International Journal of Research Publication and Reviews

Journal homepage: www.ijrpr.com ISSN 2582-7421

A Comprehensive Review of Naphthalene and its Chemistry

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ABSTRACT:

Naphthalene, a white, crystalline polycyclic aromatic hydrocarbon (PAH) with the formula C10H8, has captivated the scientific community for decades. This review delves into the intricate details of naphthalene, exploring its unique structure, fascinating properties, and diverse applications, supported by a comprehensive literature survey. Comprised of two fused benzene rings, naphthalene exhibits high melting and boiling points due to strong intermolecular forces. Its aromatic character makes it susceptible to various reactions, including electrophilic aromatic substitution, oxidation, and reduction, leading to valuable derivatives. Historically, naphthalene was isolated from coal tar, but now modern catalytic processes offer efficient alternatives. Its applications are wide-ranging, including the production of phthalic acid (a key building block in polymers, paints, and pharmaceuticals), acting as a moth repellent, and serving as an intermediate in organic synthesis. Furthermore, research is actively exploring the potential of naphthalene in developing novel materials for electronics and energy storage, and its derivatives are being investigated for their therapeutic potential against various diseases. This review highlights the enduring significance of naphthalene, showcasing its journey from a coal tar byproduct to a versatile molecule with countless applications. The future holds immense promise, with exciting possibilities in materials science, drug discovery, and environmental remediation.

Keywords: Naphthalene, Fused benzene rings, Coal tar, Phthalic acid production,

INTRODUCTION:

Naphthalene, a seemingly simple molecule with the formula C10H8, has captivated the attention of scientists and industrialists for centuries. Its seemingly straightforward structure, consisting of two fused benzene rings, belies a remarkable depth of chemical complexity and diverse applications (Fig 1). From its humble beginnings as a component of coal tar to its current status as a versatile building block in modern industry, naphthalene has consistently held a place of prominence in the world of chemistry.

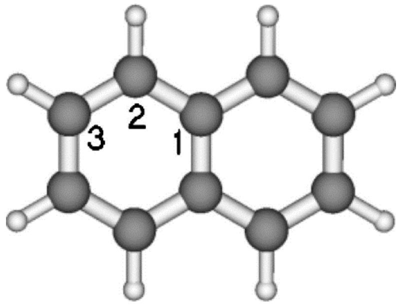
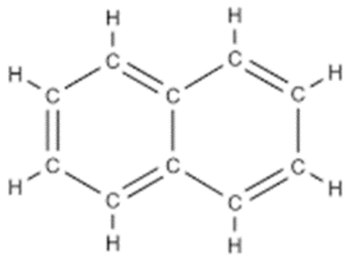


Fig 1. The structure of naphthalene, featuring two fused benzene rings.

The allure of naphthalene stems from its unique combination of intrinsic properties and readily accessible reactive sites. Its aromatic character, arising from the delocalization of its pi electrons, grants it exceptional stability and reactivity towards electrophilic aromatic substitution reactions, forming the basis for its extensive use in organic synthesis. [(1)] Beyond its aromatic nature, naphthalene possesses other noteworthy physical properties. Its high melting and boiling points, attributed to strong intermolecular forces, dictate its behavior in various processing and purification techniques. [(2)] The historical significance of naphthalene is undeniable. Its initial isolation from coal tar marked the beginning of its journey into the industrial world. However, modern times have witnessed a shift towards more efficient and environmentally friendly production methods, such as catalytic processes derived from petroleum feedstocks. [(3)] The diverse applications of naphthalene are a testament to its remarkable versatility. It stands as the cornerstone for the production of phthalic acid, a vital component in plastics, paints, and pharmaceuticals. Its effectiveness as a moth repellent has ensured its place in countless households around the world. [(4)] This comprehensive review delves into the fascinating world of naphthalene, exploring its structure, properties, synthesis, reactions, and diverse applications. Through a detailed examination of the literature and an insightful analysis of its chemical properties, we aim to unveil the enigma of this remarkable molecule and shed light on its continued significance in the world of chemistry.

