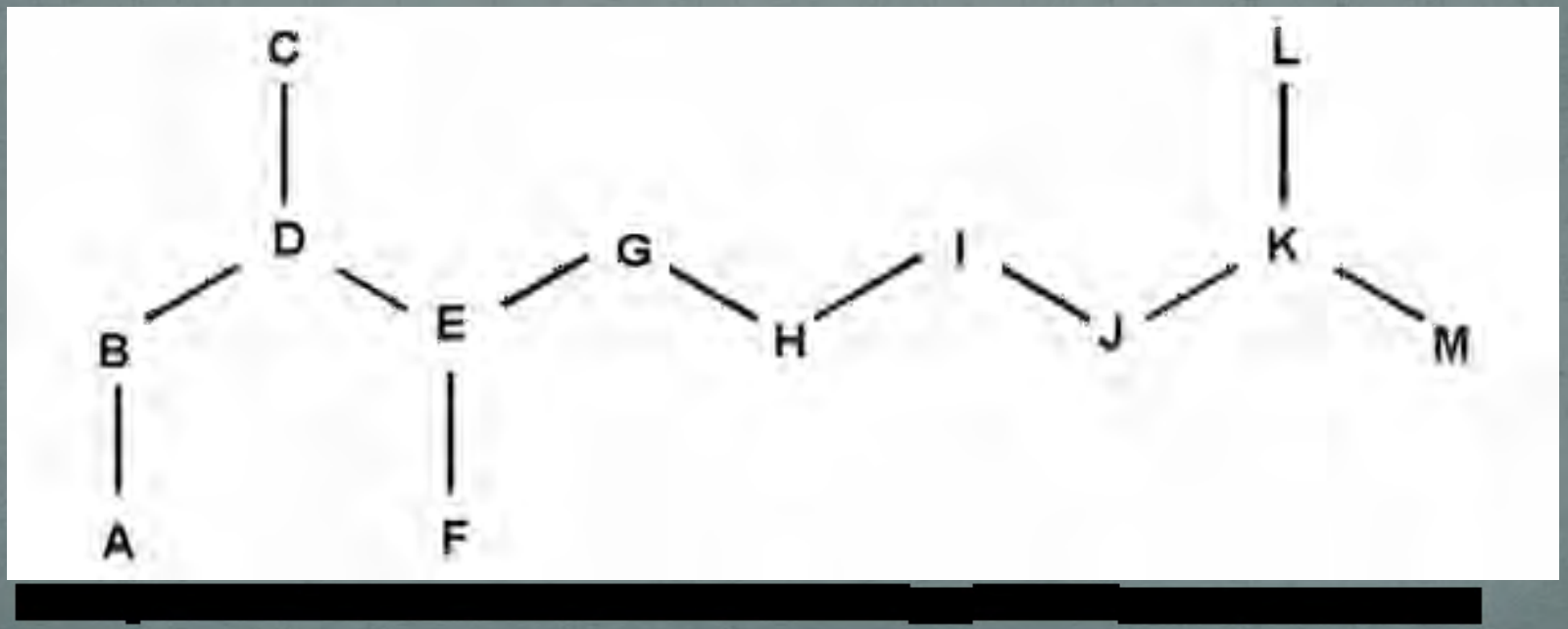
- Organic Compounds→Graph
- SHC→Tree Network



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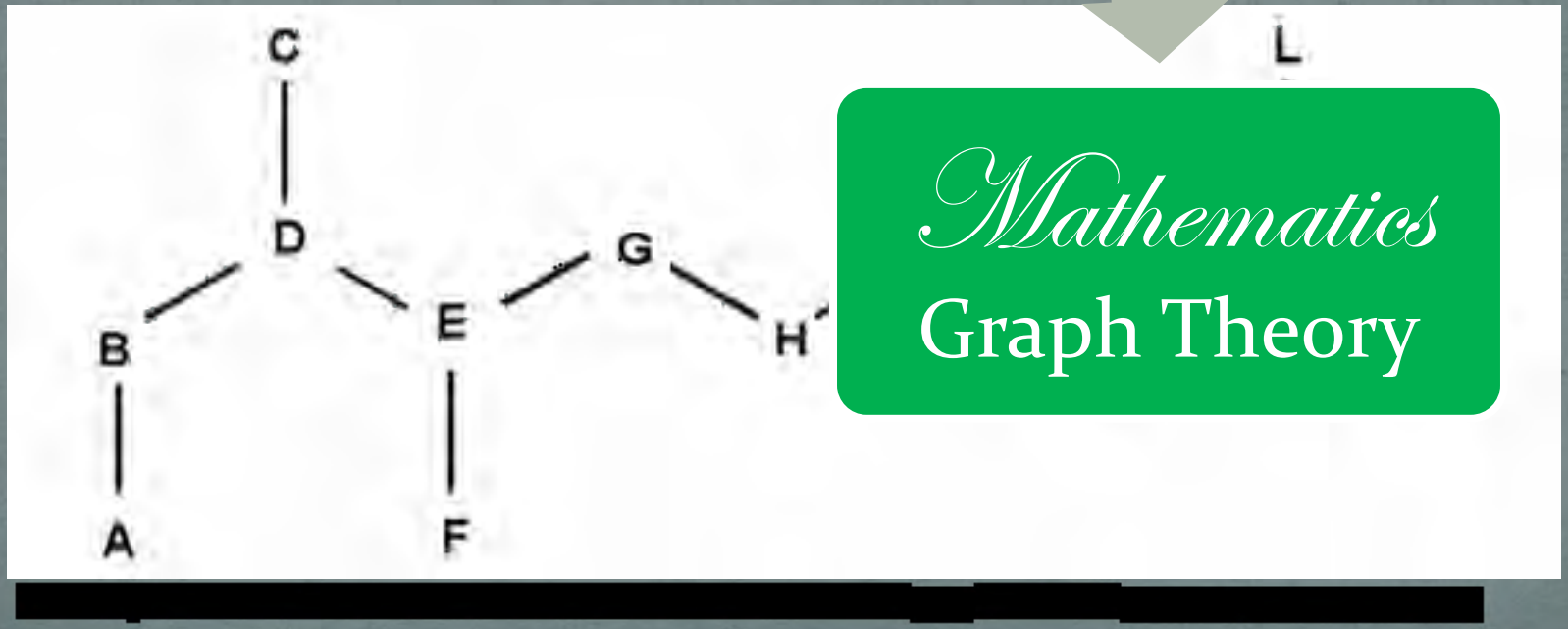
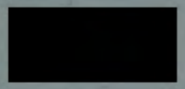
Chemistry
Organic Compounds

