UNIVERSITETET I OSLO

Kapittel 15

Benzen og aromatisitet

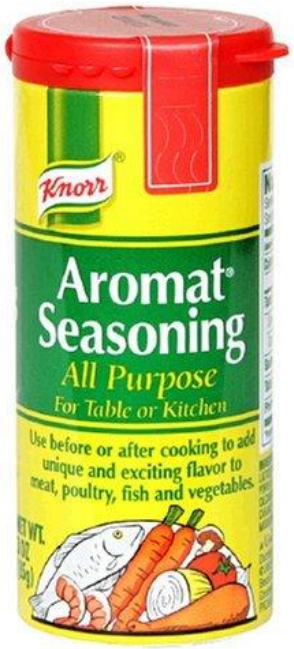
Aromatiske forbindelser

Main Entry: **[1]ar·o·mat·ic**
Pronunciation: \ˌa-rə-ˈma-tik, ˌer-ə-\
Function: *adjective*
Date: 14th century

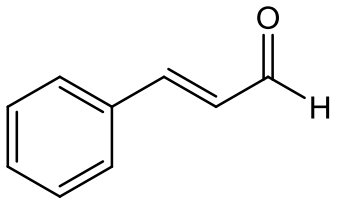
1 : of, relating to, or having aroma: **a** : FRAGRANT **b** : having a strong smell **c** : having a distinctive quality
2 *of an organic compound* : characterized by increased chemical stability resulting from the delocalization of electrons in a ring system (as benzene) containing usually multiple conjugated double bonds — compare ALICYCLIC , ALIPHATIC

synonyms see ODOROUS
— **ar·o·mat·i·cal·ly** \-ti-k(ə-)lē\ *adverb*
— **aro·ma·tic·i·ty** \ə-rə-mə-ˈti-sə-tē, ˌer-ə-, ə-ˌrō-mə-\ *noun*

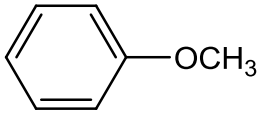
- En klasse forbindelser som historisk sett ble forbundet med en spesiell aroma (duft)



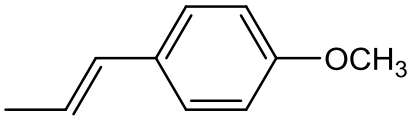
Noen eksempler på aromatiske forbindelser



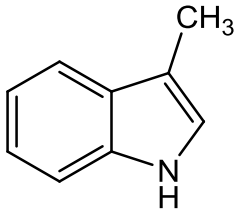
cinnamaldehyd
(kanel)



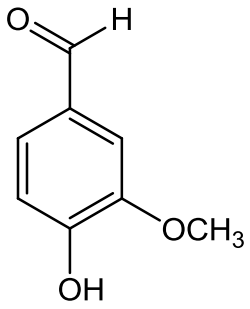
anisol
(anis)



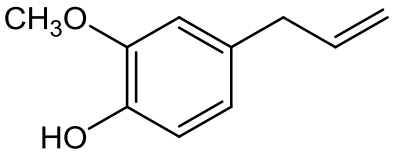
anethol
(anis, lakris, fennikel)



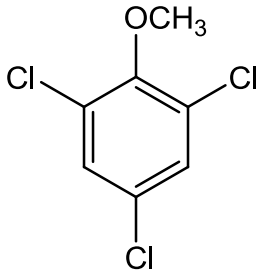
skatol
(kloakk)



vanillin
(vanilje)



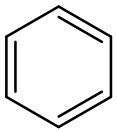
eugenol
(muskat, kanel, basilikum, nellik)



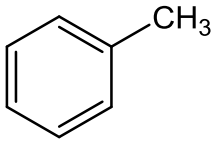
2,4,6-trikloranisol
("korkesyke")

Navnsetting

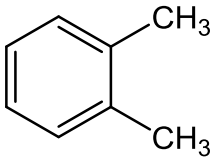
En hel del trivialnavn må kunnes – alle er tillatt av IUPAC



