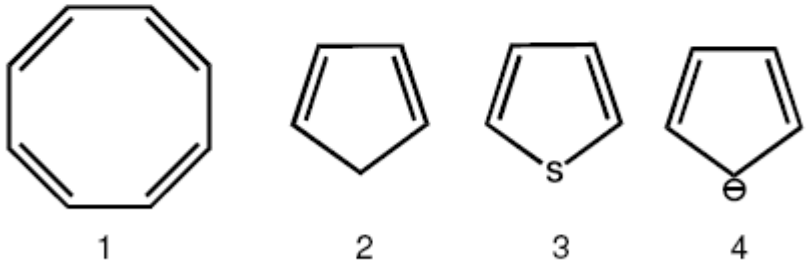
Compostos aromáticos e heteroaromáticos

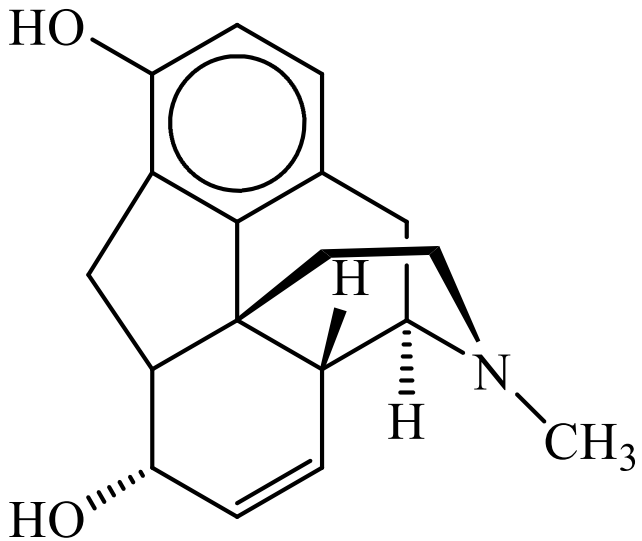
Aromático *vs.* insaturado

- ✓ Estabilidade maior dos compostos aromáticos
- ✓ Planaridade do anel e conjugação das insaturações
- ✓ A aromaticidade e a regra de Hückel

Regra de Hückel: o número de elétrons π deve ser igual a 4n+2, dando n um número inteiro