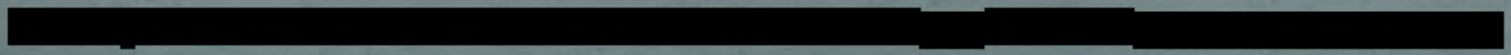


Mathematics
Graph Theory

2. Transformation

- Longest MC→Diameter of Graph
- Best Naming→Simulation & Comparing





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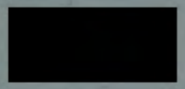
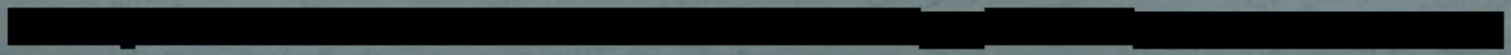
- Longest MC→Diameter of Graph
- Best Naming→Simulation & Comparing
- Grouping Side Chains→Isomorphic of Graph





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- Longest MC→Diameter of TN
- Grouping Side Chains (SC)→IsomorphiTrees

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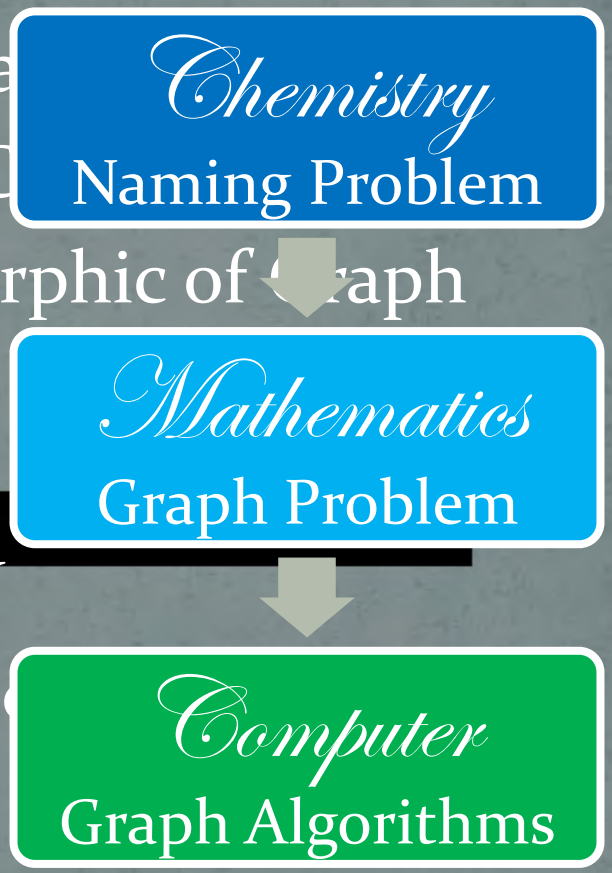
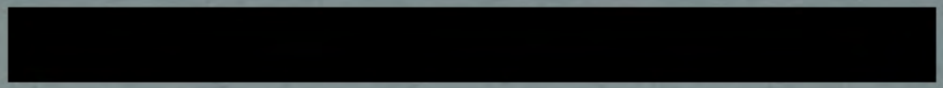
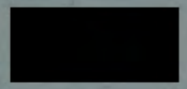
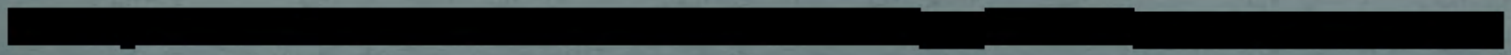


2. Transformation -- Rationality







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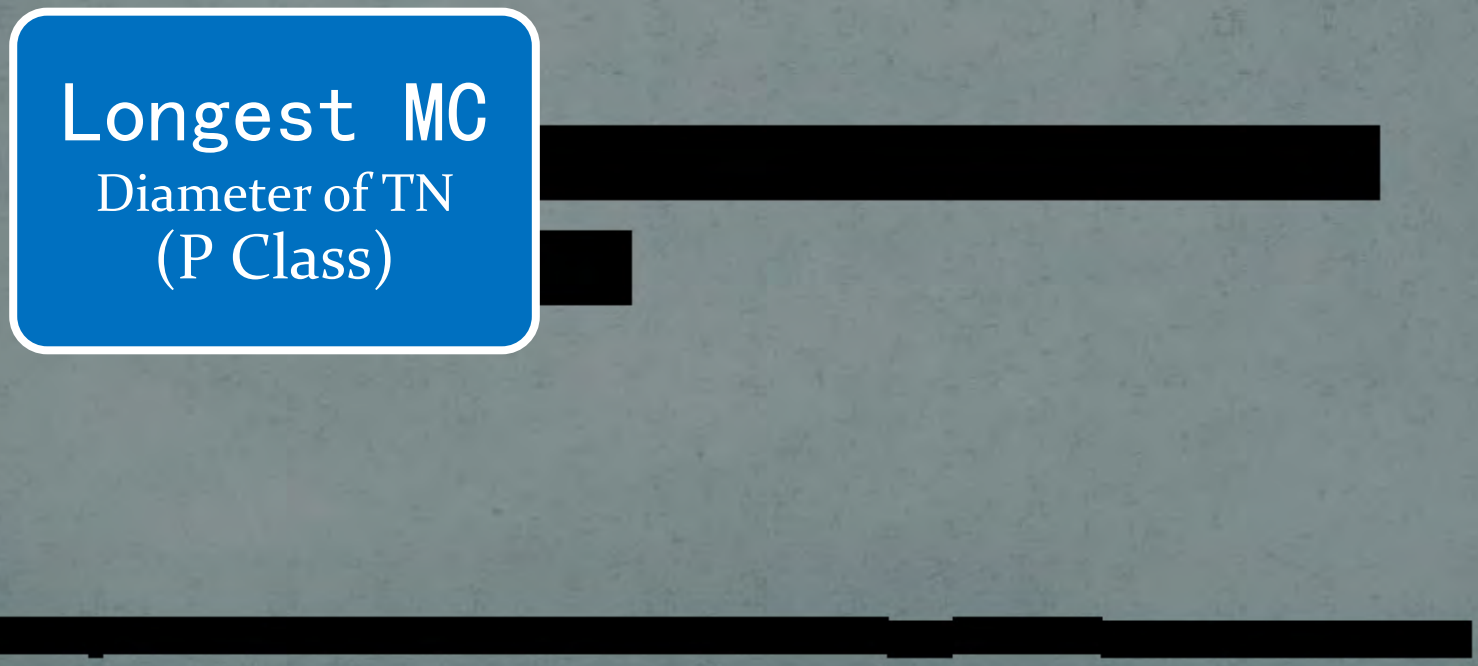