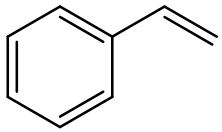
benzen



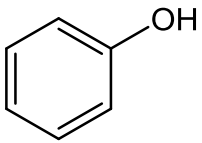
toluen



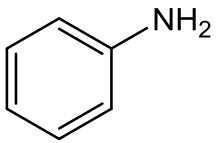
orto-xylen



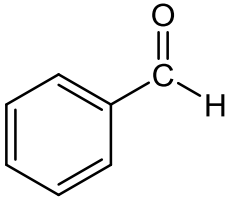
styren



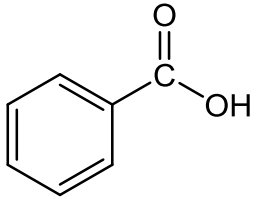
fenol



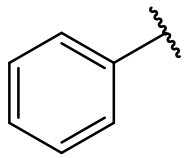
anilin



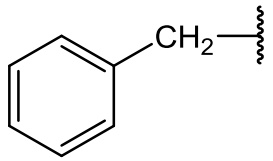
benzaldehyd



benzosyre



fenyl
(C_6H_5-, Ph, ϕ)



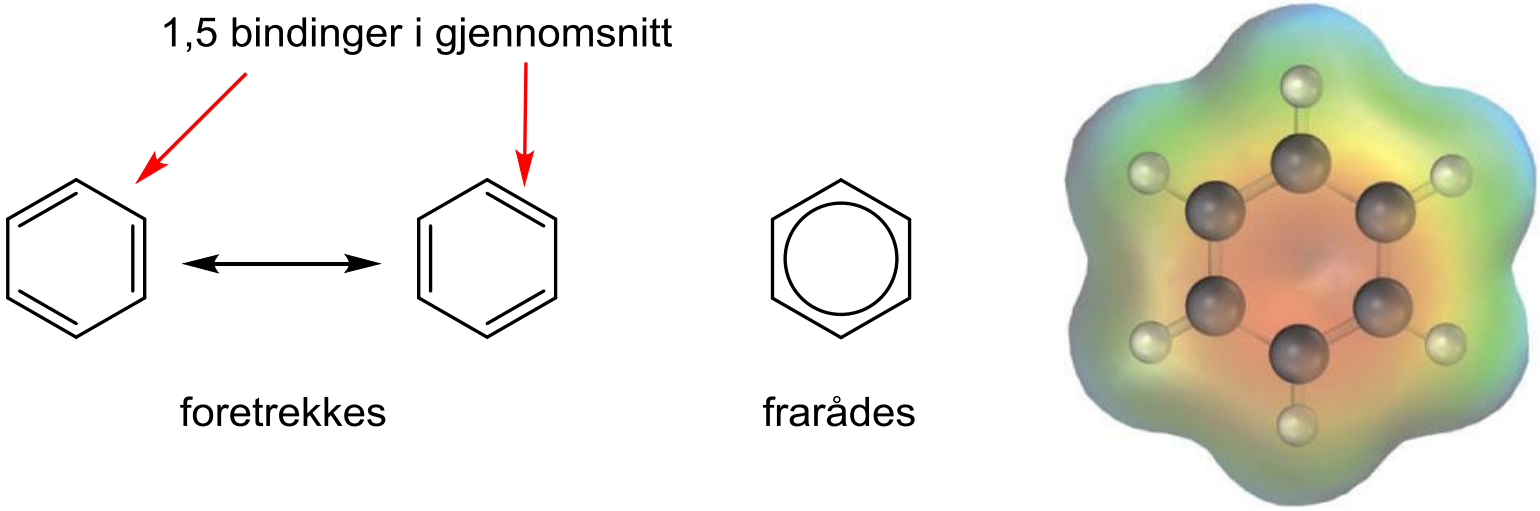
benzyl
($C_6H_5CH_2$-)

Navnsetting

- Monosubstituerte benzener navnsettes som andre hydrokarboner, med *–benzen* som stammen i navnet
- Disubstituerte benzener navnsettes med forstavelsene
  - orto- (1,2-disubstituert)
  - meta- (1,3-disubstituert)
  - para- (1,4-disubstituert)
- Tri- og flersubstituerte nummereres
  - De lavest mulige nummer brukes
  - Substituentene listes alfabetisk
  - Trivialnavnene på forrige lysark kan utgjøre stammen, med hovedsubstituenten pr. definisjon i posisjon 1