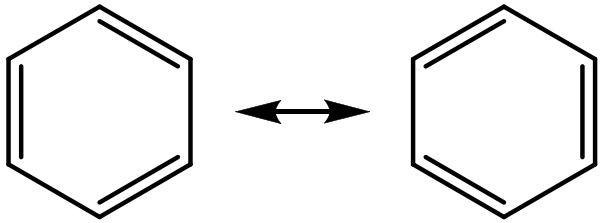


1 2 3 4



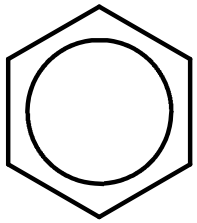
Morfina

Compostos aromáticos

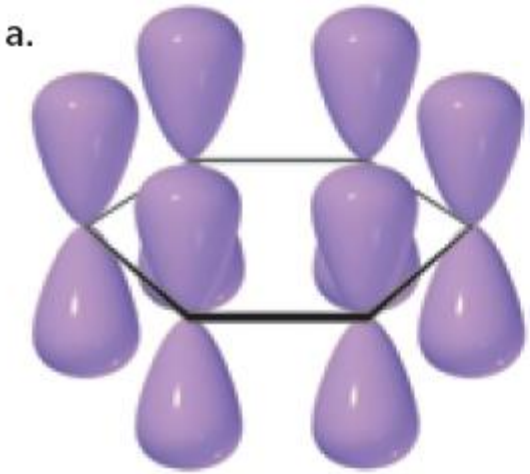


Estruturas de ressonância para o benzeno

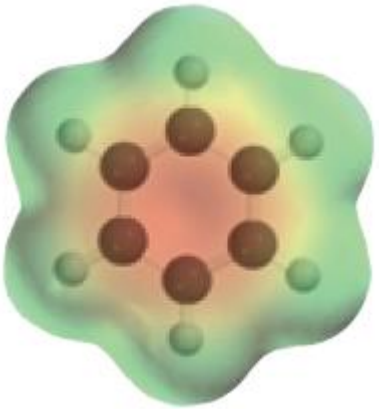
ou

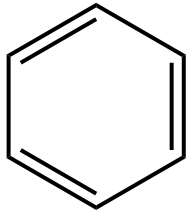


Representação do híbrido de ressonância



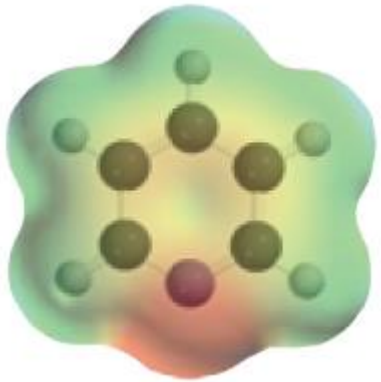
Compostos aromáticos

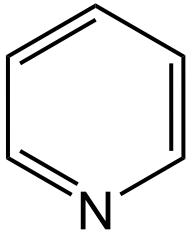




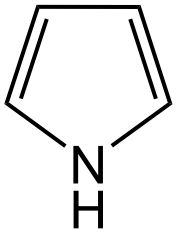
Benzeno

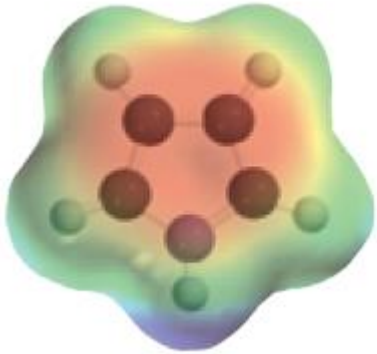
Piridina





Pirrol



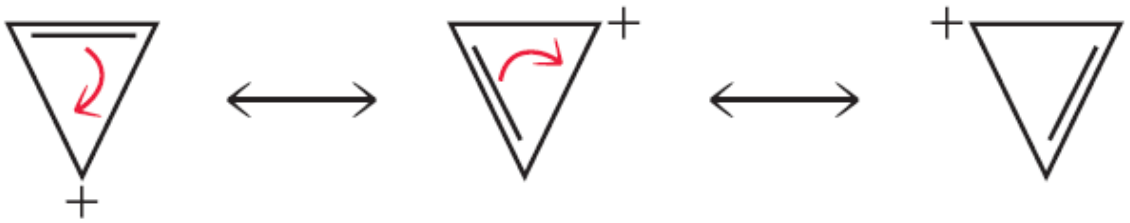


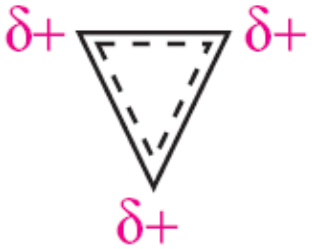
Reatividade & aromaticidade

Ciclopropeno