Structure and Properties:

Naphthalene (C10H8) is a polycyclic aromatic hydrocarbon (PAH) with a unique and fascinating structure. Its defining feature is the presence of two benzene rings fused together at adjacent carbon atoms, commonly referred to as the ortho position. This fusion leads to a planar configuration with a delocalized system of pi electrons, contributing significantly to its aromatic character. (5)



Properties: Naphthalene possesses a variety of interesting properties that are directly related to its structure. These include:

Physical properties:

- Melting point: 80.5 °C
- Boiling point: 218 °C
- Density: 1.145 g/cm3
- Solubility: Slightly soluble in water, readily soluble in organic solvents
- Appearance: White, crystalline solid with a characteristic mothball odor (6)

Chemical properties:

- Aromatic character: Naphthalene exhibits high aromaticity due to the delocalization of its pi electrons. This makes it resistant to electrophilic attack and favors electrophilic substitution reactions.
- High reactivity: The presence of reactive sites, particularly the α-carbon positions on the benzene rings, makes naphthalene susceptible to a variety of reactions, including electrophilic aromatic substitution, oxidation, reduction, and Diels-Alder reactions.
- Moth repellent: The unique odor of naphthalene acts as a powerful deterrent to moths, leading to its widespread use in mothballs and other pest control products. (7)

Synthesis of Naphthalene:

Naphthalene, the captivating molecule with the formula C10H8, has fascinated chemists for centuries. Its unique structure, consisting of two fused benzene rings, has fueled innovation in various synthesis methods, leading to its widespread application in numerous industries. This review explores the diverse pathways for naphthalene synthesis, tracing its journey from historical extraction to modern catalytic advancements.

1. Coal Tar Extraction- The earliest known method for obtaining naphthalene involved isolating it from coal tar, a byproduct of coal distillation (Figure 2). This crude process involved collecting the tar, then fractionally distilling it to separate different components based on their boiling points. Naphthalene, with its relatively high boiling point of 218°C, could be isolated and further purified through various crystallization techniques.

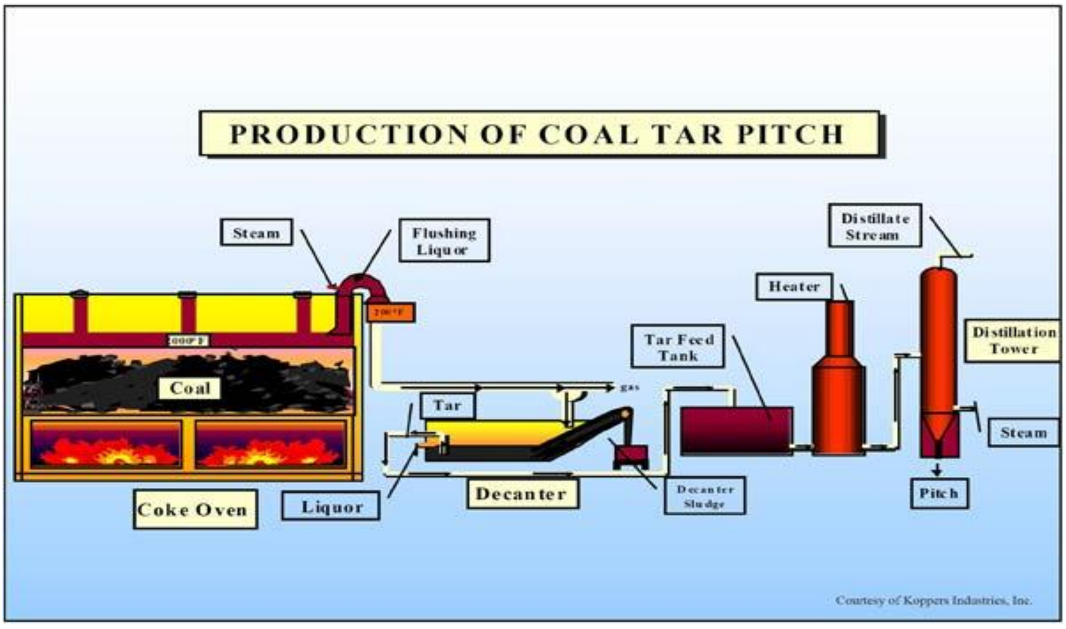


Fig 2. Coal tar distillation, a historical method for naphthalene extraction. [8]

While this method served as the primary source of naphthalene for many years, it had limitations. The reliance on coal as a feedstock raised environmental concerns, and the separation process was inefficient and laborious. [9]

Modern Evolution: Catalytic Processes

With the advancement of chemical technology, more efficient and environmentally friendly synthesis methods for naphthalene emerged. Catalytic processes now play a crucial role in its production, primarily relying on petroleum-derived feedstocks.

