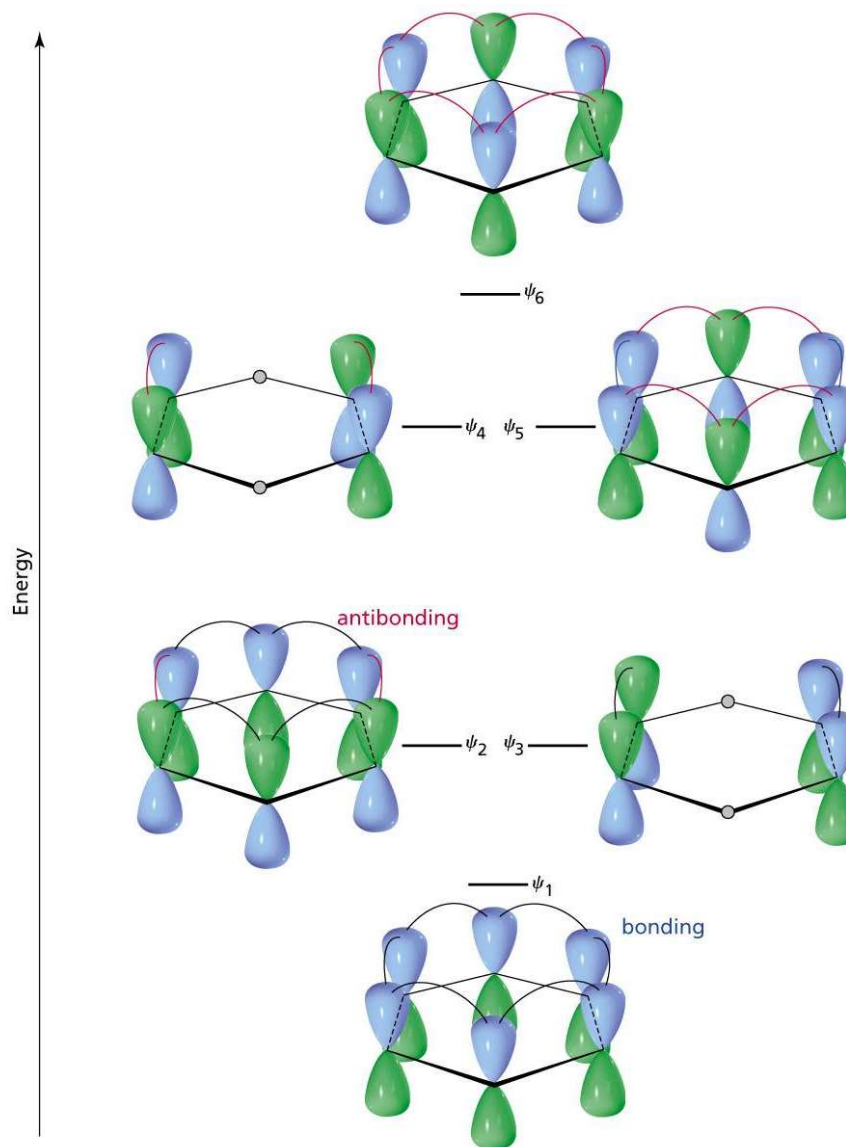
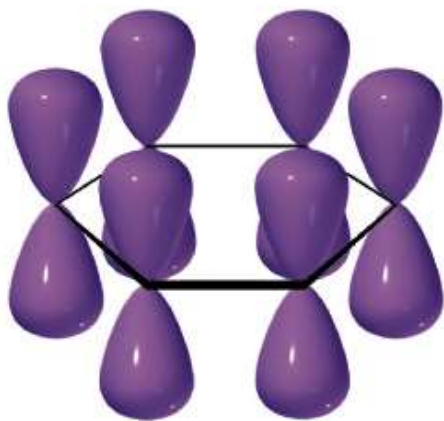
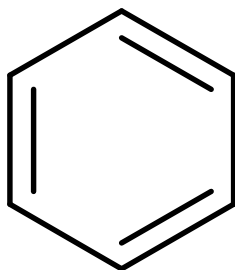
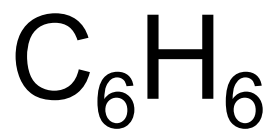