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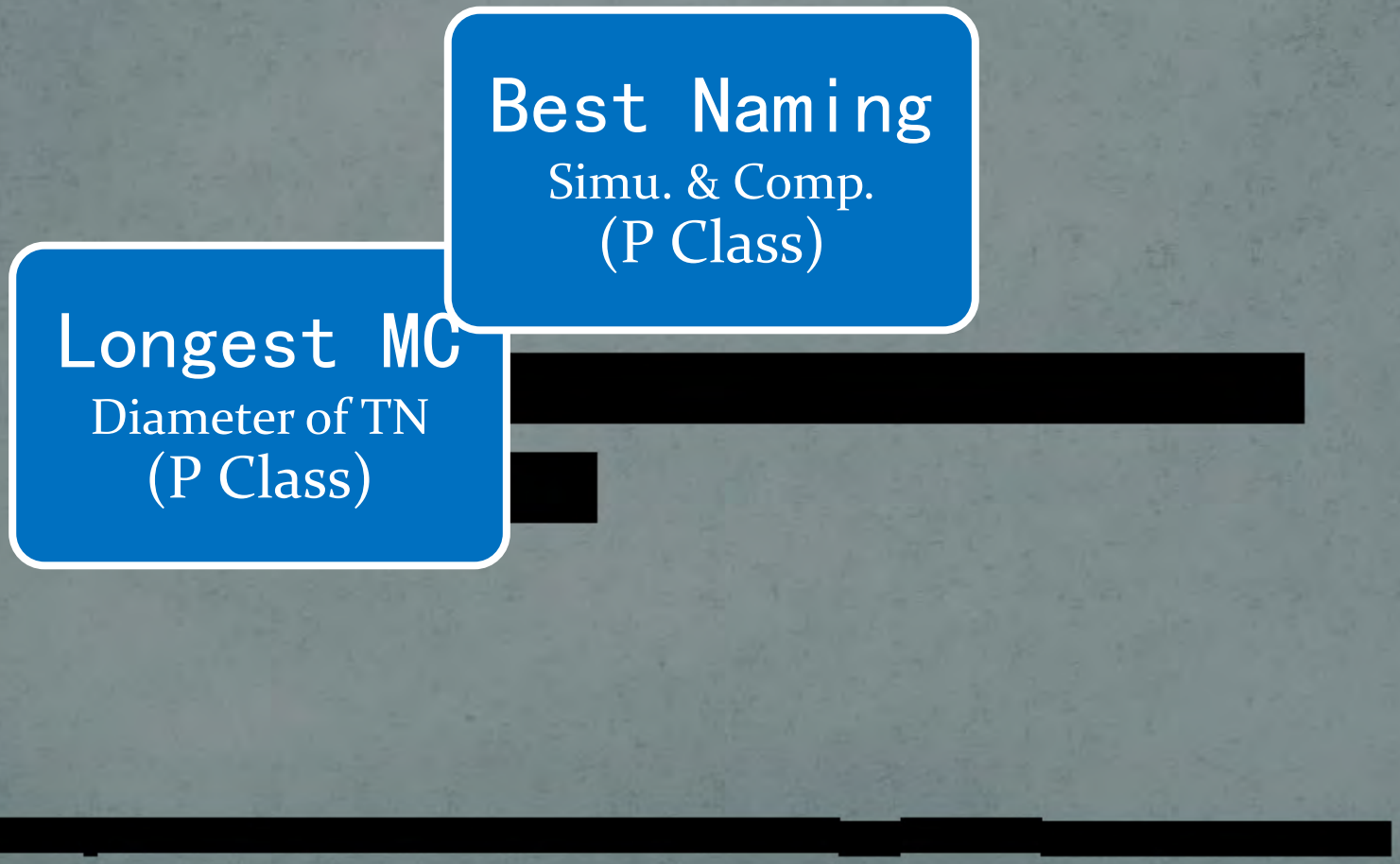

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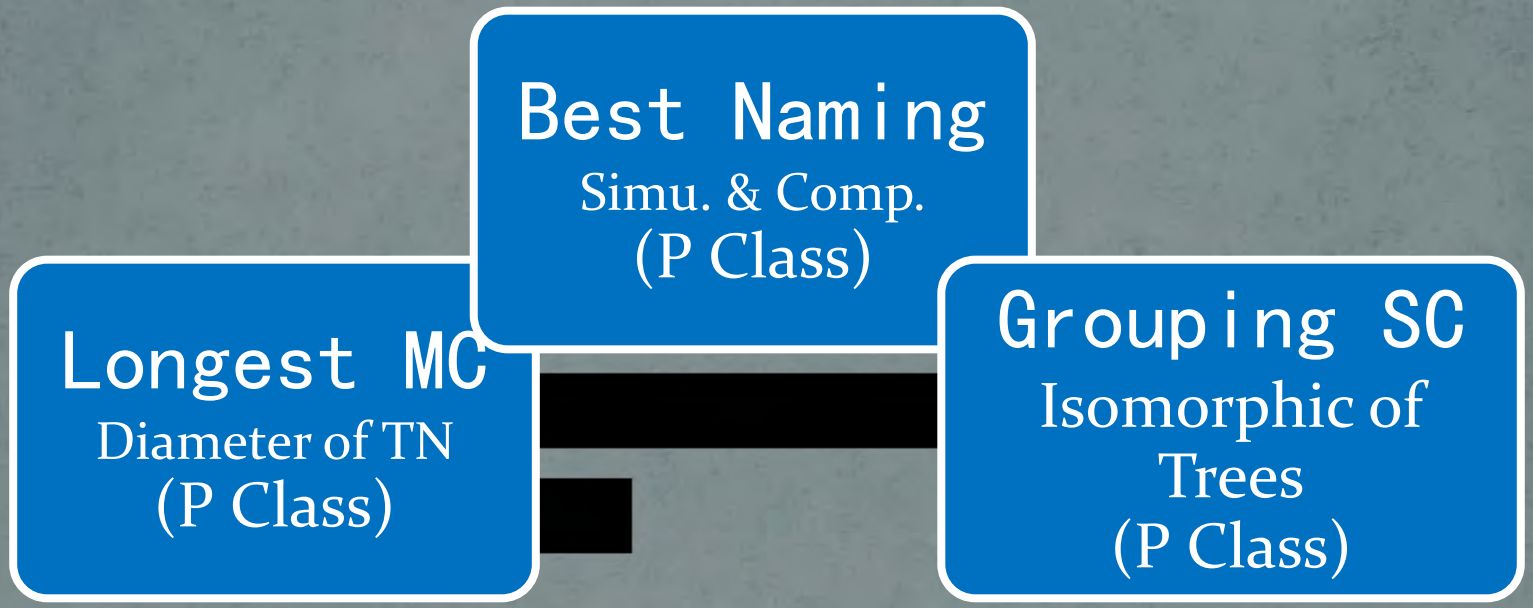