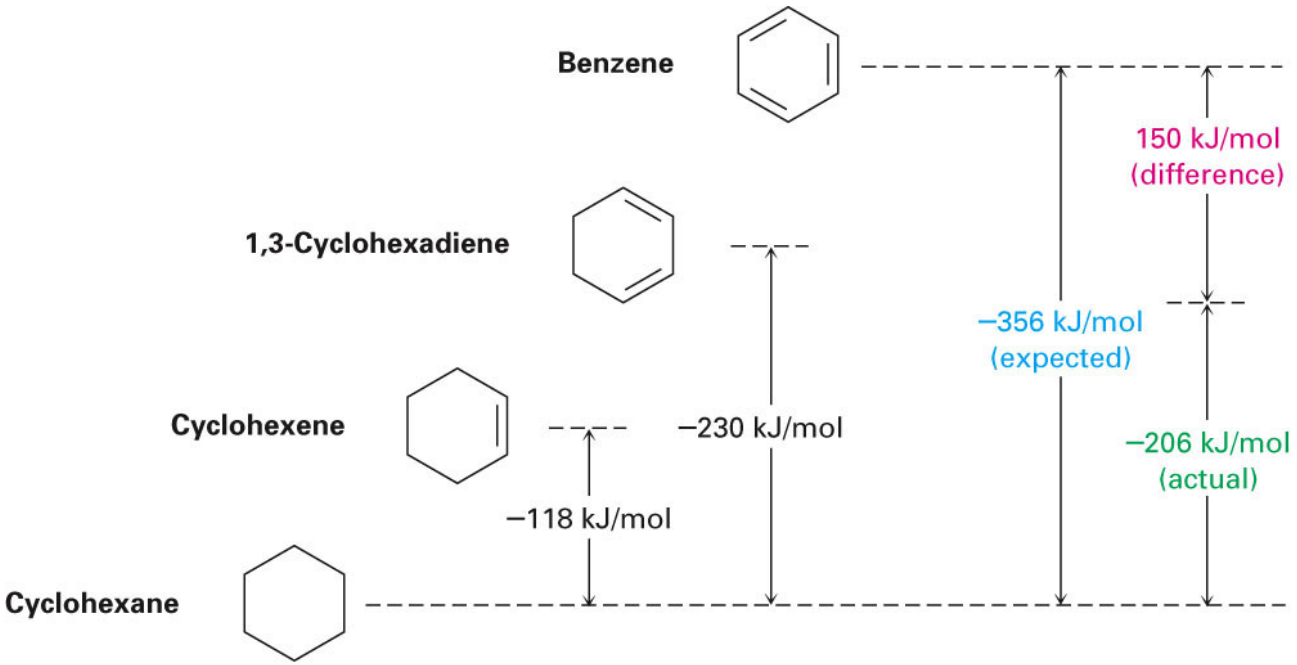
Benzen: Struktur

- Benzen er mindre reaktivt enn typiske alkener
  - Substitusjonsreaksjoner, ikke addisjonsreaksjoner !
- Alle karbon-karbon bindinger i benzen er identiske
  - Bindingsavstander ca. midt mellom C-C og C=C
  - Beskrives med to resonansstrukturer
  - 6 sp^2-hybridiserte karbonatomer i ring
  - "π-elektronsky" over og under ringen