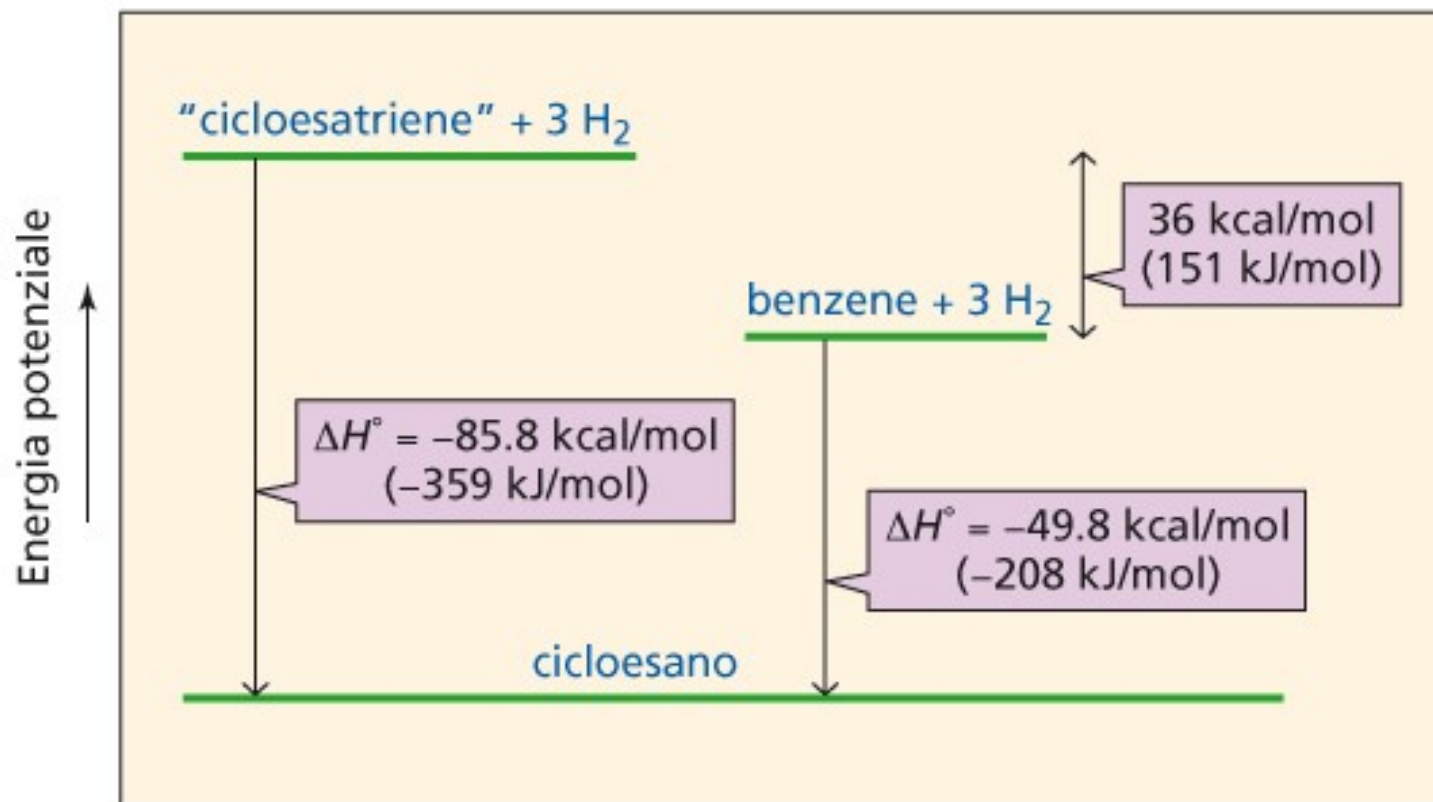
Benzene e aromaticità

Un breve riepilogo

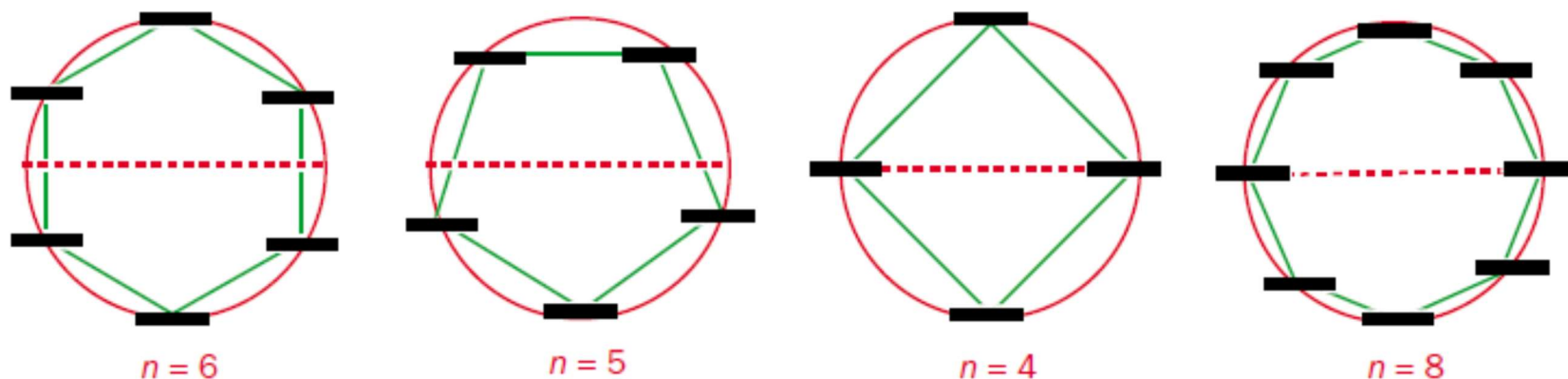


Benzene e aromaticità

Un breve riepilogo



Composti Aromatici: $4n+2$ elettroni

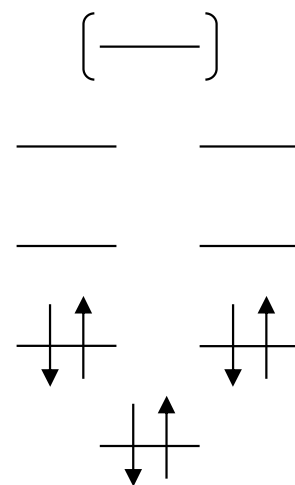
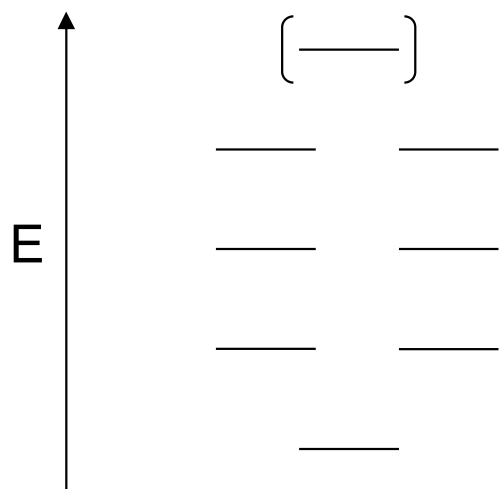


Metodo empirico per valutare l'energia degli orbitali. Si disegna il poligono regolare corrispondente con un vertice puntato verso il basso. L'energia degli orbitali corrisponde ai vertici del poligono. Orbitali sotto il centro del poligono sono di legame, orbitali all'altezza del centro del poligono sono di non legame, orbitali sopra il centro del poligono sono di antilegame.