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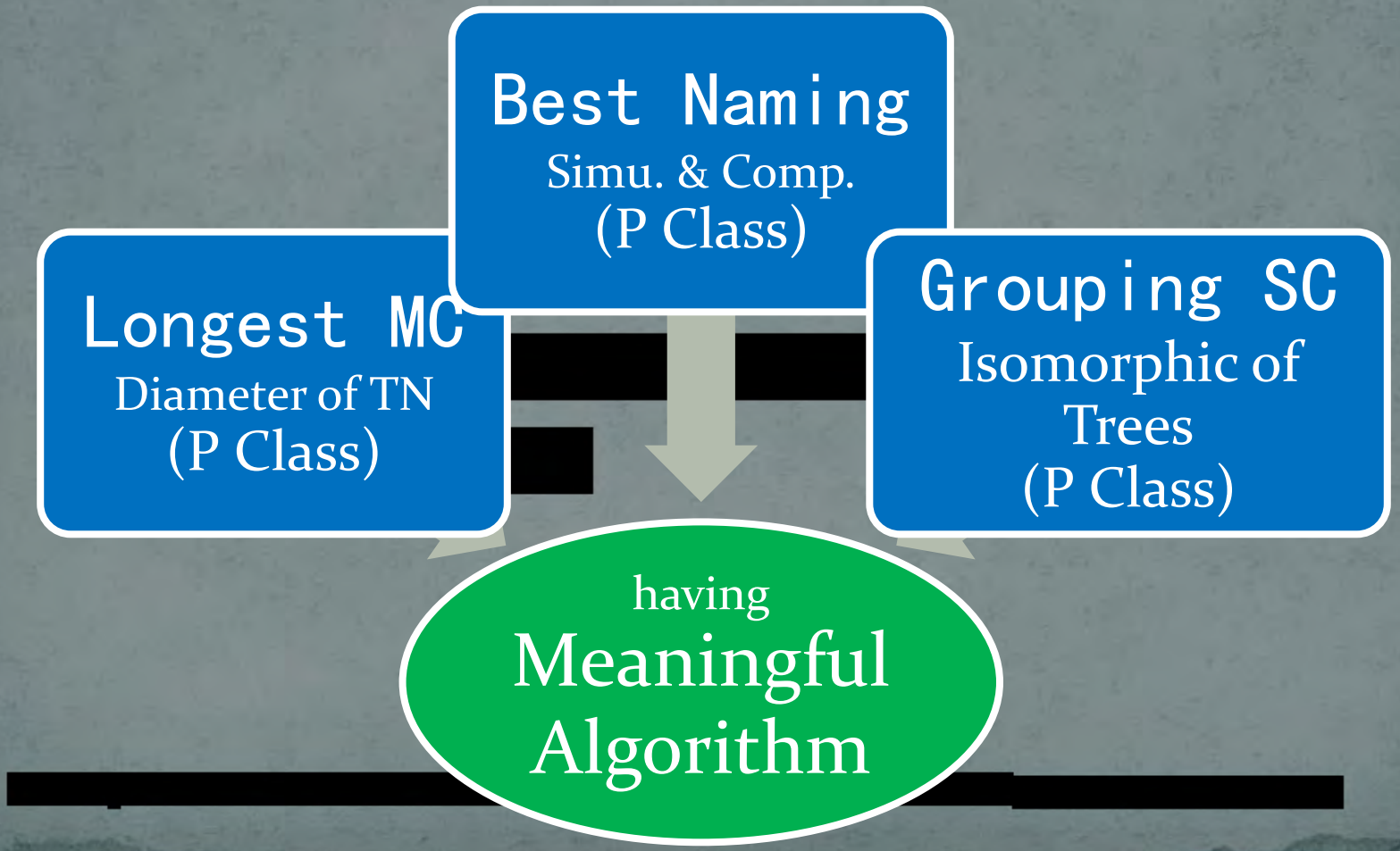

3.1. Algorithms

算法 3 饱和链烃和一价饱和链烃基系统命名算法

▷Procedure $Naming(\mathbb{G})$
if 过程$Naming(\mathbb{G})$是第一次调用
 then
  对$\mathbb{G}$中所有取代基$\mathbb{Z}$进行复杂性比较的预处理
if $\mathbb{G}$是烃
 then
  $\mathbb{D} \leftarrow FindD(\mathbb{G})$
 else
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将$Count(\mathbb{S})$最大的直径$\mathbb{S} \in \mathbb{D}$存入集合$\mathbb{R}$
for each $\mathbb{S} \in \mathbb{R}$ do
 for each $\mathbb{Z} \in \mathbb{P}_{\mathbb{S}}$ do
  if $Hash(Rank(\mathbb{Z})) = \text{NULL}$ then
   $\mathbb{K} = \mathbb{K} \cup \{\mathbb{Z}\}$
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 对侧链$\mathbb{Z}$调用$Naming(\mathbb{Z})$进行系统命名$\mathbb{A}_{\mathbb{Z}}$
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$\mathbb{S} \in \mathbb{R}'$中，侧链序号和最小的命名为$\mathbb{S}_g$
将$\mathbb{M}_{\mathbb{S}_g}$中对侧链的命名按照顺序输出并用短线连接，最后输出碳原子数为$card(\mathbb{D})$的直链烷烃的习惯命名