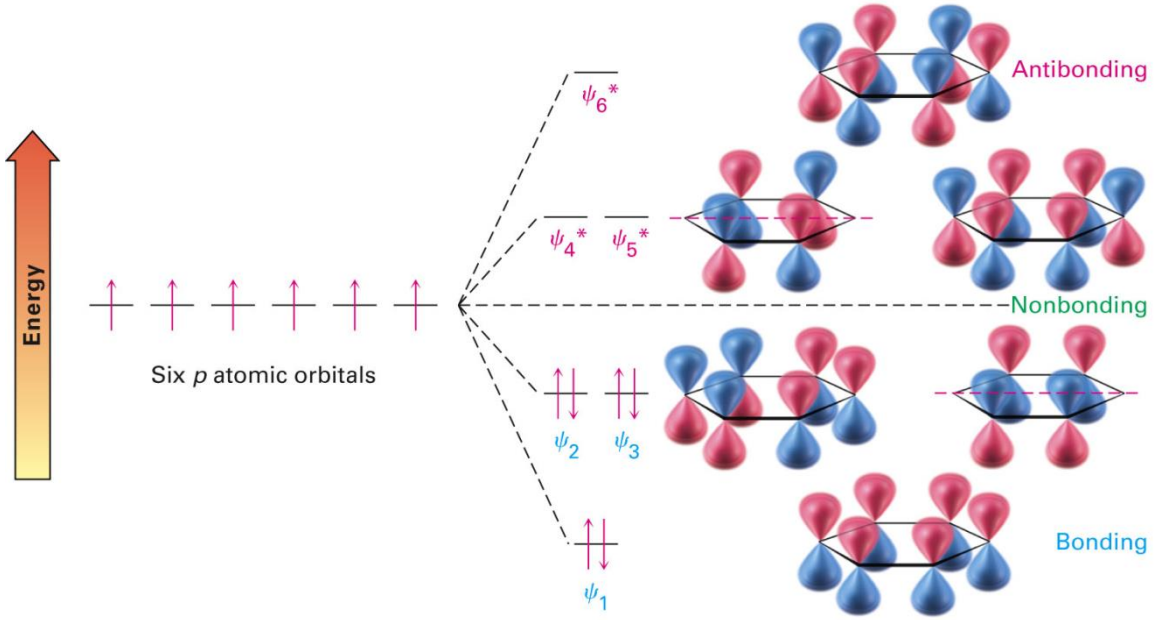
Benzen: Stabilitet

- Hydrogenering av en C=C binding i et alken frigjør 118 kJ/mol
- Fullstendig hydrogenering av benzen frigjør 206 kJ/mol
  - Dette er ca. 150 kJ/mol mindre energi enn 3 x alkenets hydrogeneringsvarme
  - Benzen må derfor være 150 kJ/mol mer stabilt enn 3 alkener i utgangspunktet



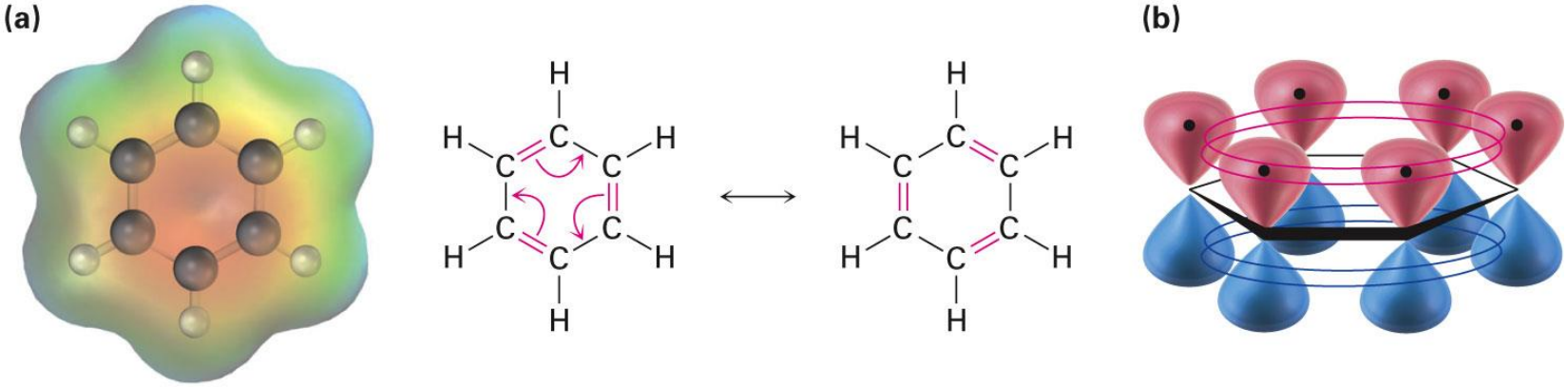
Benzen: π-orbitaler

- Normalt C-H og C-C σ-bindingssystem mellom sp^2-hybridiserte C-atomer
- Utvidet π-bindingssystem
  - Overlapp mellom alle 6 p-orbitaler
  - 6 p-orbitaler kombineres og gir 6 π-orbitaler
  - 3 bindende π-orbitaler utgjør en elektronrik "π-elektronsky" med utstrekning over og under ringens plan



Six benzene molecular orbitals

Benzen:
Resonans og “π-elektronsky”