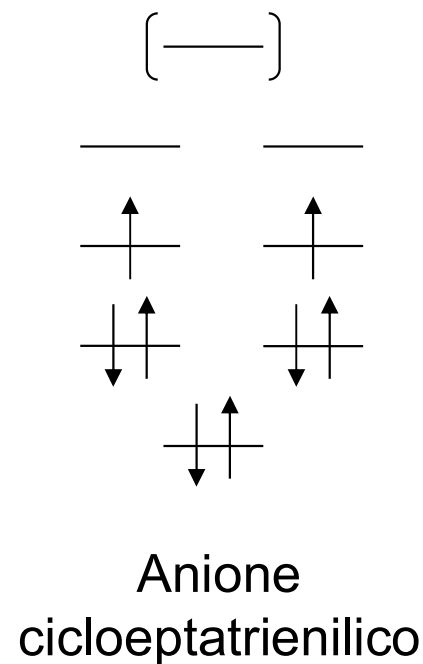
Il sistema è aromatico quando tutti gli orbitali di legame sono riempiti.

Composti Aromatici: Regola di Huckel

Sono aromatici composti che presentano un sistema coniugato ciclico contenente $4n+2$ elettroni (2, 6, 10, 14, 18, ...)



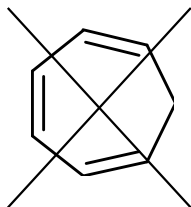
Ione trolilio



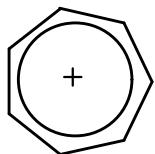
Anione
cicloeptatrienilico

Composti Aromatici

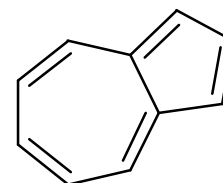
Anelli a 7 atomi:



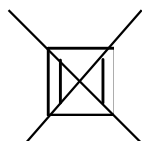
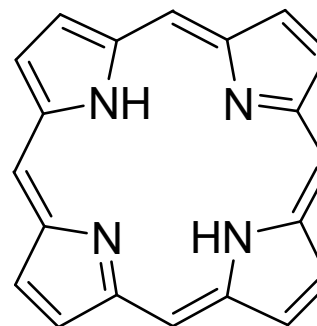
cicloeptatriene



Ione tropilio

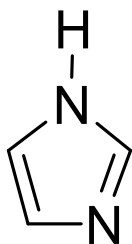
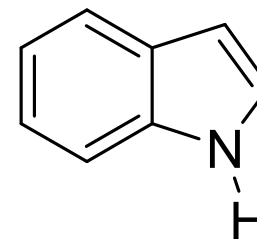
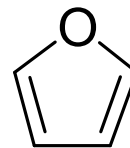
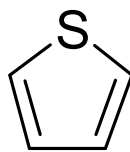
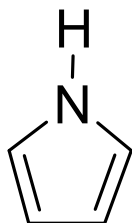
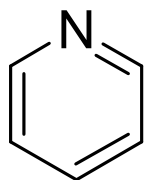
Anione
cicloeptatrienilicoAzulene
($\mu = 0.8$ D)

Altri anelli:

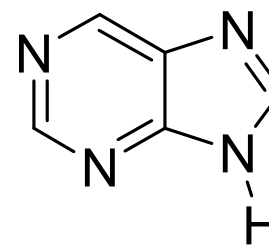
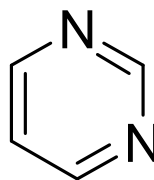
Catione
ciclopropenilicoCiclobutadiene
(4e, antiaromatico)

Porfina (18e)

Composti eteroaromatici

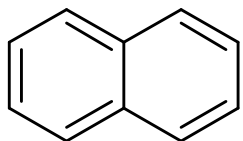


Amminoacidi
(His)

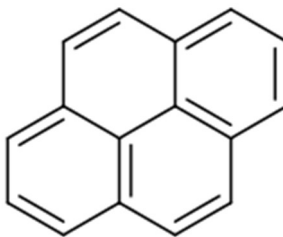


Nucleobasi,
caffeina

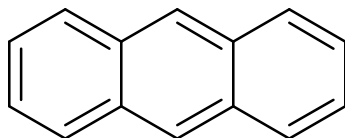
Composti aromatici: quali sono?