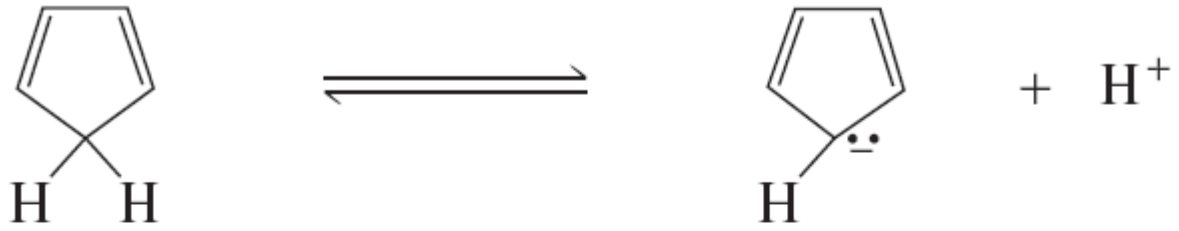
cátion

ânion





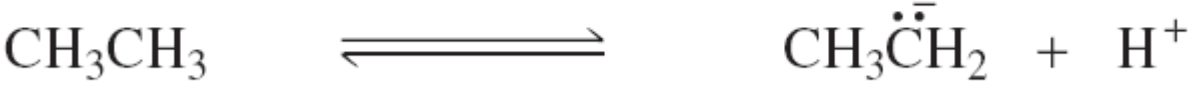
Reatividade & aromaticidade



Ciclopentadieno

$pK_a = 15$

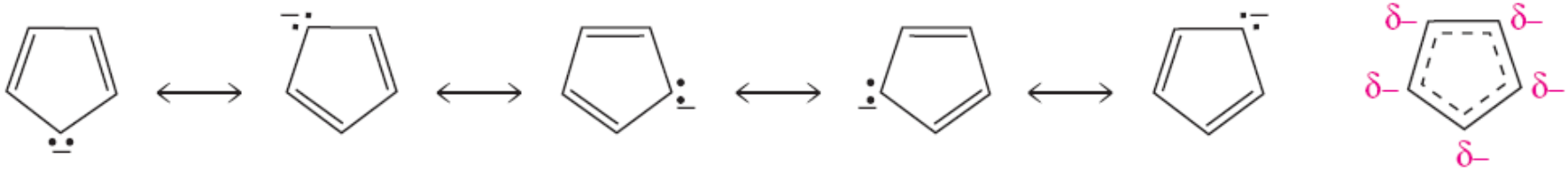
Base conjugada



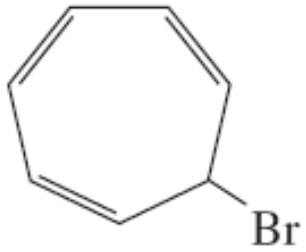
etano

$pK_a = 50$

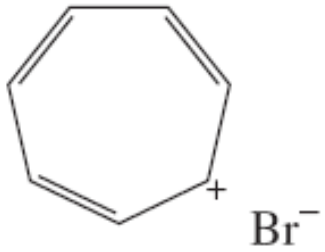
Base conjugada



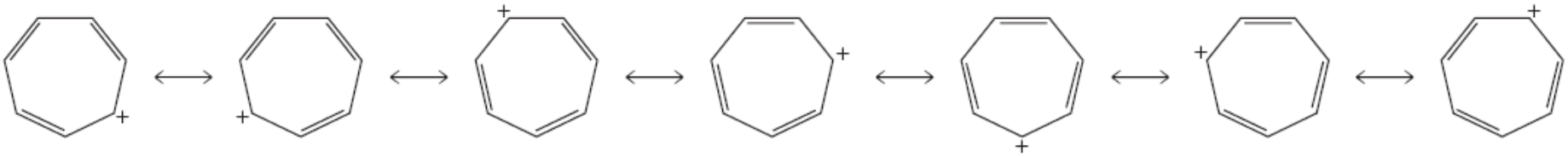
Reatividade & aromaticidade

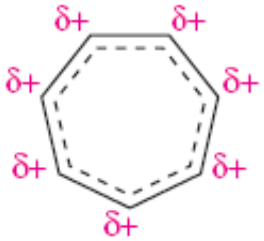


7-bromociclohepta-1,3,5-trieno

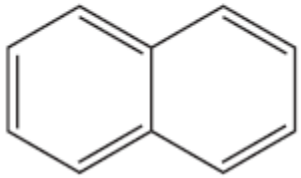


íon tropílio

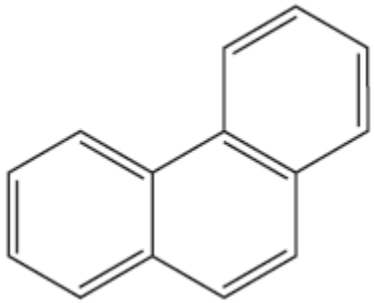




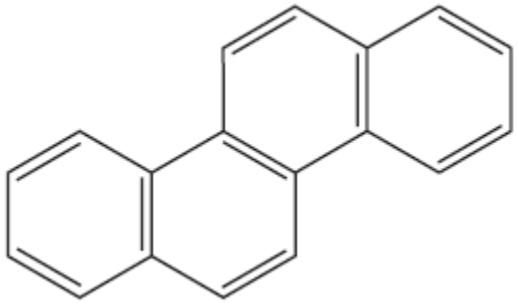
Compostos aromáticos policíclicos e heteroaromáticos