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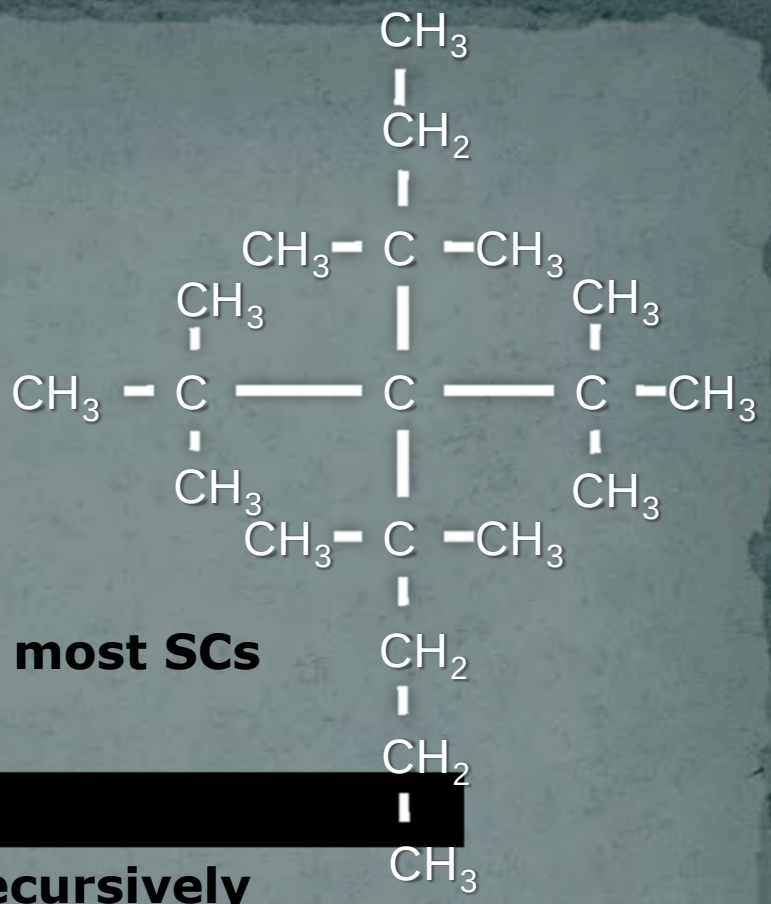

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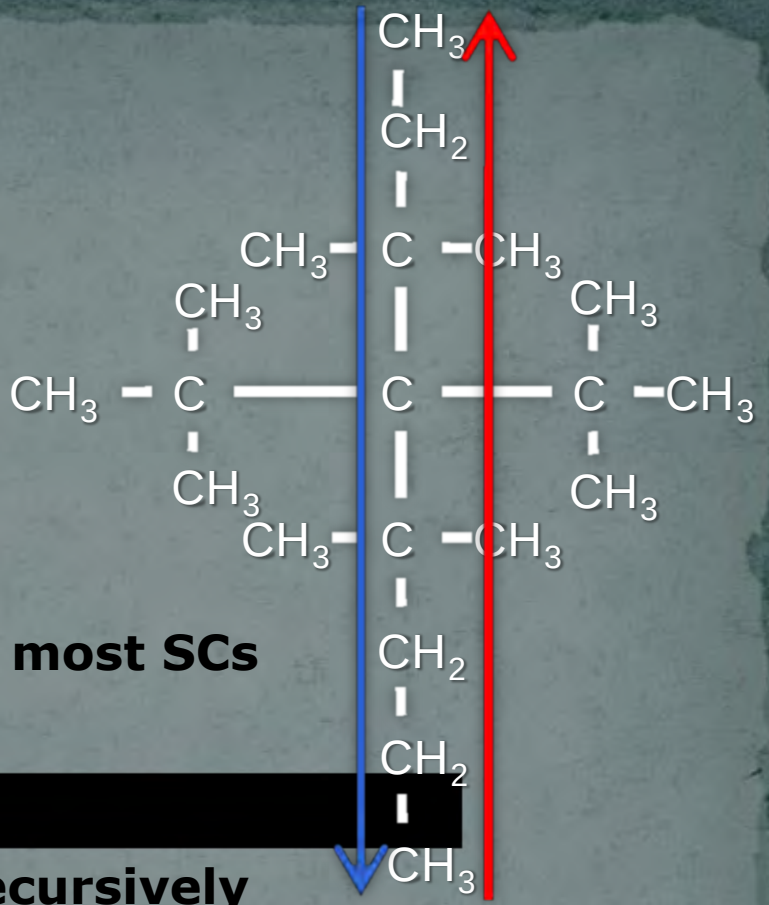

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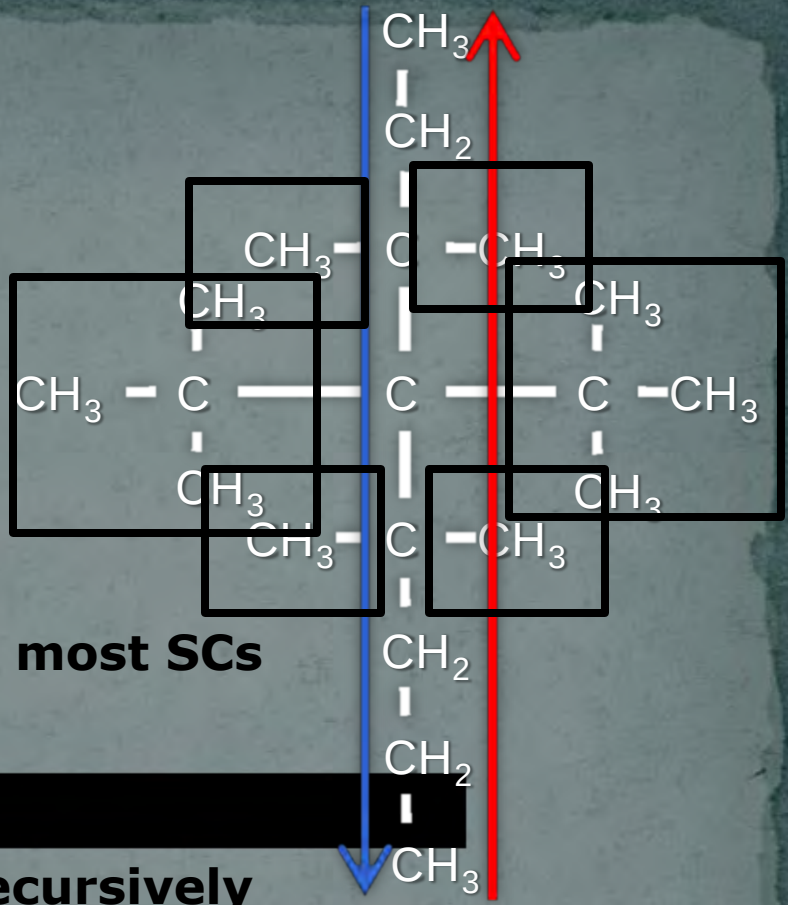

