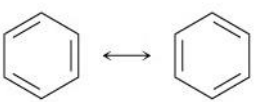
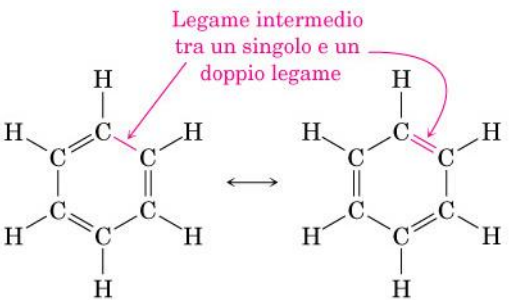
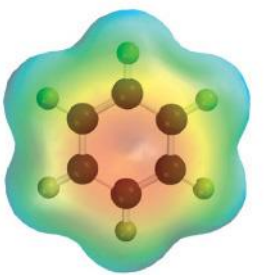
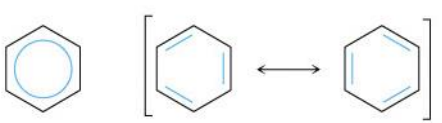
Benzene e aromaticità




Legame intermedio
tra un singolo e un
doppio legame





Rappresentazioni alternative del benzene.
La rappresentazione con il cerchio deve essere usata con attenzione dal momento che non indica in numero degli elettroni π nell'anello.

Il benzene è più stabile di un teorico ”cicloesatriene”

FIGURA 15.2 Confronto dei calori di idrogenazione per il cicloesene, l'1,3-cicloesadiene e il benzene. Il benzene risulta di 150 kJ/mole (36 kcal/ mol) più stabile di quanto ci si potrebbe aspettare per il "cicloesatriene".

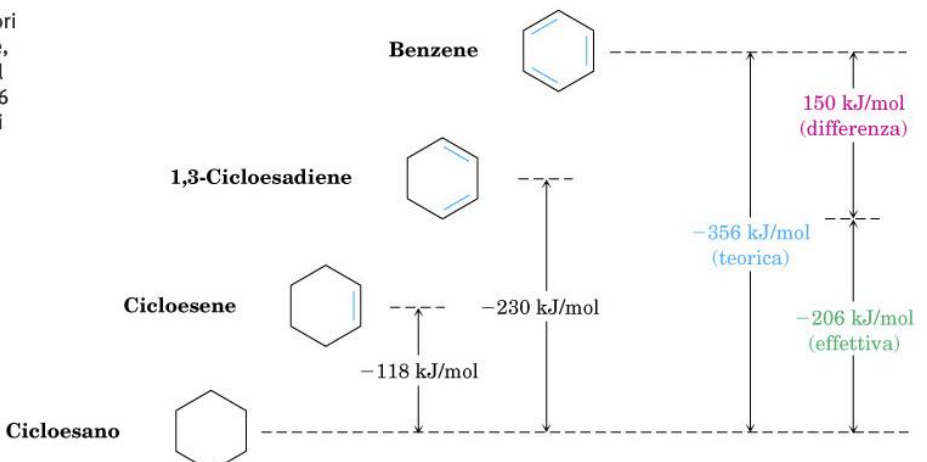
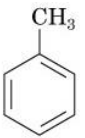
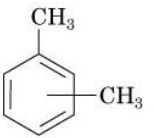


FIGURA 15.1 Alcuni idrocarburi aromatici presenti nel catrame di carbone.

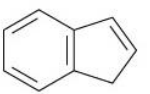
Benzene
(p.e. 80°C)



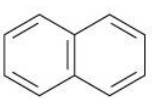
Toluene
(p.e. 111°C)



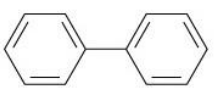
Xilene
(p.e. orto, 144°C;
meta, 139°C; para, 138°C)



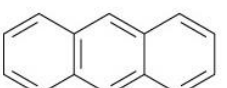
Indene
(p.e. 182°C)



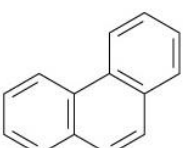
Naftalene
(p.f. 80°C)



Bifenile
(p.f. 71°C)