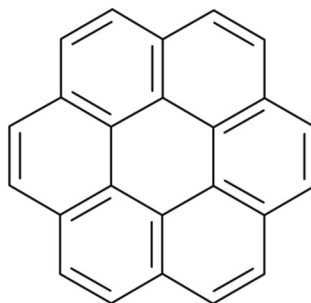
naftalene



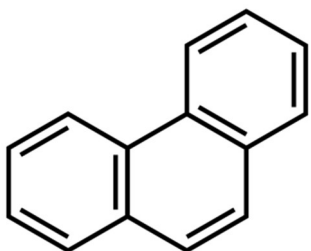
pirene



antracene



coronene



fenantrene

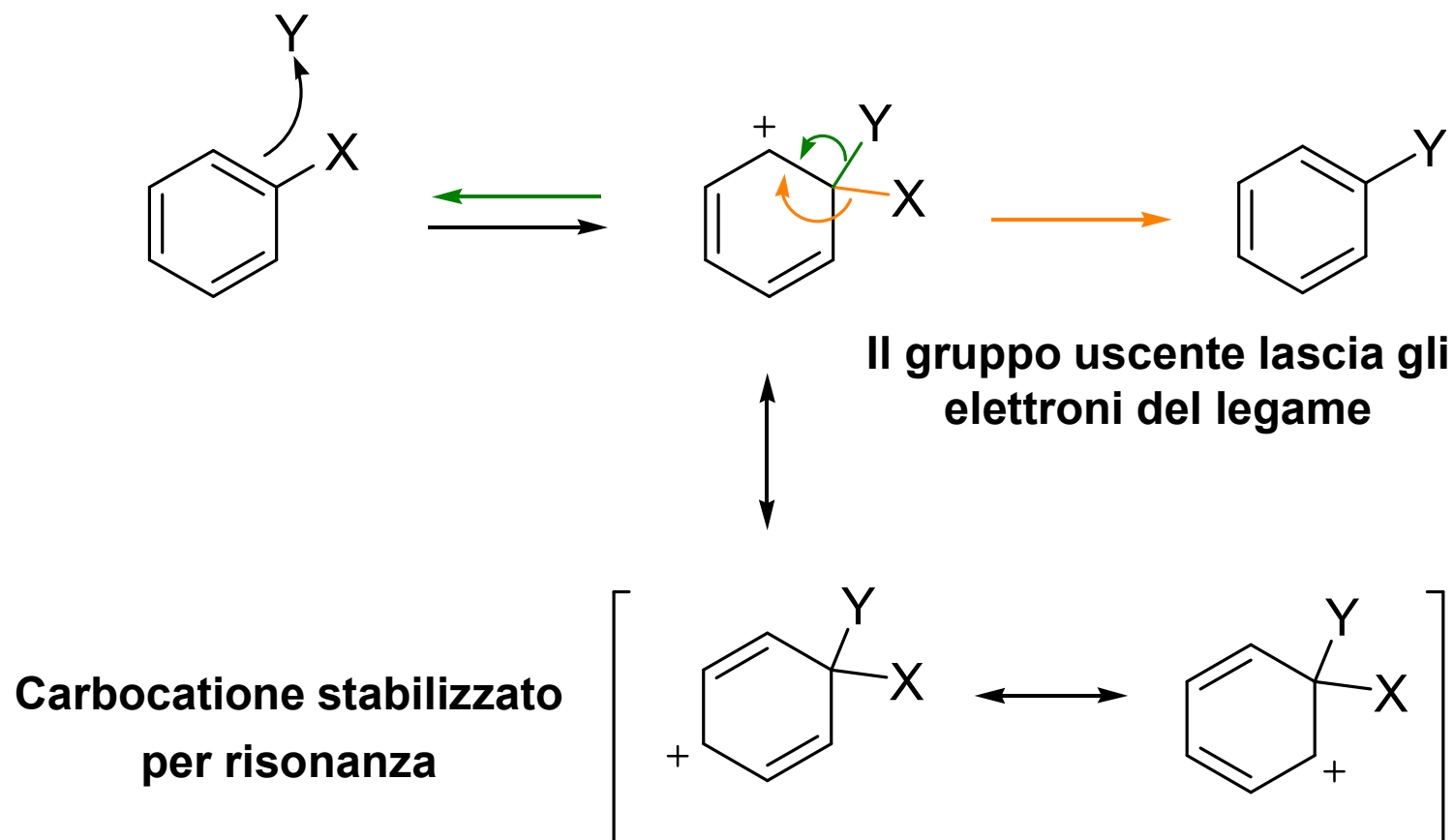


corannulene

Composti aromatici: quali sono?

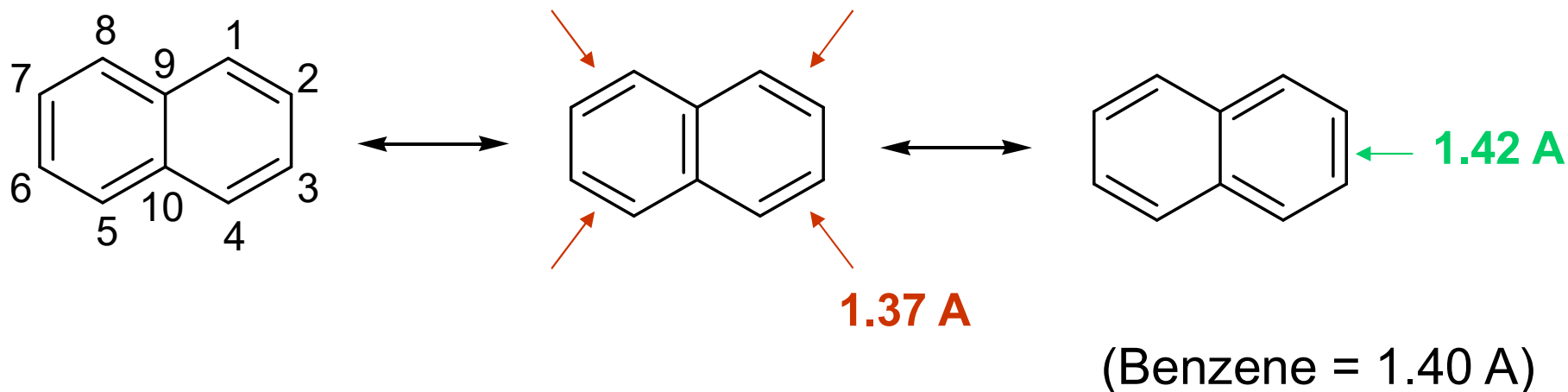
- **$4n+2$** elettroni in sistema π delocalizzato (sempre)
- Corrente di anello (NMR downfield shift, 6-9 ppm, sempre)
- Molto stabili $\Rightarrow$ poco reattivi (non sempre)
- Reazioni di sostituzione elettrofilica (non sempre)
- Formule di risonanza di Kekulé (no)