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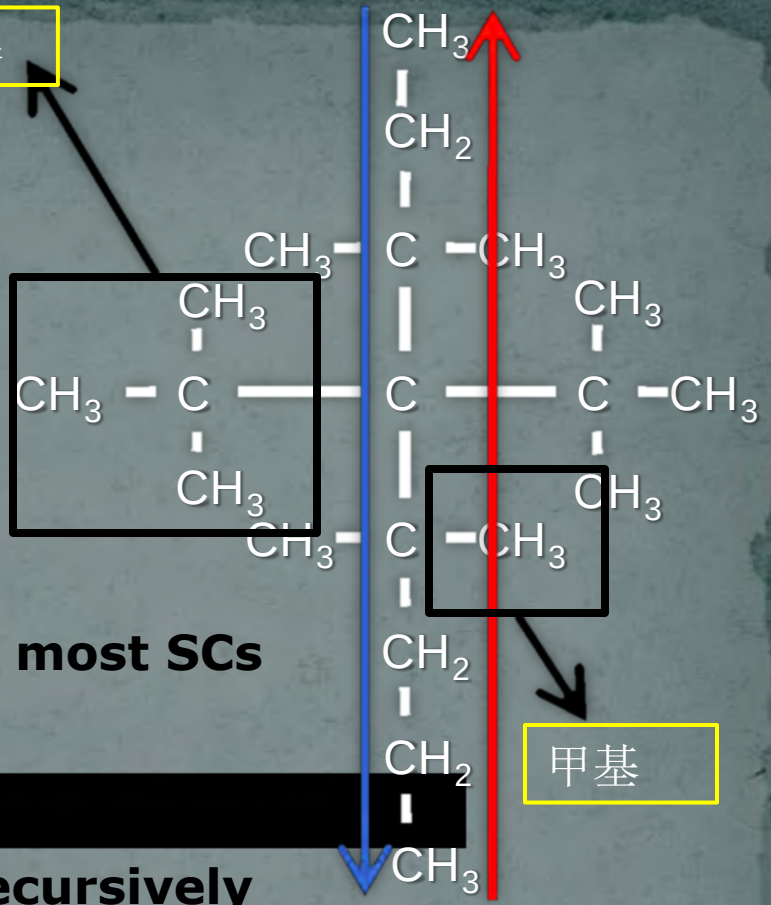

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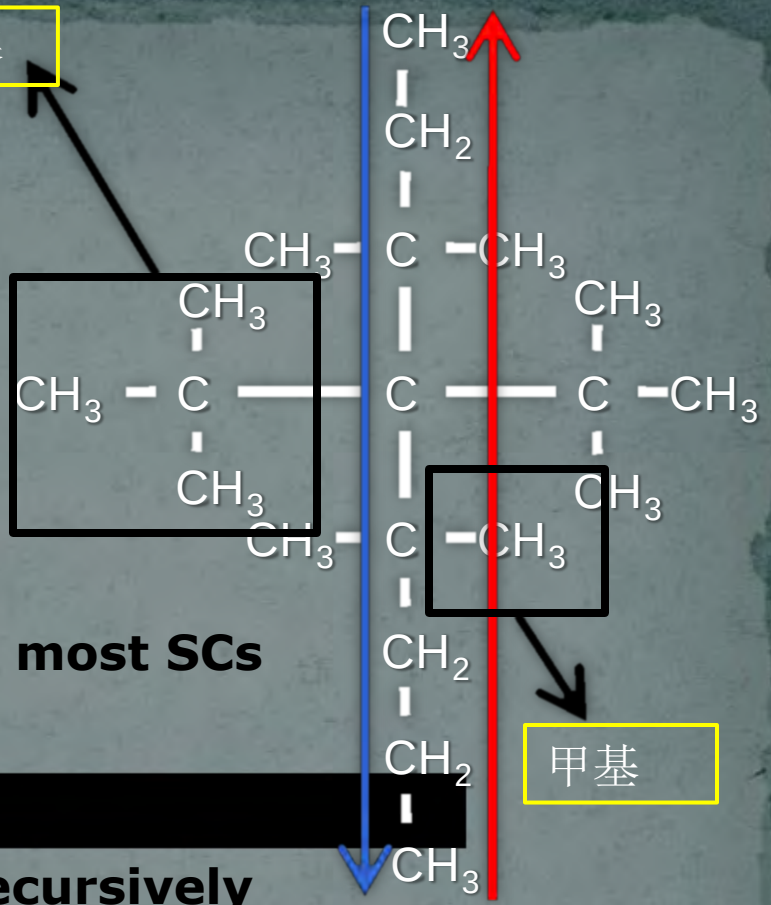