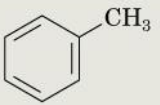
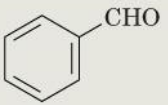
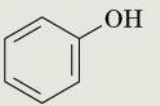
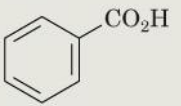
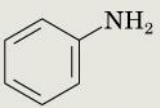
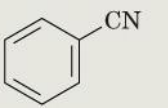
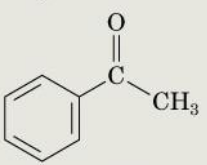
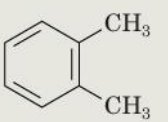
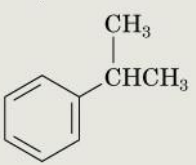
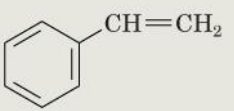


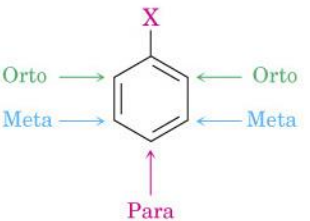
Antracene
(p.f. 216°C)

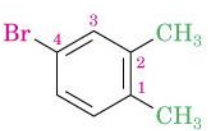


Fenantrene
(p.f. 101°C)

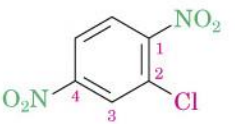
TABELLA 15.1 Nomi comuni di alcuni composti aromatici

Formula	Nome	Formula	Nome
	Toluene (p.e. 111°C)		Benzaldeide (p.e. 178°C)
	Fenolo (p.f. 43°C)		Acido benzoico (p.f. 122°C)
	Anilina (p.e. 184°C)		Benzonitrile (p.e. 191°C)
	Acetofenone (p.f. 21°C)		*orto*-Xilene (p.e. 144°C)
	Cumene (p.e. 152°C)		Stirene (p.e. 145°C)



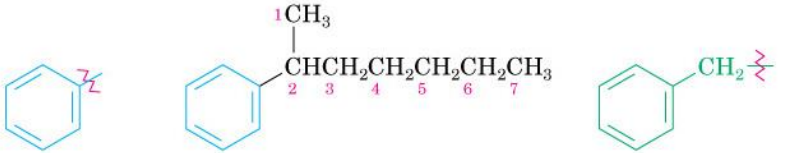


4-Bromo-1,2-dimetilbenzene



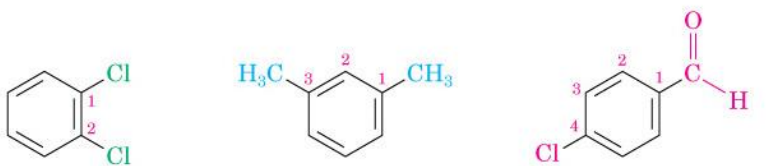
2-Cloro-1,4-dinitrobenzene

2,4,6-Trinitrotoluene (TNT)



Gruppo fenilico **2-Fenileptano** **Gruppo benzilico**

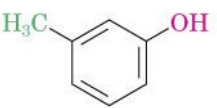
I benzeni disostituiti vengono denominati usando i prefissi ***orto- (o***
eta- (m), o ***para- (p)***. Un benzene orto-disostituito porta i due sostituen
ıll'anello in posizione 1,2, un benzene meta-disostituito ha i due sostituen
posizione 1,3, e un benzene para-disostituito presenta i sostituenti in p
zione 1,4.



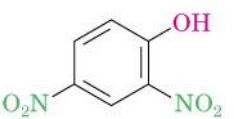
***orto*-Diclorobenzene**
1,2 disostituito

***meta*-Xilene**
1,3 disostituito

***para*-Clorobenzaldeide**
1,4 disostituito

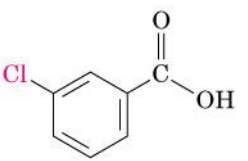


***m*-Metilfenolo**
(*m*-Cresolo)



2,4-Dinitrofenolo

2,6-Dibromo*fenolo*



***Acido m*-clorobenzoico**

Idrocarburi policiclici aromatici

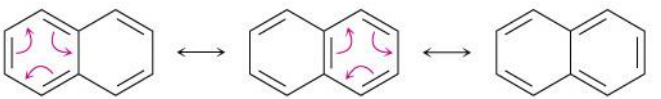
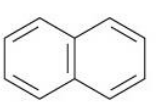
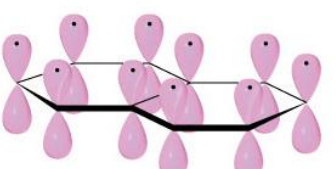
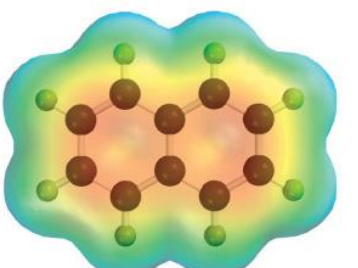


FIGURA 15.12 Il disegno degli orbitali e la mappa di potenziale elettrostatico del naftalene mostrano che i dieci elettroni π sono completamente delocalizzati su entrambi gli anelli.