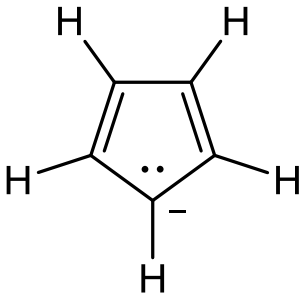


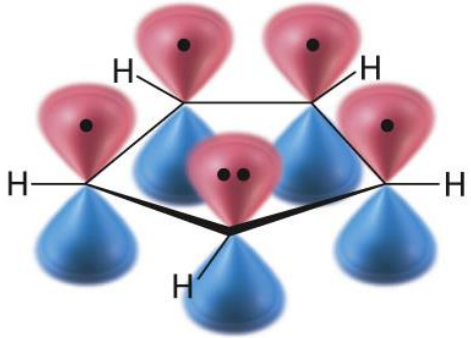
Aromatisitet: Hückels 4n+2-regel

UNIVERSITETET I OSLO

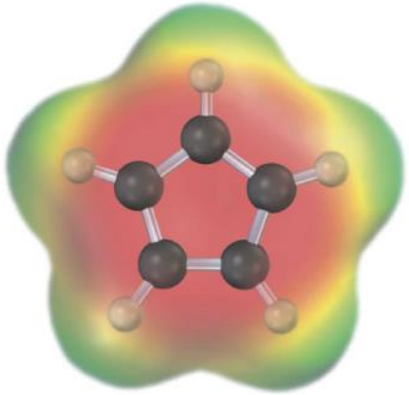
- Benzen er syklisk og plant, med konjugerte C=C bindinger
- Benzen er usedvanlig stabilt sammenlignet med alkener
- Benzen har 120° bindingsvinkler, sp^2 hybridiserte C-atomer, 6 identiske C-C bindingsavstander
- Benzen reagerer annerledes enn alkener
- Benzen beskrives med to identiske resonansstrukturer
- Mange andre ringsystemer enn benzen har lignende egenskaper
- Aromatisitet uttrykt ved Hückels 4n+2 regel:
  - Et molekyl er aromatisk (og spesielt stabilisert) hvis det har 4n+2 π-elektroner i syklisk konjugasjon (n = 0, 1, 2, 3...)
  - Et molekyl er *anti*aromatisk (og destabilisert) hvis det har 4n π-elektroner i syklisk konjugasjon (n = 1, 2, 3...)

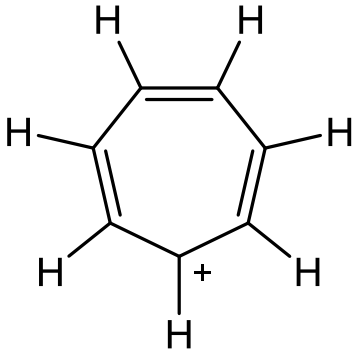
Aromatiske kationer og anioner

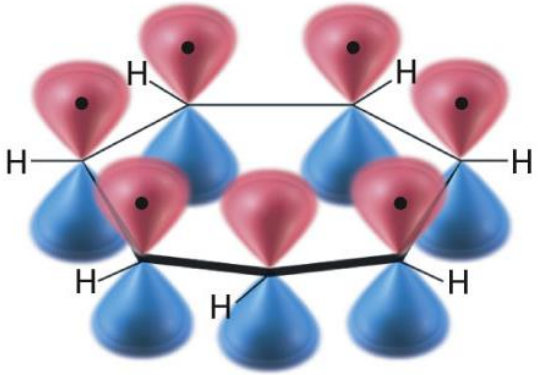




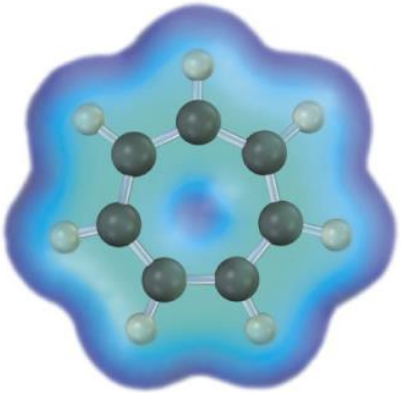
Aromatic cyclopentadienyl anion
with six π electrons