1. Dealkylation:

This method involves the removal of alkyl groups from aromatic hydrocarbons like alkylbenzenes, using catalysts such as zeolites or metal oxides (Figure 4). The dealkylation process typically occurs at high temperatures (450-650°C) and pressures.

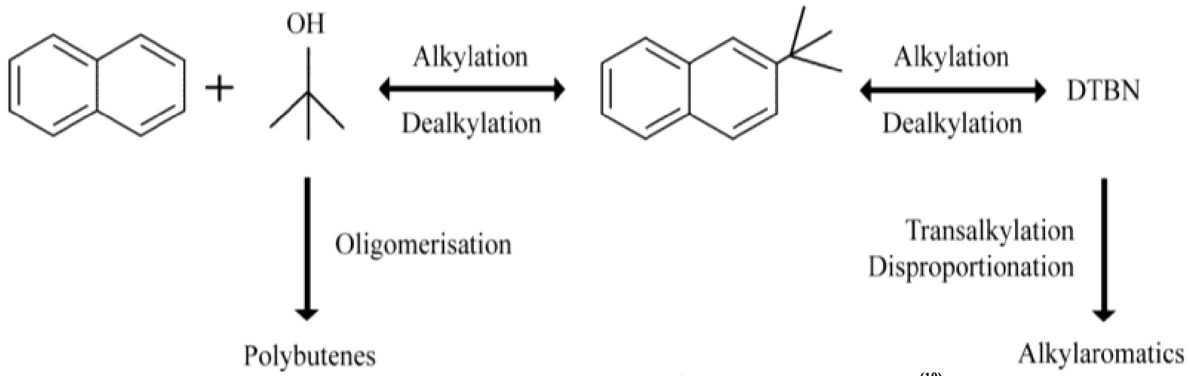


Fig 4. Dealkylation reaction, a modern method for naphthalene synthesis. [10]

2. Haworth synthesis of naphthalene:

The Haworth synthesis may be synthesized, the following stages are taken:

- 3-benzoylpropionic acid is given via Benzene's craft acylation reaction with succinic anhydride.
- The second stage is the 3-benzoylpropionic acid reaction of Clemmenson, which results in 4-phenyl butanoic acid. Clemmensen reaction is observed in the presence of zinc amalgam and hydrochloric acid.
- The development of the ring structure of α-tetralene by elimination of the water molecule will result in this product being heated in the presence of strong sulphuric acid.
- Tetrahydronaphthalene is produced through the Clemmenson reaction of α-tetralene. Clemmensen reaction is observed in the presence of zinc amalgam and hydrochloric acid.
- Tetrahydronaphthalene dehydrogenation produces naphthalene in the presence of selenium.

So, the reactions according to the steps are given below:

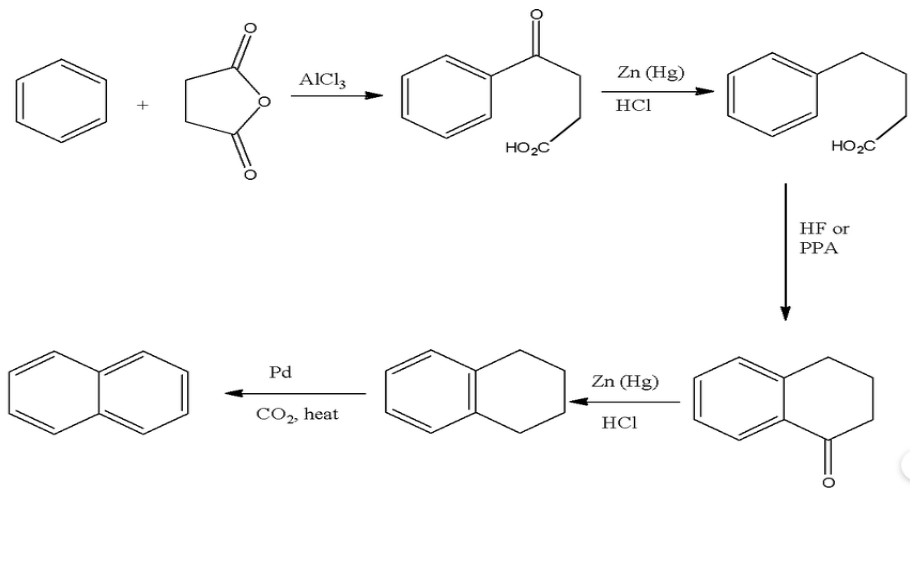
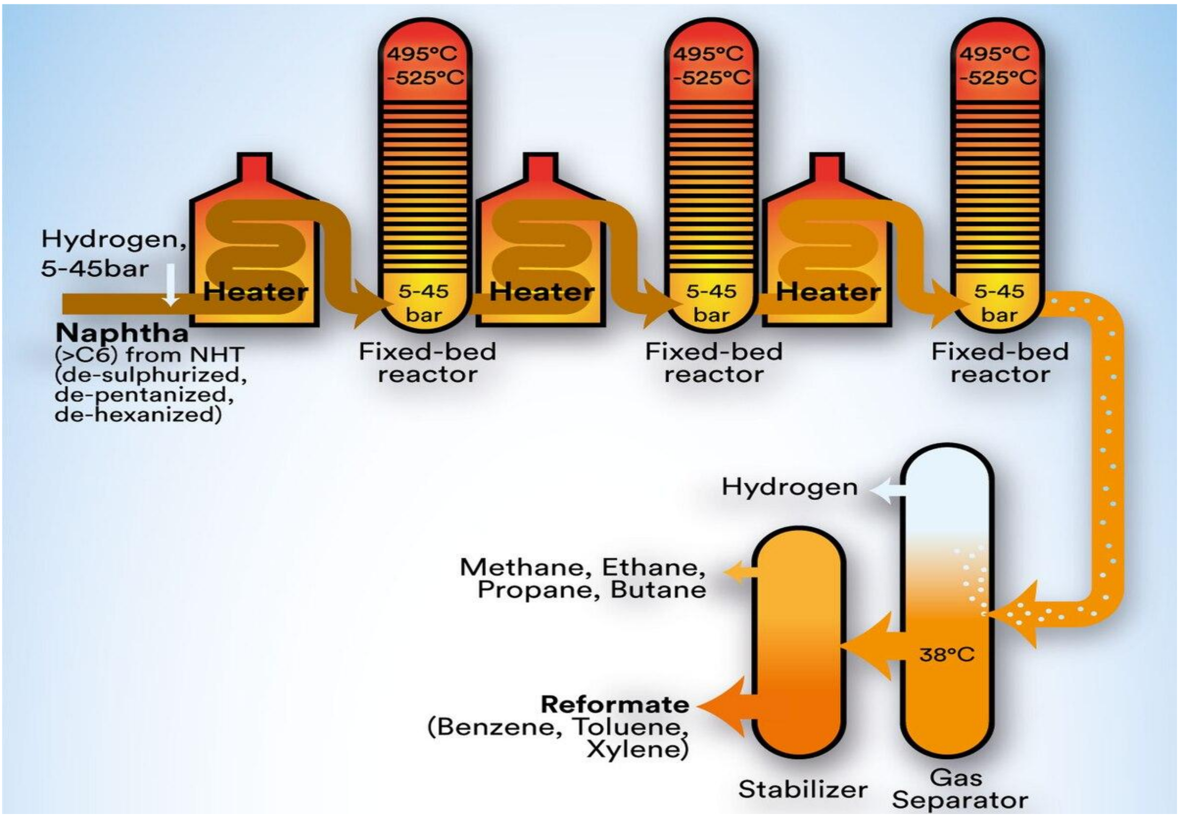


Fig 5. Haworth synthesis of naphthalene [11]

3. Catalytic Reforming:

Catalytic reforming involves transforming light naphtha fractions from crude oil into heavier hydrocarbons, including naphthalene. The process occurs under high temperatures (500-550°C) and pressures (20-50 atm) in the presence of a catalyst. This catalyst, typically platinum or rhenium supported on alumina, promotes the cracking and cyclization reactions responsible for naphthalene formation.