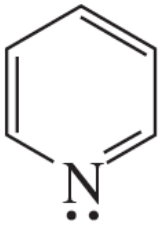
naftaleno



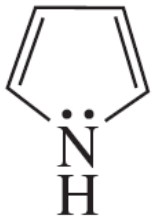
fenantreno



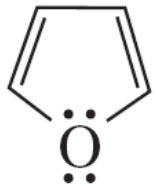
criseno



piridina



pirrol



furano

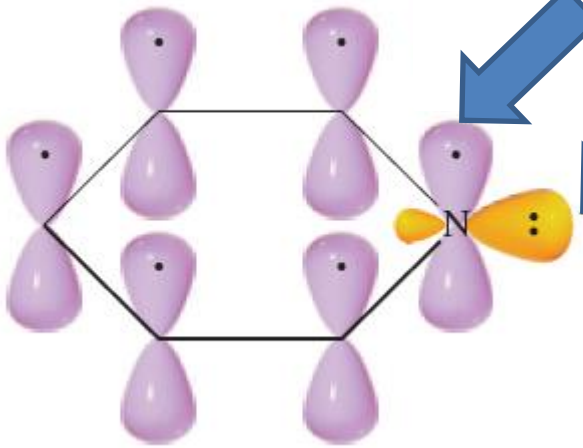
tiofeno

Compostos aromáticos policíclicos e heteroaromáticos

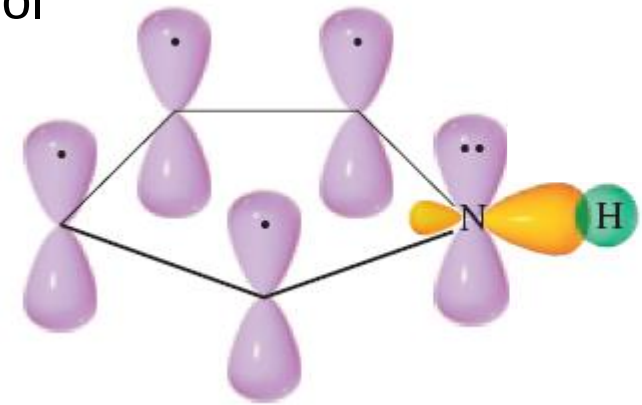
Orbital *p* que interage no sistema aromático

Orbital sp^2 fora do sistema aromático

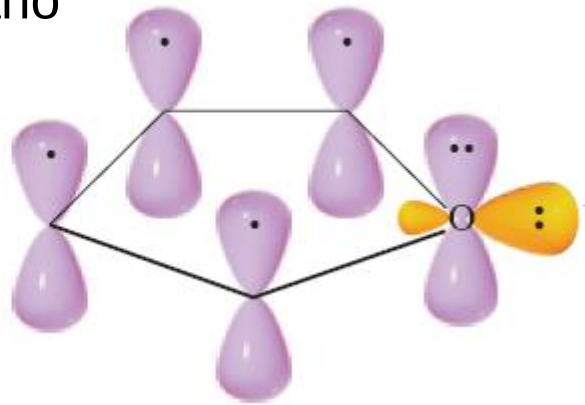
piridina



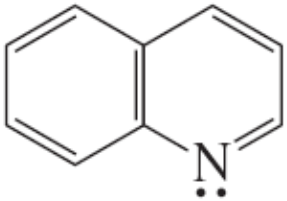
pirrol



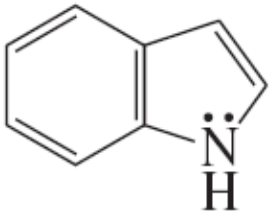
furano



Outros compostos heteroaromáticos

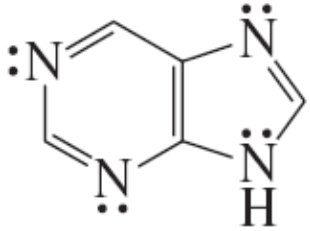


quinolina

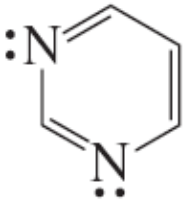


indol

imidazol



purina



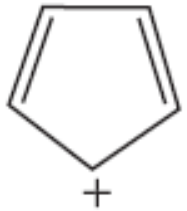
pirimidina

Bases nitrogenadas

Compostos antiaromáticos

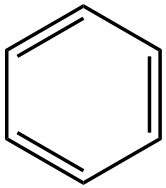
✓ Compostos antiaromáticos são menos estáveis dos que os não aromáticos e os aromáticos