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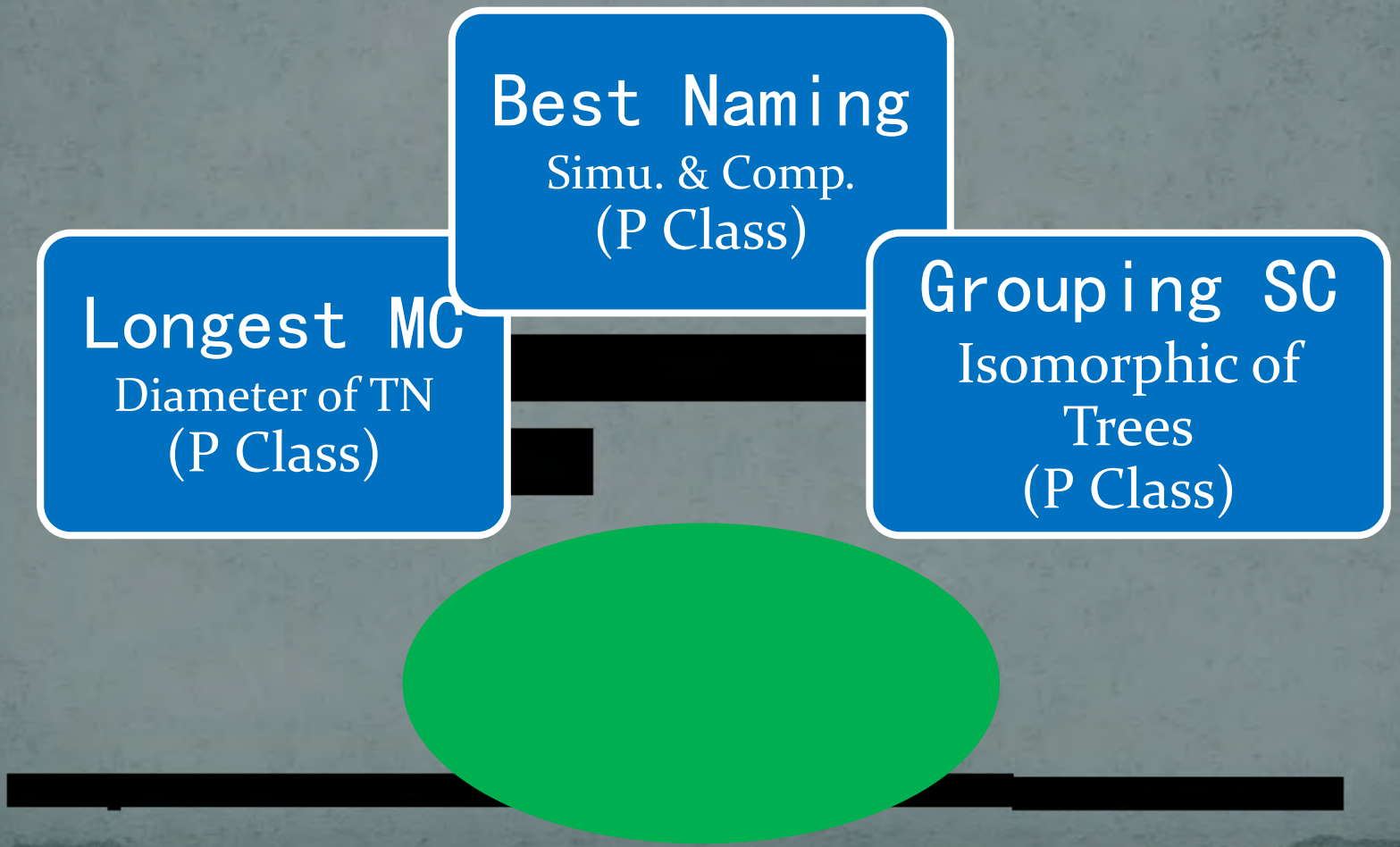
将$\mathbb{M}_{\mathbb{S}_g}$中对侧链的命名按照顺序输出并用短线连接，最后输出碳原子数为$card(\mathbb{D})$的直链烷烃的习惯命名

- **Sorting SCs**
- **Get Dia. of TN**
- **Get the MC with most SCs**
- **Grouping SCs**
- **Naming SC Recursively**
- **Connecting Numbers and SCs**
- **Sorting SCs**
- **Choosing the Best Naming**
- **Output in Natural Language**

3,3,5,5 四甲基 4,4 二(1,1-二甲基乙基)
4,4,6,6 四甲基 5,5 二(1,1-二甲基乙基)

2. Transformation -- Rationality



3.1. Algorithms

算法 3 饱和链烃和一价饱和链烃基系统命名算法

▷Procedure $Naming(\mathbb{G})$
if 过程$Naming(\mathbb{G})$是第一次调用
 then
  对$\mathbb{G}$中所有取代基$\mathbb{Z}$进行复杂性比较的预处理
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将$Count(\mathbb{S})$最大的直径$\mathbb{S} \in \mathbb{D}$存入集合$\mathbb{R}$
for each $\mathbb{S} \in \mathbb{R}$ do
 for each $\mathbb{Z} \in \mathbb{P}_{\mathbb{S}}$ do
  if $Hash(Rank(\mathbb{Z})) = \text{NULL}$ then
   $\mathbb{K} = \mathbb{K} \cup \{\mathbb{Z}\}$
  将$\mathbb{Z}$的地址存入$Hash(Rank(\mathbb{Z}))$
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 对侧链$\mathbb{Z}$调用$Naming(\mathbb{Z})$进行系统命名$\mathbb{A}_{\mathbb{Z}}$
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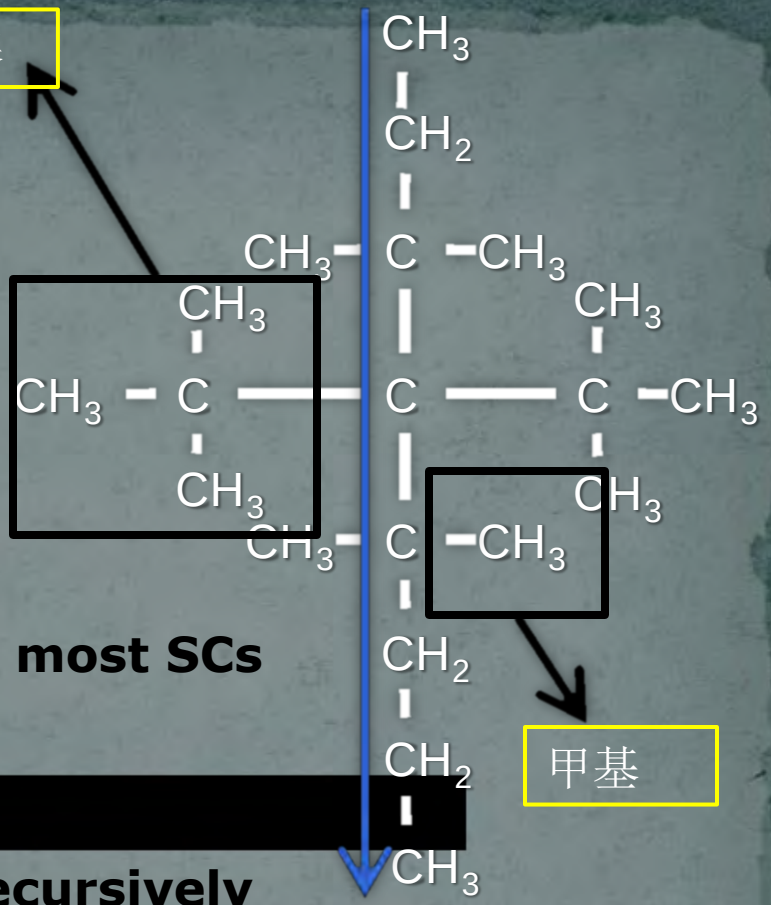
- **Choosing the Best Naming**
- **Output in Natural Language**