Cycloheptatrienyl cation
six π electrons

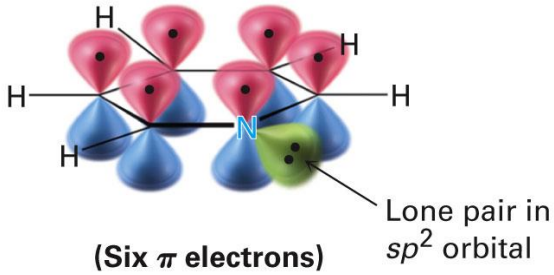


Aromatiske heterosykliske forbindelser

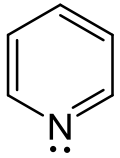
UNIVERSITETET I OSLO

Heterosykliske ringer (hvor ett eller flere atomer er ikke-karbon) kan også være aromatiske, forutsatt at π-systemet har 4n+2 p-elektroner

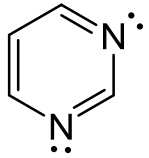
Pyridine



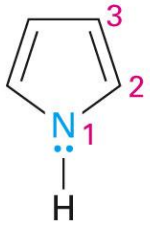
(Six π electrons)



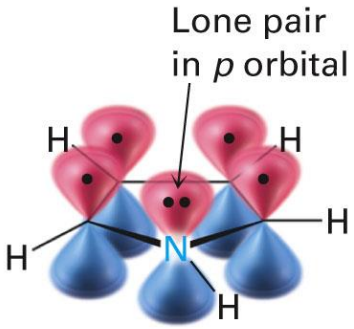
pyridin



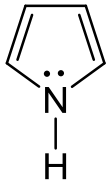
pyrimidin



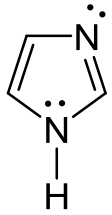
Pyrrole



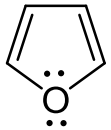
(Six π electrons)



pyrrol



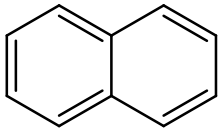
imidazol



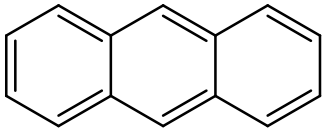
furan

Polysykliske aromatiske hydrokarboner (PAH)