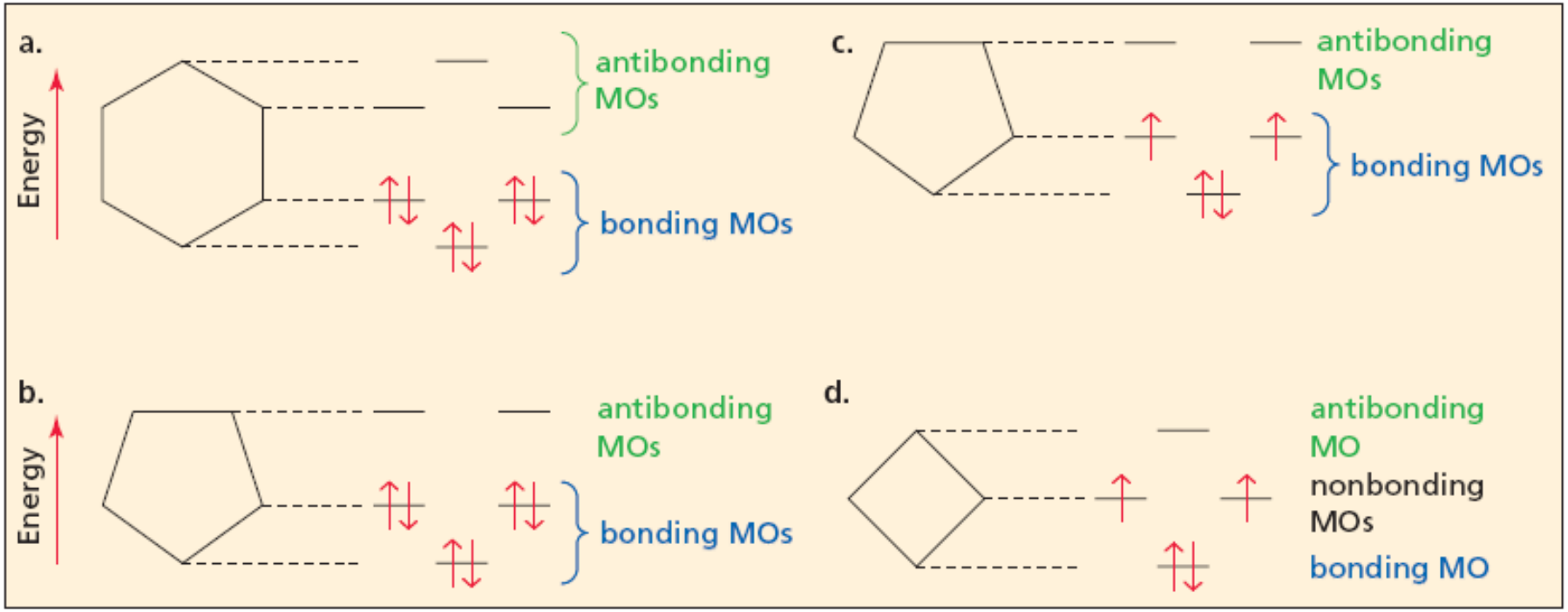
✓ São planos, com duplas ligações alternadas e número de elétrons $\pi = 4n$