Fig 6. Continuous Catalytic reforming



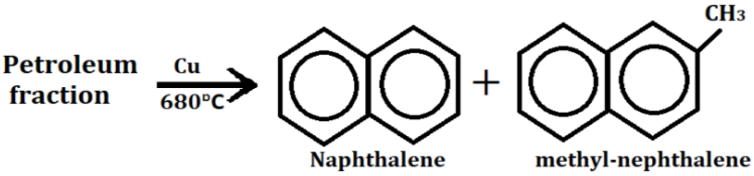
Reaction Mechanism:

The exact reaction mechanism for naphthalene formation is complex and involves several intermediate steps. However, the general pathway involves:

- Dehydrogenation: Removal of hydrogen atoms from naphtha molecules, leading to the formation of olefins.
- Aromatization: Cyclization and aromatization of olefins to form naphthene intermediates.
- Dehydrocyclization: Further dehydrogenation and cyclization of naphthene intermediates to yield naphthalene. [12]

4. From petroleum:

When petroleum fraction is passed over copper (Cu) as a catalyst at 680°C then naphthalene and methyl naphthalene are formed.



Preparation of naphthalene

After this, methyl naphthalene is separated and further converted into naphthalene by heating with hydrogen under process. [13]

5. From 4-phenyl-1-butene:

When 4-phenyl-1-butene is react with red hot calcium oxide, then naphthalene is formed. (13)

Chemical Reactions of Naphthalene:

Naphthalene, with its unique fused-ring structure and aromatic character, exhibits a rich tapestry of chemical reactions. This review dives deep into the intricate details of these reactions, providing structures and relevant literature sources.

1. Electrophilic Aromatic Substitution (EAS):

This is the most common reaction of naphthalene, involving the replacement of a hydrogen atom with an electrophile (E+) at one of the benzene rings. It occurs under mild conditions and can be directed to specific positions using various catalysts and substituents.

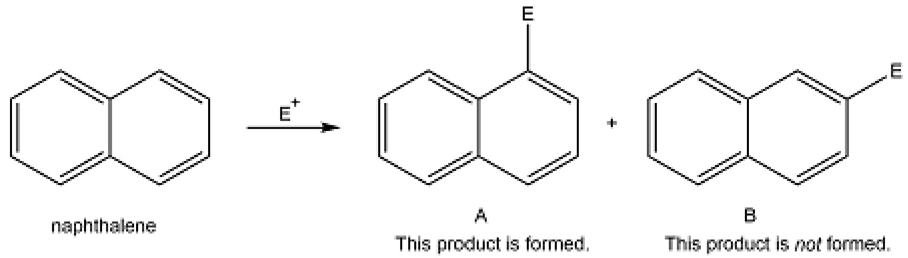


Fig 7. Naphthalene structure and EAS reaction (13)

Examples:

- Nitration with nitric acid: Forms 1-nitronaphthalene (C10H7NO2).
- Sulfonation with sulfuric acid: Forms 1-naphthalenesulfonic acid (C10H7SO3H).
- Halogenation with chlorine or bromine: Forms various halogenated naphthalene (e.g., 1-chloronaphthalene (C10H7Cl)). **(14)**

2. Oxidation:

Naphthalene can be oxidized by strong oxidizing agents like potassium permanganate (KMnO4) or chromic acid (H2CrO4). The specific product depends on the reaction conditions and the oxidizing agent used.