Sostituzione elettrofila aromatica

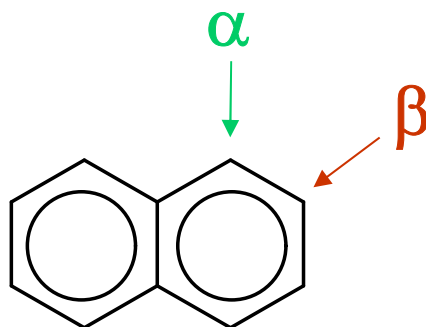


Anelli aromatici condensati: aromatici policiclici

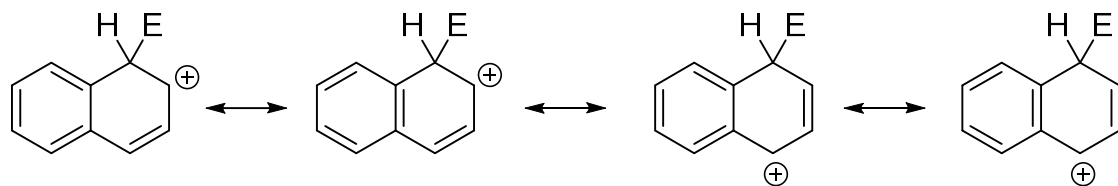
Naftalene



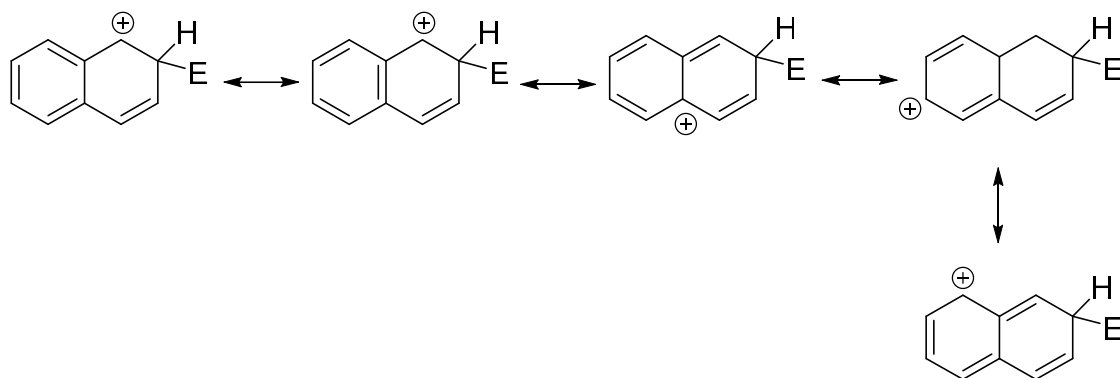
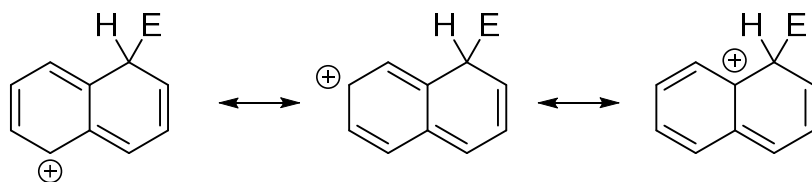
Energia di coniugazione 255 kJ/mol