3,3,5,5-四甲基-4,4-二(1,1-二甲基乙基)辛烷

$$O(m^2) + O(n^2) + O(n^3) + O(m^3) = O(n^3)$$

3.1. Algorithms – Time Complexity

算法 3 饱和链烃和一价饱和链烃基系统命名算法

▷Procedure $Naming(\mathbb{G})$
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 then
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 then
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  if $Hash(Rank(\mathbb{Z})) = \text{NULL}$ then
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for each $\mathbb{Z} \in \mathbb{K}$ do
 对侧链$\mathbb{Z}$调用$Naming(\mathbb{Z})$进行系统命名$\mathbb{A}_{\mathbb{Z}}$
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- **Sorting SCs** $O(m^2)$
- **Get Dia. of TN** $O(n^2)+(2m-1)\times O(n)=O(n^2)$
- **Get the MC with most SCs** $2m \times n \times O(n) = O(n^3)$
- **Grouping SCs**
- **Naming SC Recursively**
- **Connecting Numbers and SCs**
- **Sorting SCs** $O(m^3)$
- **Choosing the Best Naming**
- **Output in Natural Language**

$$O(m^2) + O(n^2) + O(n^3) + O(m^3) = O(n^3)$$

3.1. Algorithms – Time Complexity

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appx. 1k carbons/sec

$O(m^2)$

$O(n^2)+(2m\text{-}1)\times O(n)=O(n^2)$

$2m \times n \times O(n)$
$=O(n^3)$

$O(m^3)$

$$O(m^2) + O(n^2) + O(n^3) + O(m^3) = O(n^3)$$

3.2. Optimized Algorithms

算法 3 饱和链烃和一价饱和链烃基系统命名算法

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- **Naming SC Recursively**
- **Connecting Numbers and SCs**
- **Sorting SCs** $O(m^3)$
- **Choosing the Best Naming**
- **Output in Natural Language**

$$O(m^2) + O(n^2) + O(n^3) + O(m^3)$$

$$= O(n^3)$$

3.2. Optimized Algorithms

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if 过程$Naming(\mathbb{G})$是第一次调用

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$\mathbb{D} \leftarrow FindD\&Count(\mathbb{G})$

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for each $\mathbb{S} \in \mathbb{R}$ do

for each $\mathbb{Z} \in \mathbb{P}_S$ do

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- **Sorting SCs** $O(m^2)$
- **Get MC with longest dia. and most SCs on the same time** $O(n^2)$
- **Grouping SCs** [redacted]
- **Naming SC Recursively**
- **Connecting Numbers and SCs**
- **Sorting SCs** $O(m^2 \log m)$
- **Choosing the Best Naming**
- **Output in Natural Language** [redacted]

$$O(m^2) + O(n^2) + O(n^2) + O(m^2 \log m) = O(n^2 \log n)$$

3.2. Optimized Algorithms

算法 3 饱和链烃和一价饱和链烃基系统命名算法

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3.2. Optimized Algorithms

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▷Procedure *Naming*(𝔾)
if 过程*Naming*(𝔾)是第一次调用
 then
  对𝔾中所有取代基ℤ进行复杂性比较的预处理
if 𝔾是烃
 then
  $\mathbb{D} \leftarrow FindD\&Count(\mathbb{G})$
 else
  $\mathbb{D} \leftarrow FindD\&Count(\mathbb{G})$
将[redacted]最大的直径[redacted]存入集合ℝ
for each $\mathbb{S} \in \mathbb{R}$ do
 for each $\mathbb{Z} \in \mathbb{P}_S$ do
  if $Hash(Rank(\mathbb{Z})) = \text{NULL}$ then
   $\mathbb{K} = \mathbb{K} \cup \{\mathbb{Z}\}$
  将ℤ的地址存入$Hash(Rank(\mathbb{Z}))$
for each $\mathbb{Z} \in \mathbb{K}$ do
 对侧链ℤ调用$Naming(\mathbb{Z})$进行系统命名$\mathbb{A}_Z$
for each $\mathbb{S} \in \mathbb{R}$ do
 for each $\mathbb{Z} \in \mathbb{K}$ do
  将$Hash(Rank(\mathbb{Z})) \cap \mathbb{S}$的标号与$\mathbb{A}_Z$连接后，存入该直径的侧链系统命名集合$\mathbb{M}_S$
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- **Sorting SCs** $O(m^2 \log m)$
- **Choosing the Best Naming**
- **Output in Natural Language**

appx. 10k carbons/sec

$O(n^2)$

4.1. Conclusions

- **SHC→Tree Network in Graph Theory**
- **Getting MC and Grouping SCs→Diameters and** isomorphism of TN
- **Give Chinese Systematic Naming Algorithm (CSNA) based on Diameter and Isomorphism Algorithms**
- **Optimize the Algorithm to Get Better Performance**
- **CSNA: Efficient and Fast**

4.2. Future Work

- Accurate Computing Complexity Estimation
- Pattern Matching :
  - Generating TNs from Expressions
- Generalization

Thanks

Thanks for Your Attention [redacted]

[1] [redacted]