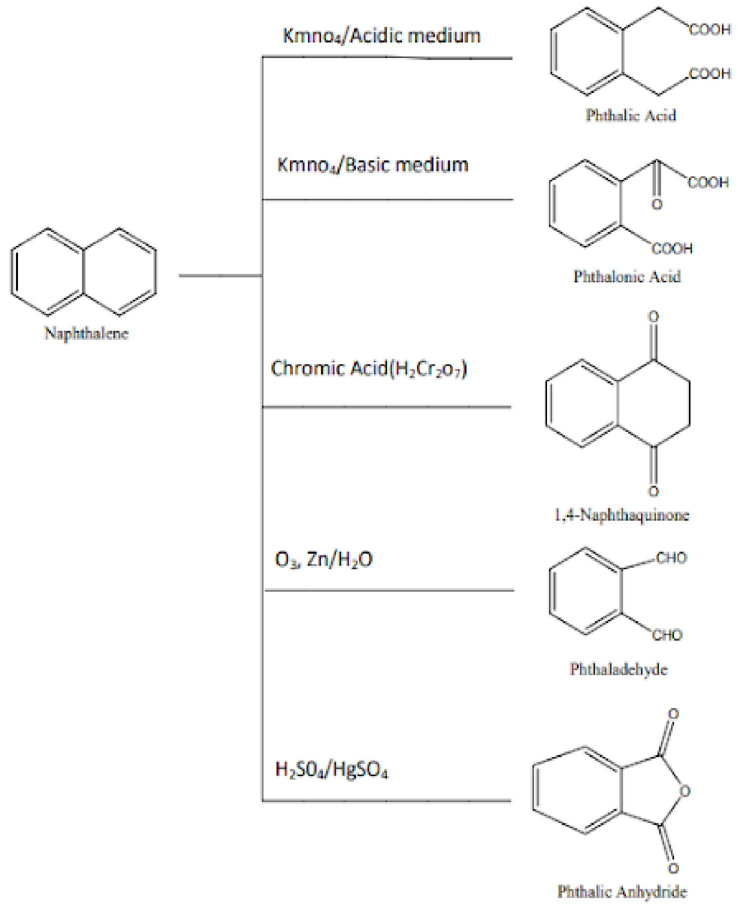


Fig 8. Oxidation of naphthalene [15]

3. Reduction:

Naphthalene can be reduced by hydrogen gas (H2) in the presence of catalysts like nickel (Ni) or platinum (Pt) to form 1,2-dihydronaphthalene (tetralin).

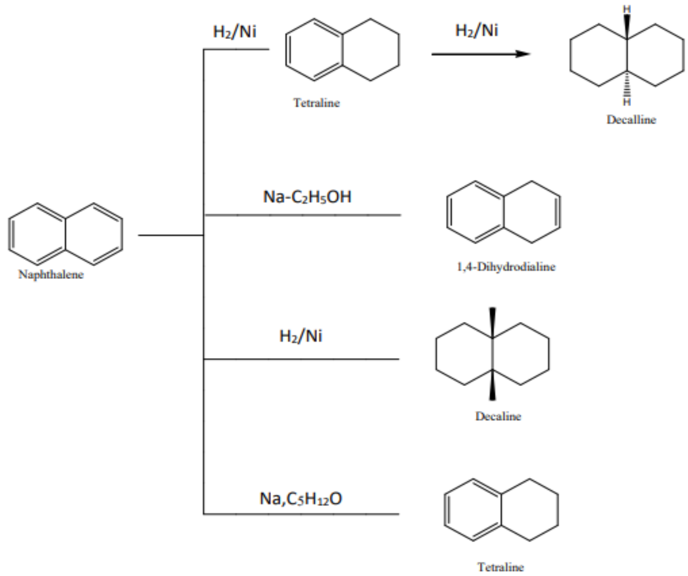


Fig 9. Reduction of naphthalene [15]

4. Diels-Alder Reaction:

Naphthalene can act as a diene in Diels-Alder reactions, allowing for the construction of complex cyclic molecules with valuable properties. [16]

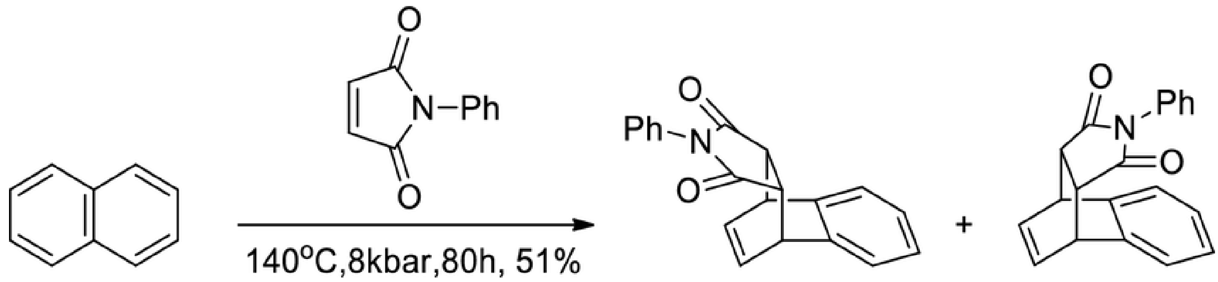


Fig 10. DA reaction naphthalene with N-phenyl-maleimide [16]