Naftalene: reattività e orientazione



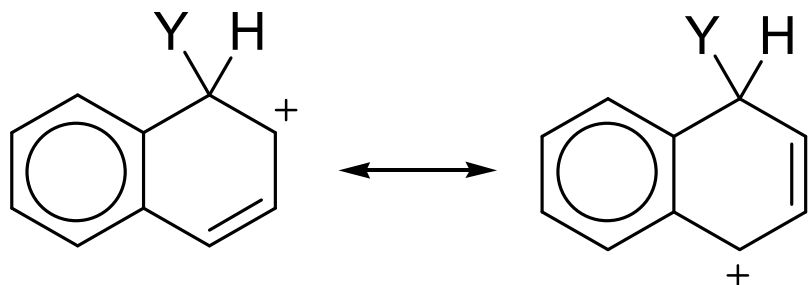
Sostituzione in α



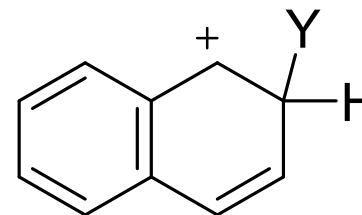
Sostituzione in β

Naftalene: reattività e orientazione

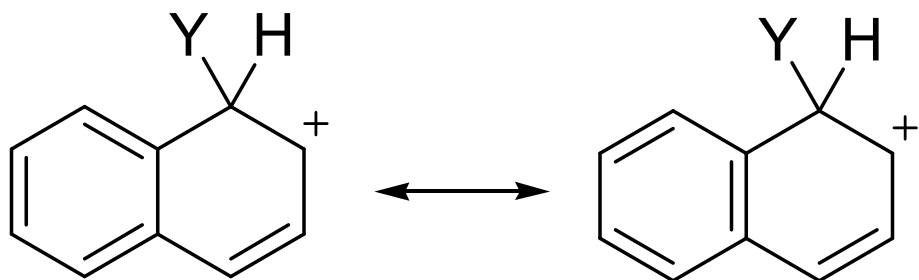
Sostituzione in α



Sostituzione in β

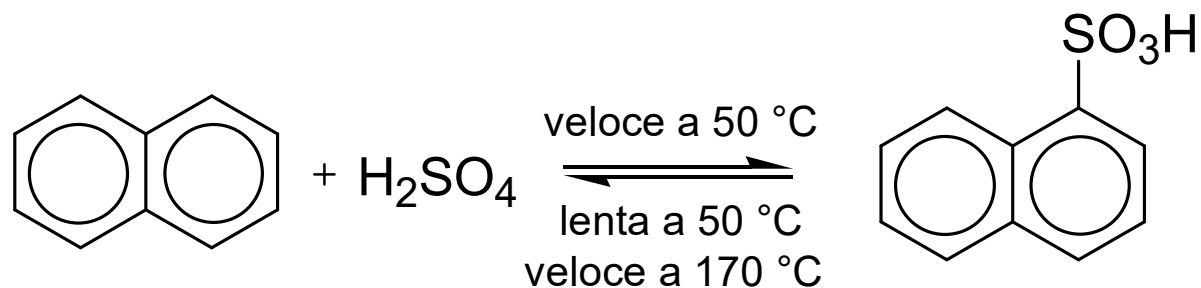
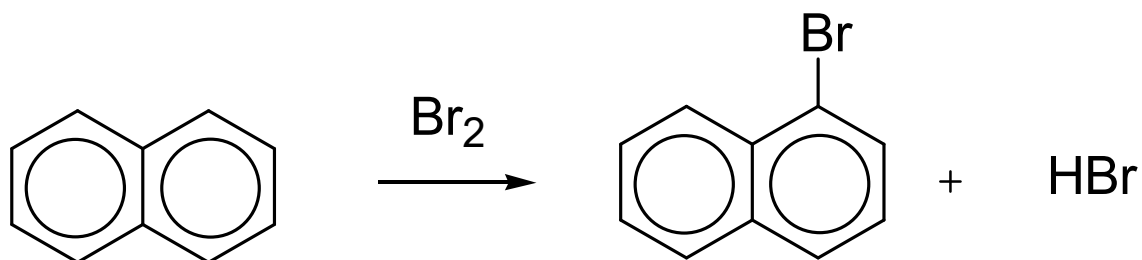


La sostituzione avviene preferenzialmente in posizione α

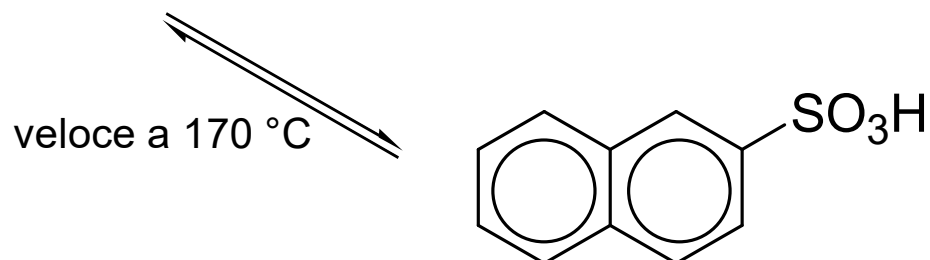


L'intermedio catione arenio ha ancora due forme di Kekulé: il naftalene è più reattivo del benzene