Naftalene

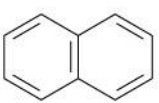




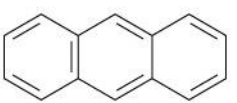
-Planare

-Ogni atomo dell'anello ha un orbitale *p*

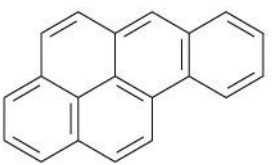
-6 elettroni π nel sistema di orbitali coniugati



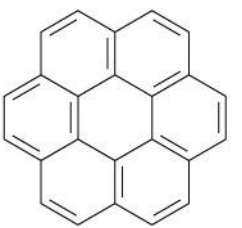
Naftalene



Antracene



Benzo[a]pirene



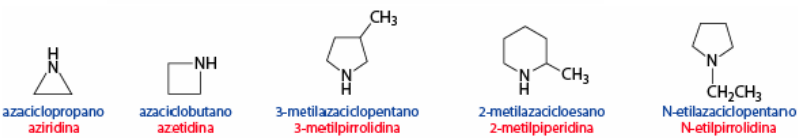
Coronene

Eterocicli aromatici

Eterocicli

Classificazione:

- Non aromatici



- Aromatici
  - PENTATOMICI
  - ESATOMICI
  - BENZOCONDENSATI
  - POLICICLICI

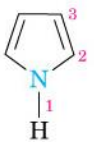
ETEROCICLI AROMATICI PENTATOMICI con 1 ETEROATOMO

pirrolo

furano

tiofene

Eterocicli aromatici a 5 termini



Pirrolo

Furano

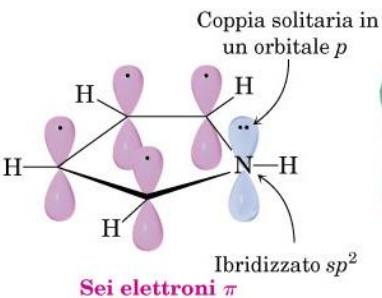
Tiofene

-Planari

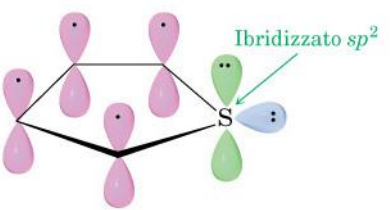
-Ogni atomo dell'anello ha un orbitale *p*

-6 elettroni π nel sistema di orbitali coniugati

FIGURA 15.9 Il pirrolo, un eterociclo aromatico a cinque termini, ha una disposizione degli elettroni π molto simile a quella dell'anione ciclopentadienile.

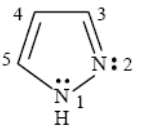


Tiofene

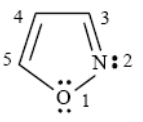


Tiofene

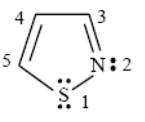
ETEROCICLICI 5 TERMINI con 2 ETEROATOMI: 1,2-