Naphthalene derivatives:

The partial list of naphthalene derivatives includes the following compounds: [17]

Name	Chemical formula	Molar mass [g/mol]	Melting point [°C]	Boiling point [°C]	Density [g/cm^3]
1-Naphthoic acid	$C_{11}H_8O_2$	172.18	157	300	
1-Naphthoyl chloride	$C_{11}H_7ClO$	190.63	16–19	190 (35 Torr)	1.265
1-Naphthol	$C_{10}H_8O$	144,17	94–96	278	1.224
1-Naphthaldehyde	$C_{11}H_8O$	156,18	1–2	160 (15 Torr)	-

1-Nitronaphthalene	$C_{10}H_7NO_2$	173.17	53–57	340	1.22
1-Fluoronaphthalene	$C_{10}H_7F$	146.16	−19	215	1.323
1-Chloronaphthalene	$C_{10}H_7Cl$	162.62	−6	259	1.194
2-Chloronaphthalene	$C_{10}H_7Cl$	162.62	59.5	256	1.138
1-Bromonaphthalene	$C_{10}H_7Br$	207.07	−2	279	1.489
1,2,7-Trimethylnaphthalene (Sapotalin)	$C_{13}H_{14}$	170.25	143	128	0.987

Applications of Naphthalene:

Naphthalene, a versatile molecule with its unique structure and properties, boasts a diverse range of applications across various industries. This review explores the numerous applications of naphthalene, providing insights into their significance and relevant literature sources.

1. Moth Repellent:

The most well-known use of naphthalene is as a moth repellent. Its characteristic odor effectively deters moths, protecting fabrics and other materials from damage. [18]

2. Chemical Production:

Naphthalene serves as a crucial building block in the production of various chemicals, including:

- Phthalic anhydride: Used in the manufacture of plastics, dyes, and resins.
- Naphthalenedisulfonic acids: Used in the production of detergents, dyes, and pharmaceuticals.
- 2-Naphthol: Used as an intermediate in the synthesis of dyes and pharmaceuticals. [19]

3. Pharmaceuticals:

Naphthalene derivatives play a vital role in the development of several pharmaceuticals, including:

- Naproxen: A nonsteroidal anti-inflammatory drug used to treat pain and inflammation.
- Warfarin: An anticoagulant medication used to prevent and treat blood clots.
- Atenolol: A beta-blocker medication used to treat high blood pressure and heart disease. [20]

4. Solvents and Lubricants:

Certain derivatives of naphthalene are used as solvents due to their high boiling points and low volatility. Additionally, some naphthalene derivatives find applications as lubricants due to their thermal stability and viscosity. [21]

5. Other Applications:

Naphthalene also finds applications in various other fields, including:

- Deodorant blocks: Releases a mild fragrance and helps absorb moisture.
- Plasticizers: Used to enhance the flexibility and processability of plastics.
- Dyes and pigments: Some naphthalene derivatives are used as colorants in various applications. [22]

CONCLUSION-

Naphthalene, with its unique structure and diverse properties, has carved a distinct niche in the realm of chemistry. Its journey, from a historical curiosity to a versatile building block, exemplifies the continuous evolution of scientific exploration. Modern synthesis methods ensure efficient and sustainable production, while its diverse reactions unlock a treasure trove of valuable products. From its crucial role in phthalic acid production to its promising applications in novel materials and therapeutics, naphthalene's potential remains boundless. As research unveils further insights into this captivating molecule, we can anticipate even greater advancements, solidifying its enduring legacy and shaping the future of chemistry across various fields.

AKNOWLEDGEMENT-

The author extends their heartfelt gratitude to Ms. Swagati A Moon for their invaluable guidance, unwavering support, and significant contributions during the creation of this review article.

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