Naftalene: orientazione

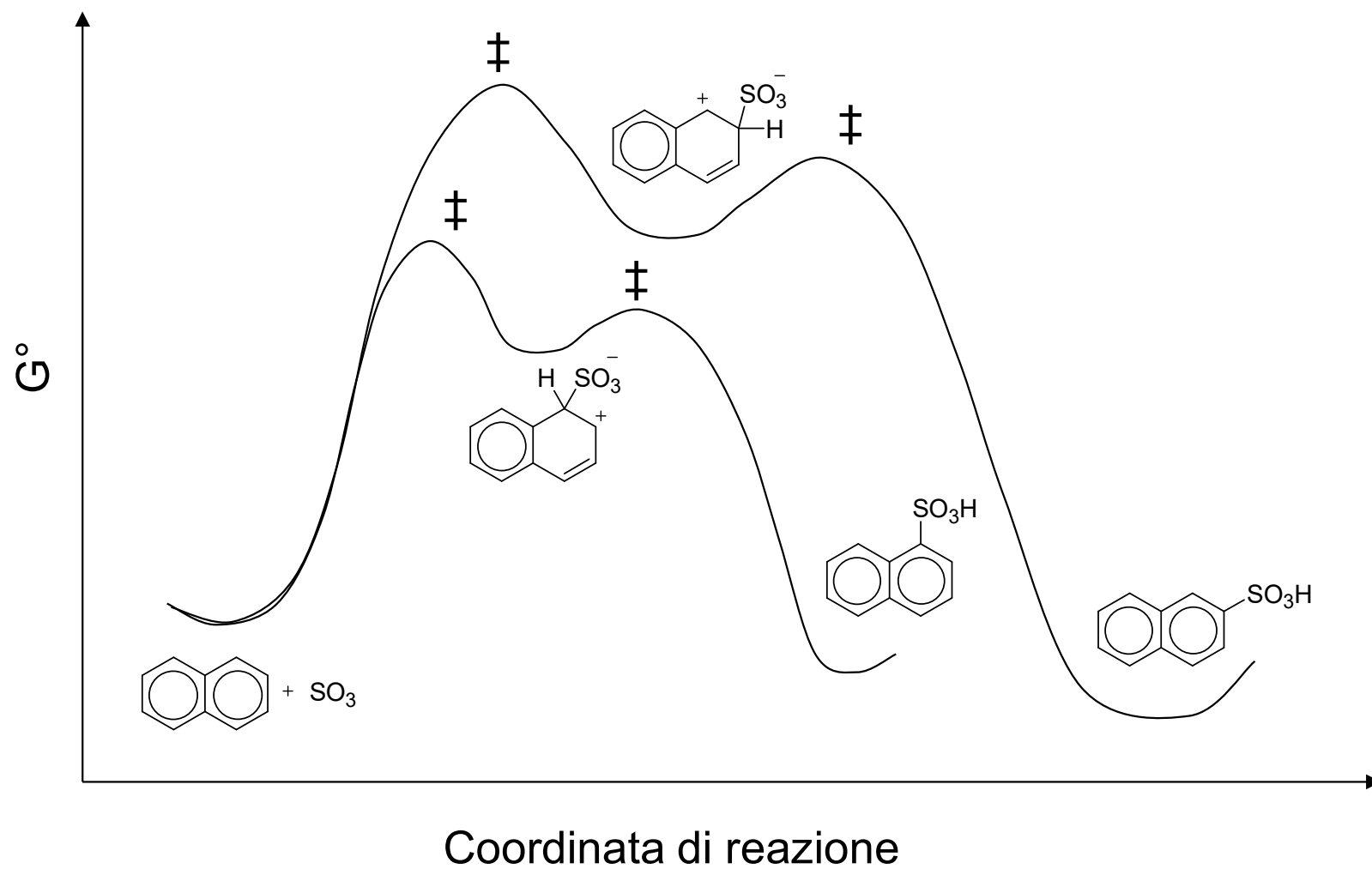


Controllo cinetico

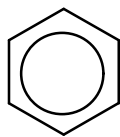
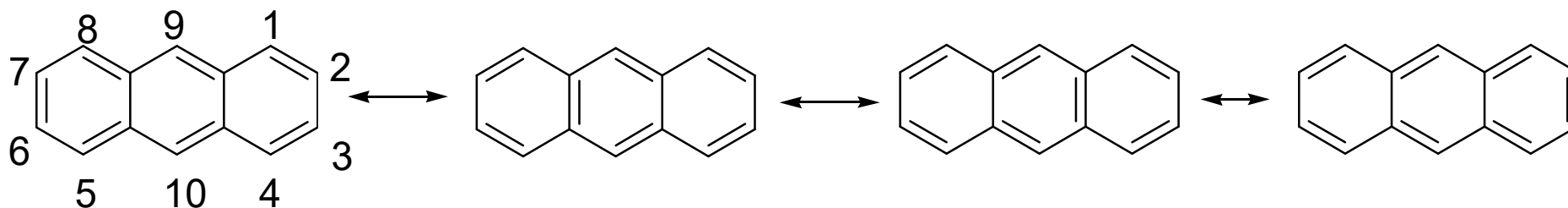


**Controllo
termodinamico**

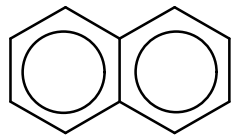
Naftalene: orientazione



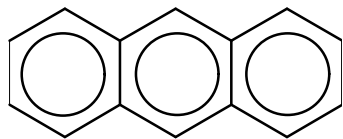
Antracene



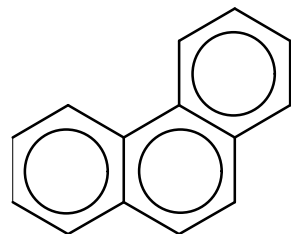
150 KJ/mol



255 KJ/mol

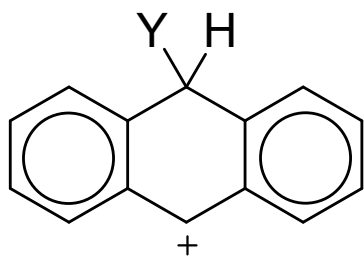


351 KJ/mol

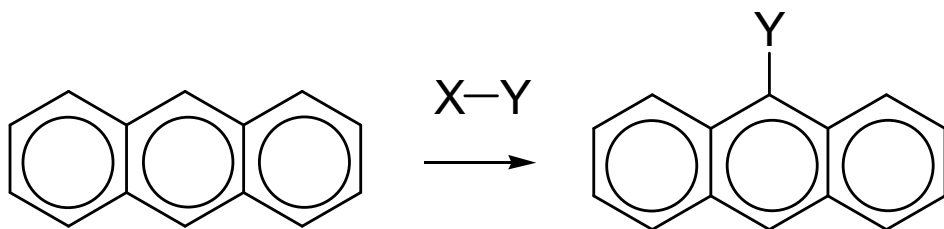


385 KJ/mol

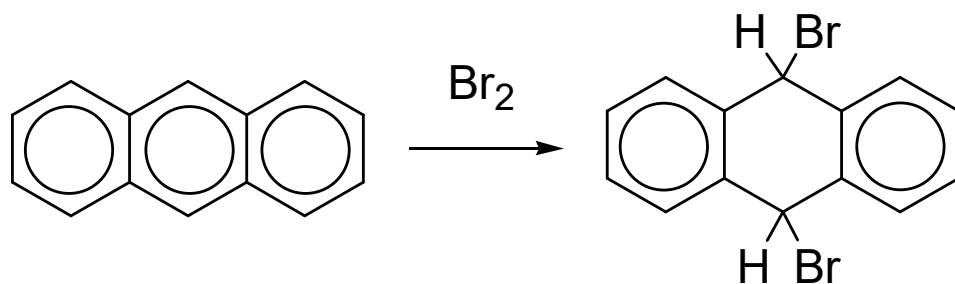
Antracene



L'intermedio catione arenio in posizione 9 ha quattro forme di Kekulé.

