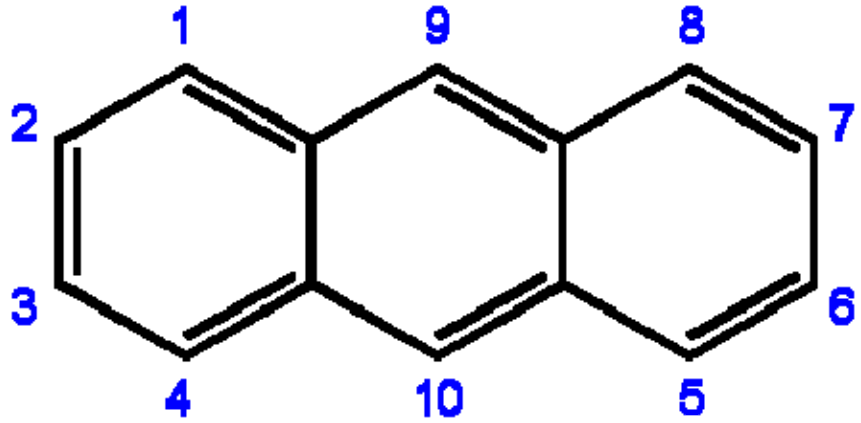
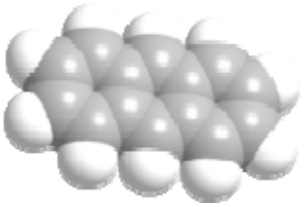
Anthracene

Anthracene[1]	
	
	
IUPAC name	Anthracene
Identifiers	
CAS number	[120-12-7]
SMILES	C12=CC=CC=C1C=C3C(C=CC=C3)=C2
Properties	
Molecular formula	$C_{14}H_{10}$
Molar mass	178.23 g mol^{-1}
Appearance	Colorless

Density	1.25 g/cm³ at 19.85 °C, Solid 0.969 g/cm³ at 220 °C, liquid
Melting point	218 °C, 491 K, 424 °F
Boiling point	340 °C, 613 K, 644 °F
Solubility in other solvents	Water: none Methanol: 0.908g per liter Hexane: 1.64g per liter
Hazards	
EU classification	Dangerous for the Environment
Except where noted otherwise, data are given for materials in their standard state (at 25 °C, 100 kPa)	

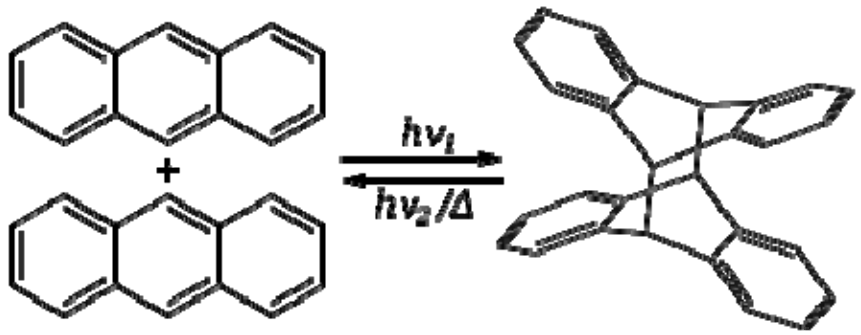
Anthracene is a solid polycyclic aromatic hydrocarbon consisting of three fused benzene rings derived from coal-tar or other residues of thermal pyrolysis. Anthracene is used in the artificial production of the red dye alizarin. It is also used in wood preservatives, insecticides, and coating materials. Anthracene is colorless but exhibits a blue (400-500 nm peak) fluorescence under ultraviolet light.

Synthesis

A classic method for the preparation of anthracene in the laboratory is by cyclodehydration of o-methyl- or o-methylene-substituted diarylketones in the so-called Elbs reaction.

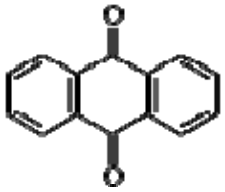
Reactions

Anthracene has the ability to photodimerize with irradiation by UV light. This results in considerable changes in the physical properties of the material.



The dimer is connected by two covalent bonds resulting from the [4+4] cycloaddition. The dimer reverts to anthracene thermally or with UV irradiation below 300 nm. The reversible bonding and photochromic properties of anthracenes is the basis of many potential applications using poly and monosubstituted anthracene derivatives. The reaction is sensitive to oxygen.

In most other reactions of anthracene, the central ring is also targeted, as it is the most highly reactive. Electrophilic substitution occurs at the "9" and "10" positions of the center ring, and oxidation of anthracene occurs readily, giving anthraquinone, $C_{14}H_8O_2$ (below).



Uses

Anthracene derivatives having a hydroxyl group are 1-hydroxyanthracene and 2-hydroxyanthracene, homologous to phenol and naphthols, and hydroxyanthracene is also called anthrol, and anthracenol.[2][3] Hydroxyanthracene derivatives are pharmacologically active, and are contained in aloe for example (specifically in the aloe latex - the references cited for this are inaccurate as they describe the aloe latex, which is typically not a part of the plant used in commerce or is removed during processing [IASC, 2009].[4][5]

Anthracene is an organic semiconductor. It is used as a scintillator for detectors of high energy photons, electrons and alpha particles. Plastics such as polyvinyltoluene can be doped with anthracene to produce a plastic scintillator that is approximately water equivalent for use in radiation therapy dosimetry. Anthracene's emission spectrum peaks at between 400 nm and 440 nm.

Bipedal derivative

In 2005, chemists at the University of California, Riverside developed the first bipedal molecule, 9,10-Dithioanthracene, which propels itself in a straight line when heated on a flat copper surface. Researchers believe the molecule has potential for use in molecular computers.

Toxicology

In spite of other polycyclic aromatic hydrocarbons (PAH), anthracene is **not** carcinogenic but has been recently included in the Substances of Very High Concern list (SVHC) by

the European Chemicals Agency (ECHA) [1] because being considered Persistent, Bioaccumulative and Toxic (PBT) for freshwater and marine ecosystems [2] within the REACH framework. Anthracene, as many other PAHs is generated during combustion processes: exposure to human happens mainly through tobacco smoke and ingestion of food contaminated with combustion products [3].

See also

- Phenanthrene
- Tetracene

References

1. NIST Chemistry WebBook Anthracene
2. 1-Hydroxyanthracene NIST datapage
3. 2-Hydroxyanthracene NIST datapage
4. TGA News
5. Herbals and Breastfeeding

External links

- International Chemical Safety Card 0825
- IARC - Monograph 32
- National Pollutant Inventory - Polycyclic Aromatic Hydrocarbon Fact Sheet
- European Chemicals Agency - ECHA

v · d · e

Polycyclic aromatic hydrocarbons

2 rings	Azulene · Naphthalene
3 rings	Acenaphthylene · **Anthracene** · Fluorene · Phenanthrene
4 rings	Chrysene · Fluoranthene · Pyrene · Tetracene · Triphenylene
5+ rings	Anthanthrene · Benzo[*a*]pyrene · Corannulene · Coronene · Dicoronylene · Helicene · Hexacene · Ovalene · Pentacene · Picene · Perylene

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Categories: Polycyclic aromatic hydrocarbons | Organic semiconductors | Phosphors and scintillators | IARC Group 3 carcinogens