Ciclobutadieno e o cátion ciclopentadienila são muito instáveis

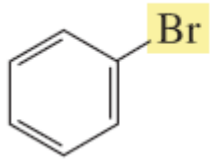
Aromático *vs.* antiaromático



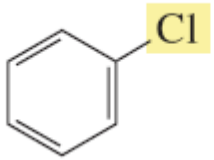


Nomenclatura

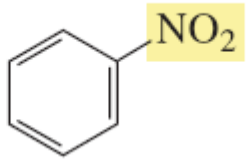
✓ Aromáticos monossubstituídos



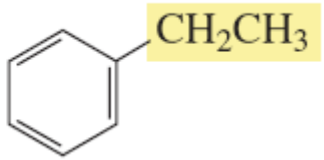
bromobenzeno



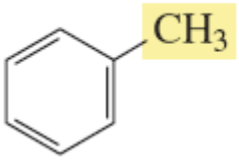
clorobenzeno



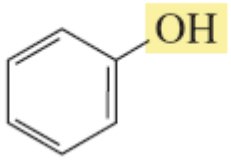
nitrobenzeno



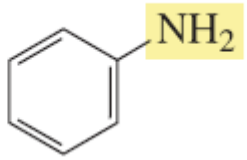
etilbenzeno



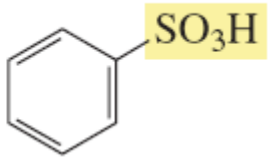
tolueno
metilbenzeno



fenol



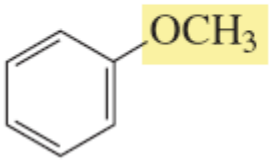
anilina



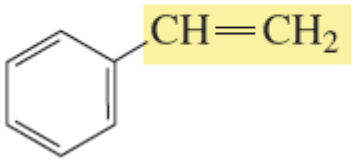
ácido benzenossulfônico

Nomenclatura

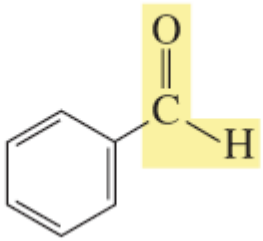
✓ Aromáticos monossubstituídos



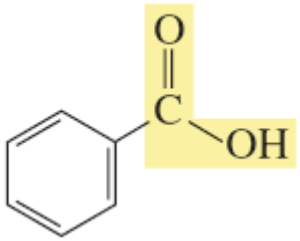
metoxibenzeno
anisol



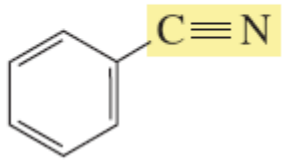
fenileteno
estireno



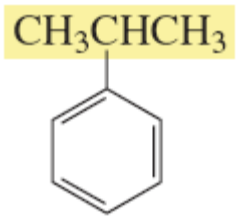
benzaldeído
aldeido benzoico



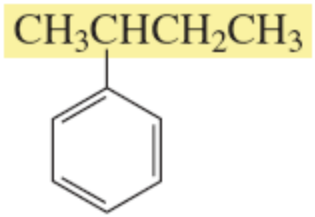
ácido benzoico



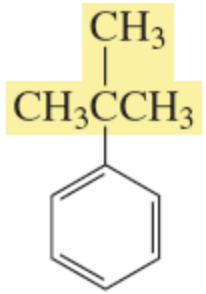
benzonitrila



isopropilbenzeno
cumeno

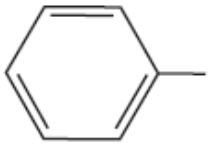


2-fenilbutano
sec-butilbenzeno

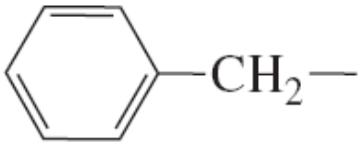


2-metil-2-fenilpropano
tert-butilbenzeno

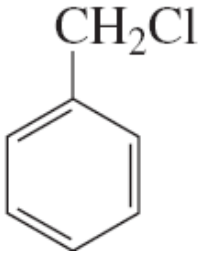
Nomenclatura (2)