pirazolo
1,2-diazolo



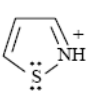
isossazolo
1,2-ossazolo



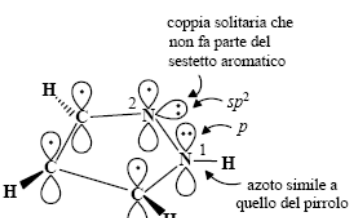
isotiazolo
1,2-tiazolo

pK_a = 2,52

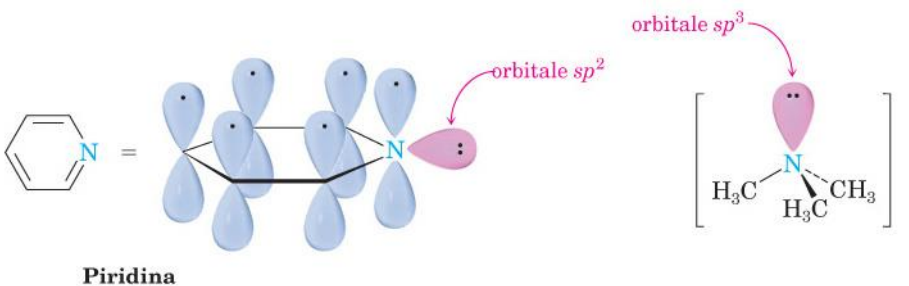
pK_a = −2,97



pK_a = −0,51

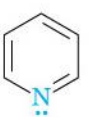


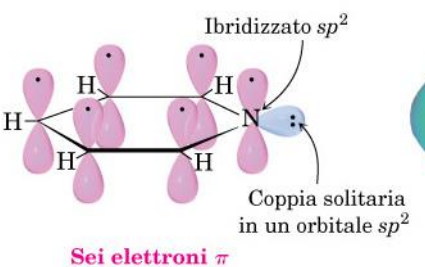
AROMATICITA':
Viene rispettata la regola di Huckel con n=1

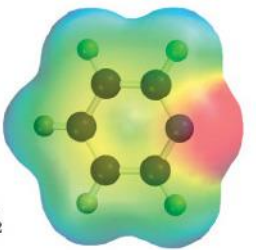


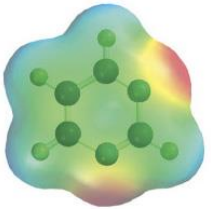
Piridina

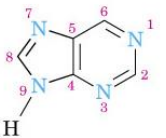
FIGURA 15.8 La piridina, un eterociclo aromatico, ha una disposizione degli elettroni π molto simile a quella del benzene.

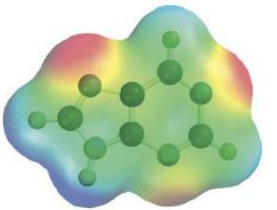






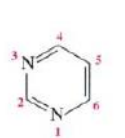




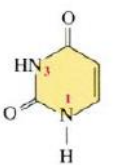


Pirimidina **Purina**

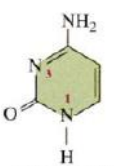
ETEROCICLI PRESENTI negli ACIDI NUCLEICI



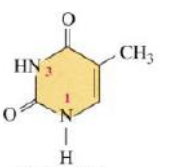
Pirimidina



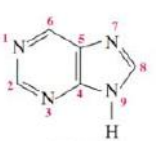
Uracile (U)



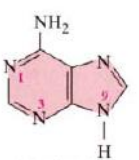
Citosina (C)



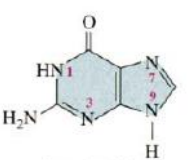
Timina (T)



Purina



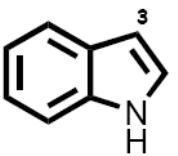
Adenina (A)



Guanina (G)

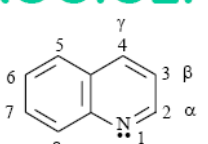
FIGURA 28.1
Nomi e abbreviazioni ad una lettera per le basi eterocicliche azotate più comuni del DNA e dell'RNA. Le basi sono numerate in maniera uguale a quella dei composti da cui hanno origine, la pirimidina e la purina.

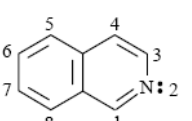
ETEROCICLI BENZOCONDENSATI



indolo

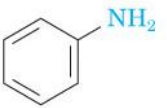
ETEROCICLI BENZOCONDENSATI





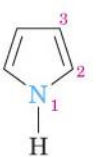
chinolina

isochinolina



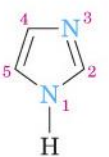
Anilina

Piridina



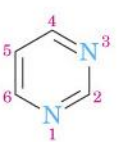
Pirrolo

Chinolina

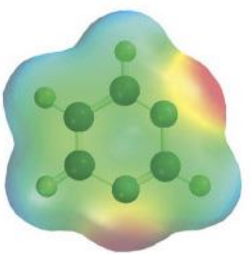


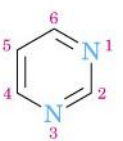
Imidazolo

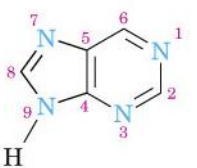
Indolo

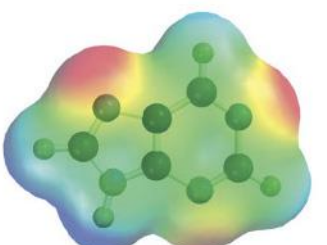


Pirimidina









Pirimidina **Purina**