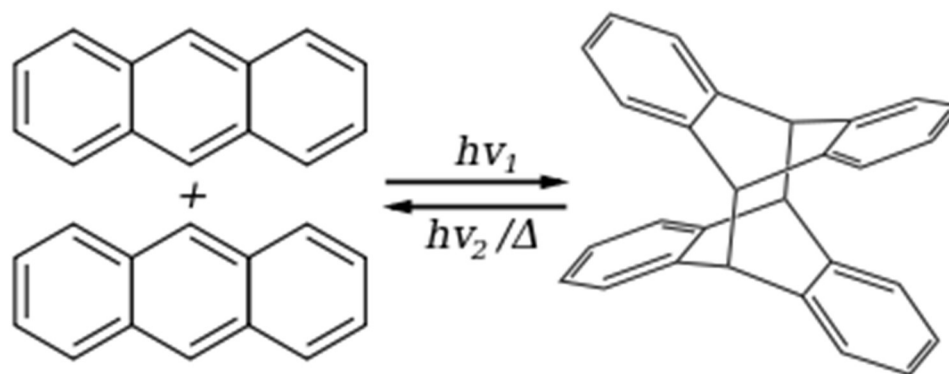
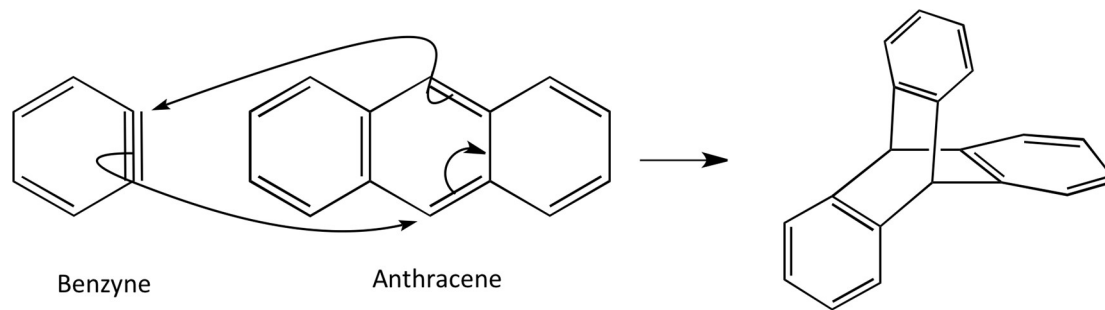
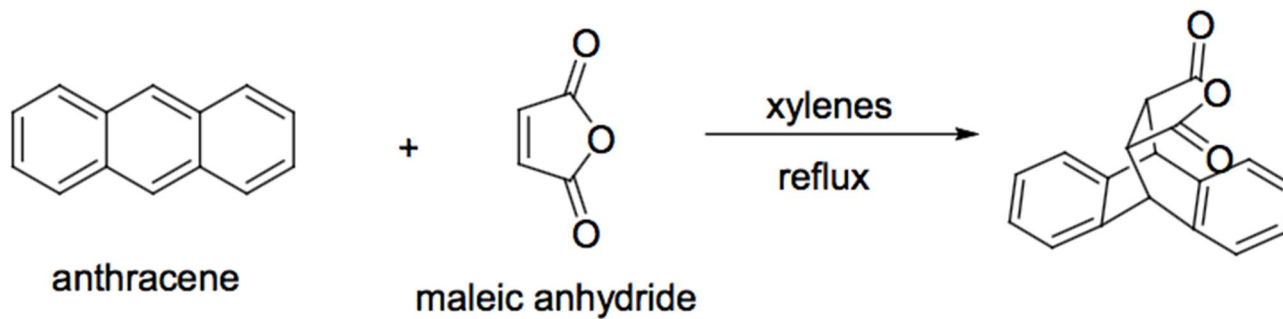


La sostituzione avviene preferenzialmente in posizione 9

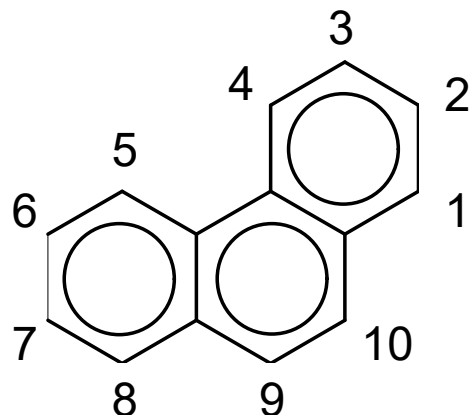


L'antracene può subire addizione alle posizioni 9,10

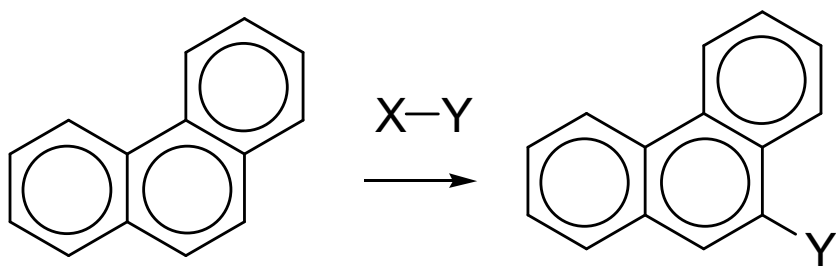
Anthracene



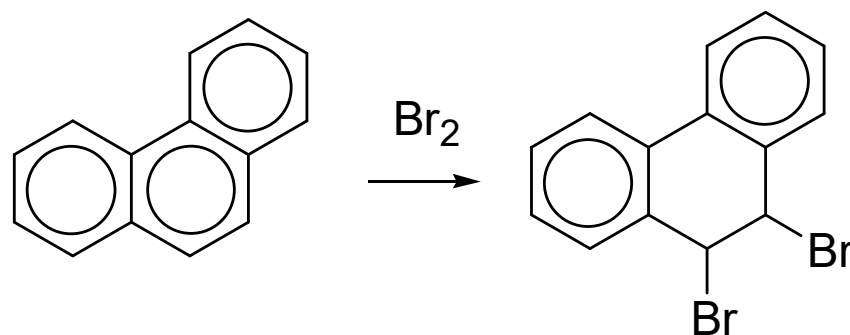
Fenantrene



Il fenantrene ha 5 formule di risonanza di Kekulé, di queste 4 hanno un doppio legame in posizione 9-10



La sostituzione avviene preferenzialmente in posizione 9



L'antracene subisce con facilità addizione alle posizioni 9,10