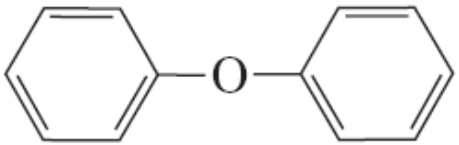
grupo fenila



grupo benzila



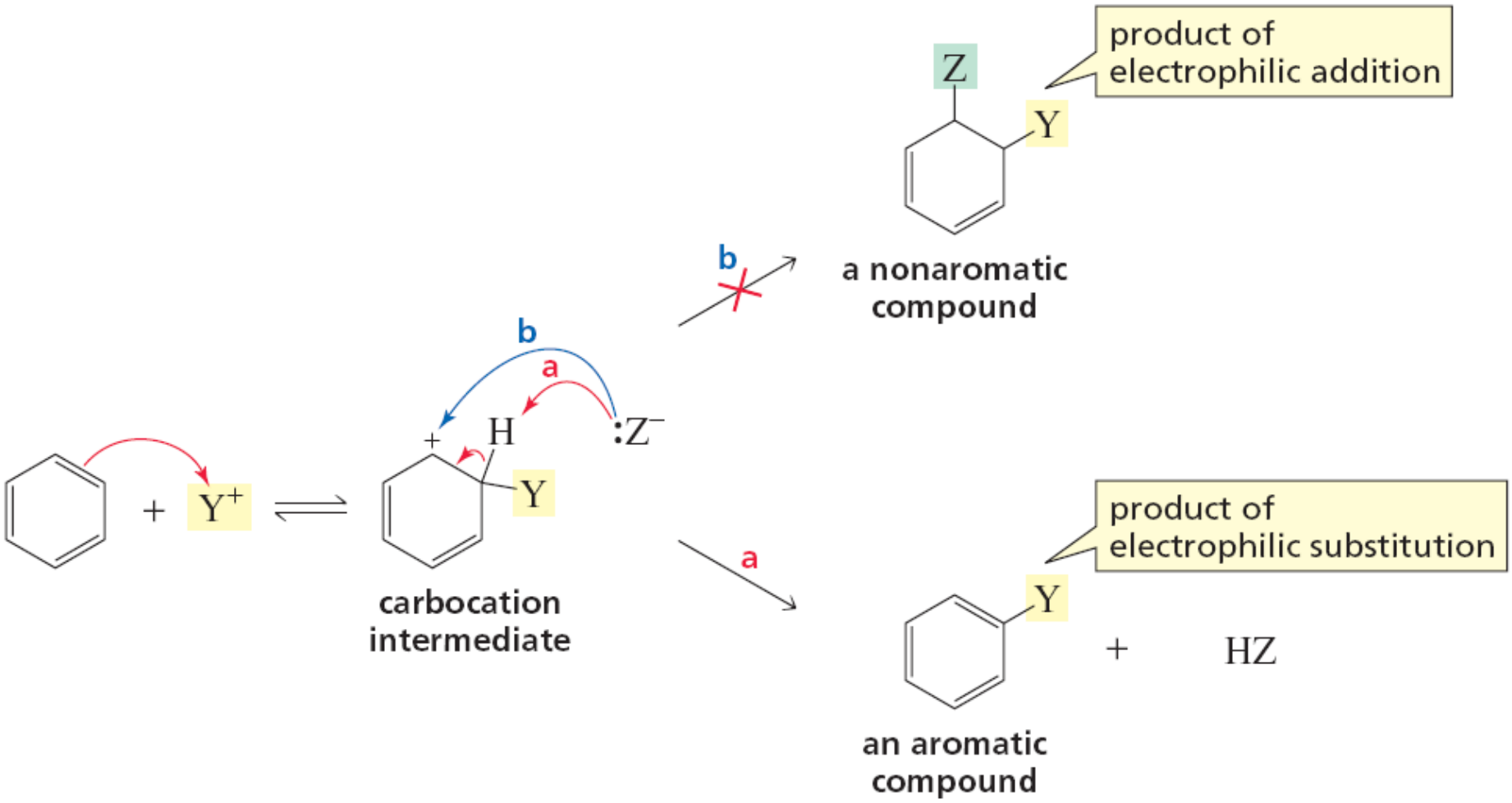
clorometilbenzeno
cloreto de benzila



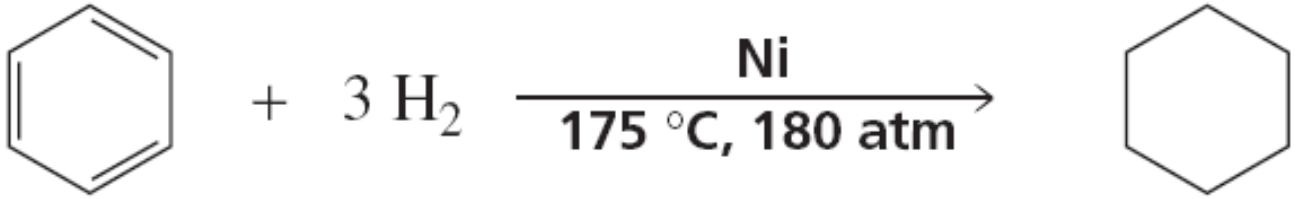
éter fenílico

éter benzílico

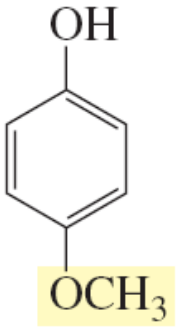
Reatividade



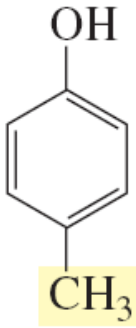
Redução do benzeno



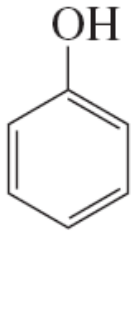
Acidez do fenol e do ácido benzoico



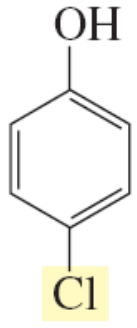
$pK_a = 10.20$



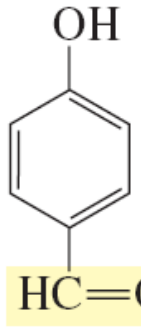