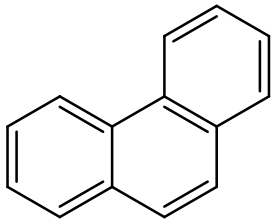
UNIVERSITETET I OSLO



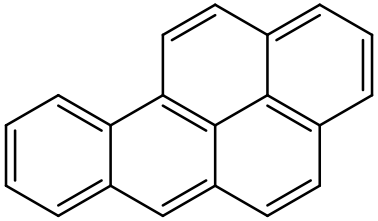
naftalen



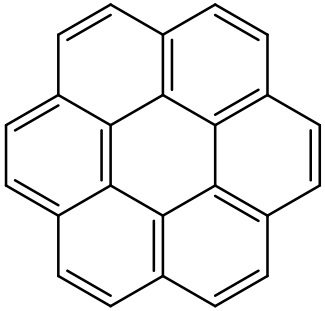
antracen



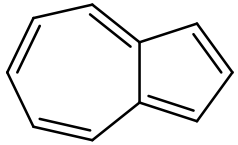
fenantren



benzo[a]pyren

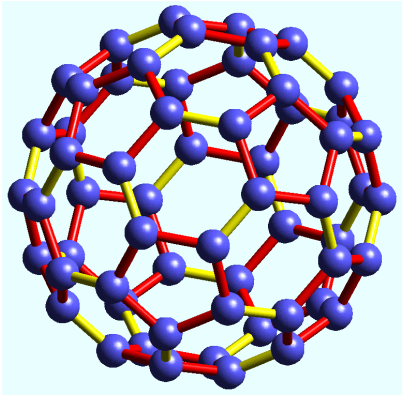


coronen

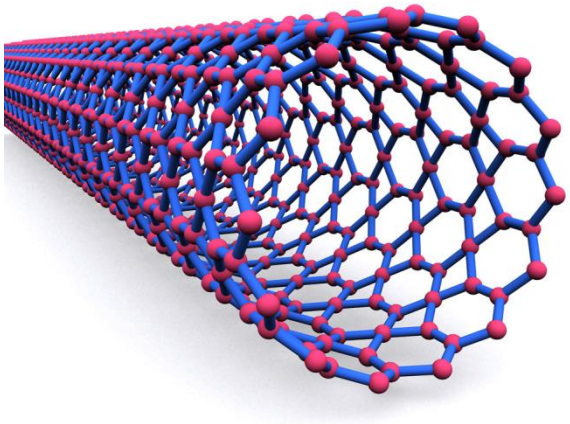


azulen

Polysykliske aromatiske forbindelser – materialkjemi

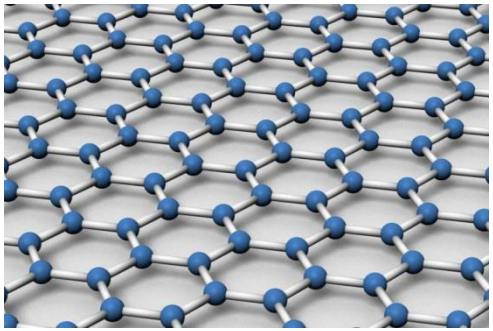


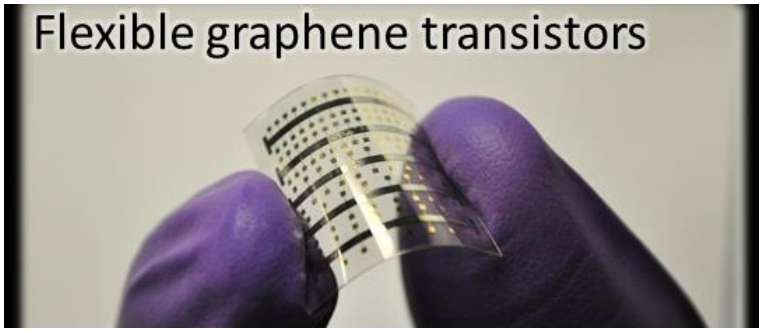
C_{60}
buckyball



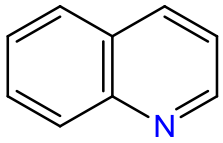
karbon
nanorør

grafen

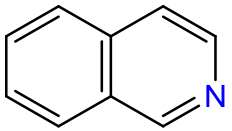




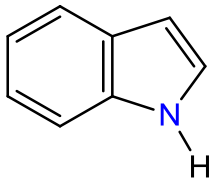
Polysykliske aromatiske forbindelser – biologisk kjemi



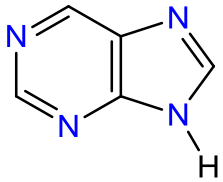
Quinolin



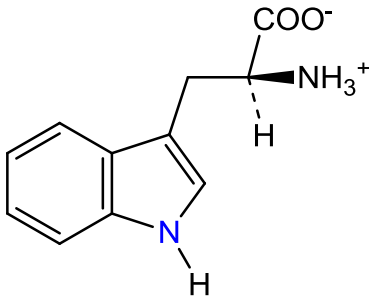
Isoquinolin



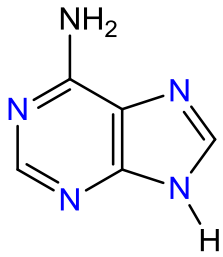
Indol



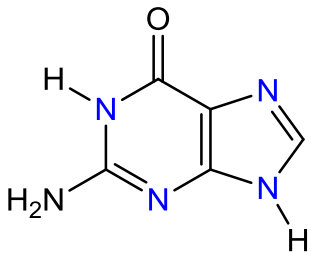
Purin



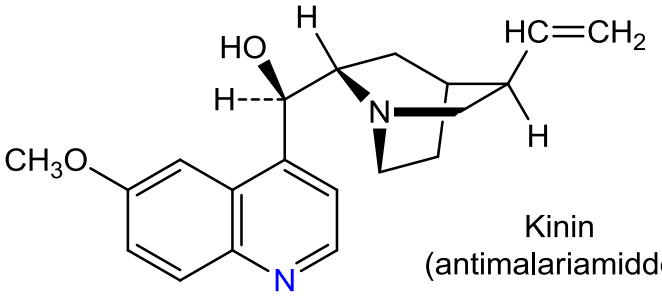
Tryptophan
(aminosyre)



Adenin
(i DNA og RNA)



Guanin
(i DNA og RNA)



Kinin
(antimalariamiddel)