$pK_a = 10.19$



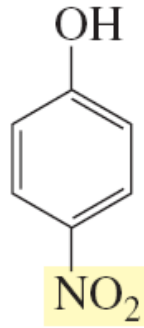
$pK_a = 9.95$



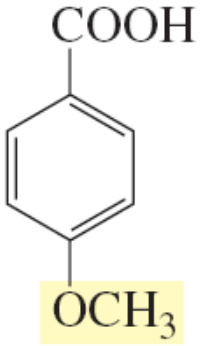
$pK_a = 9.38$



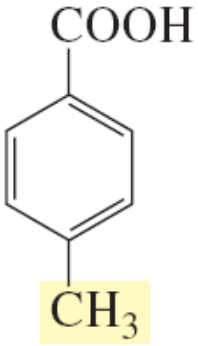
$pK_a = 7.66$



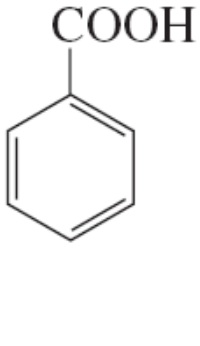
$pK_a = 7.14$



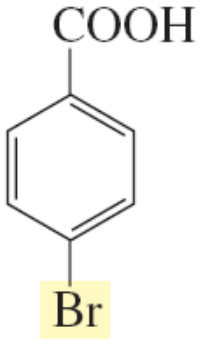
$pK_a = 4.47$



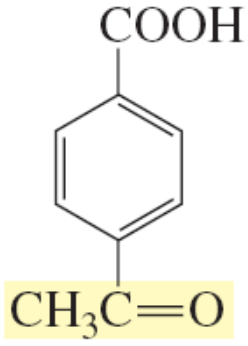
$pK_a = 4.34$



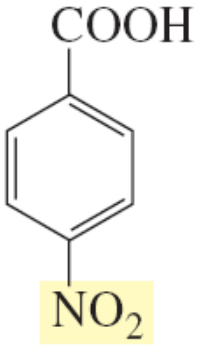
$pK_a = 4.20$



$pK_a = 4.00$

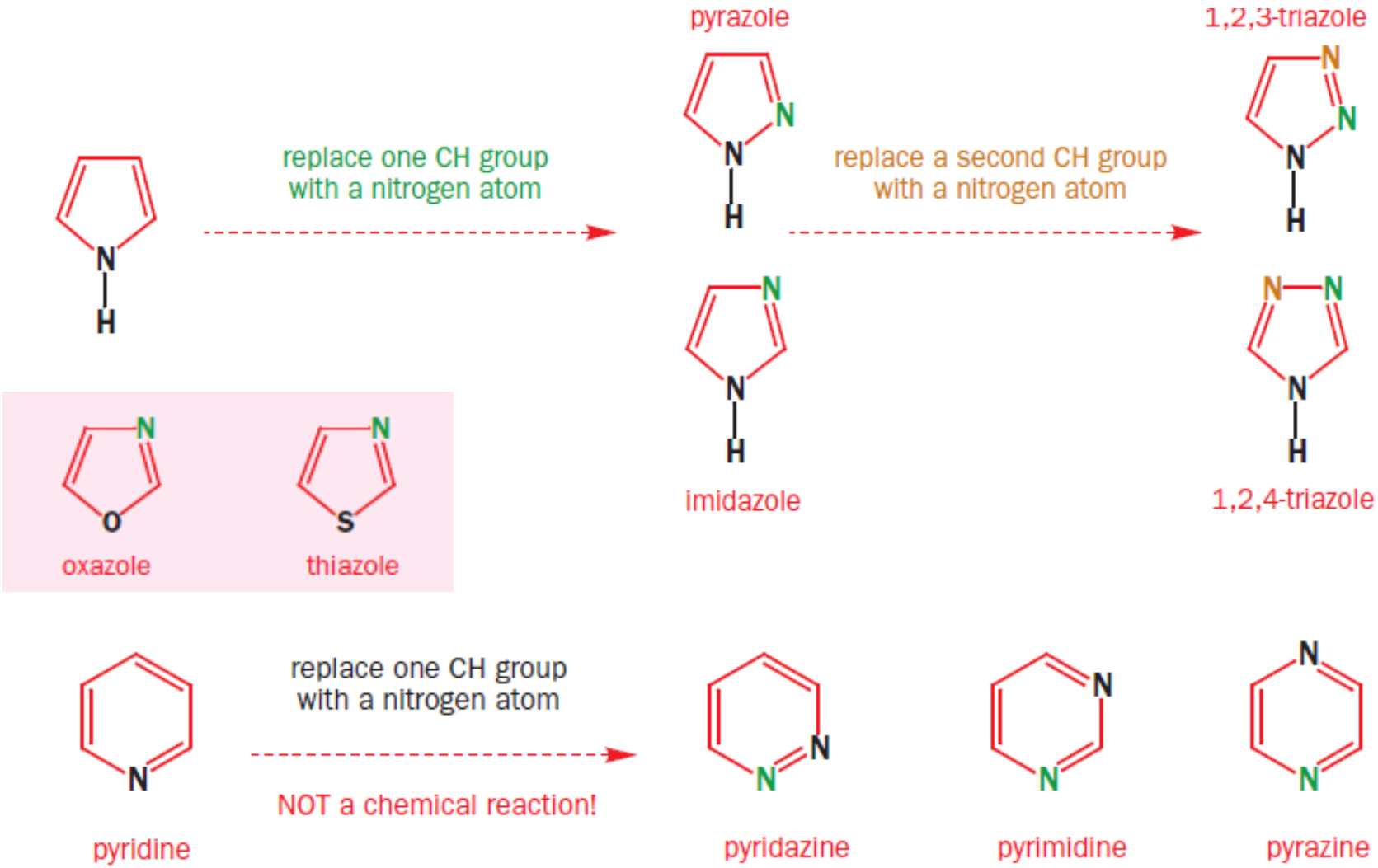


$pK_a = 3.70$

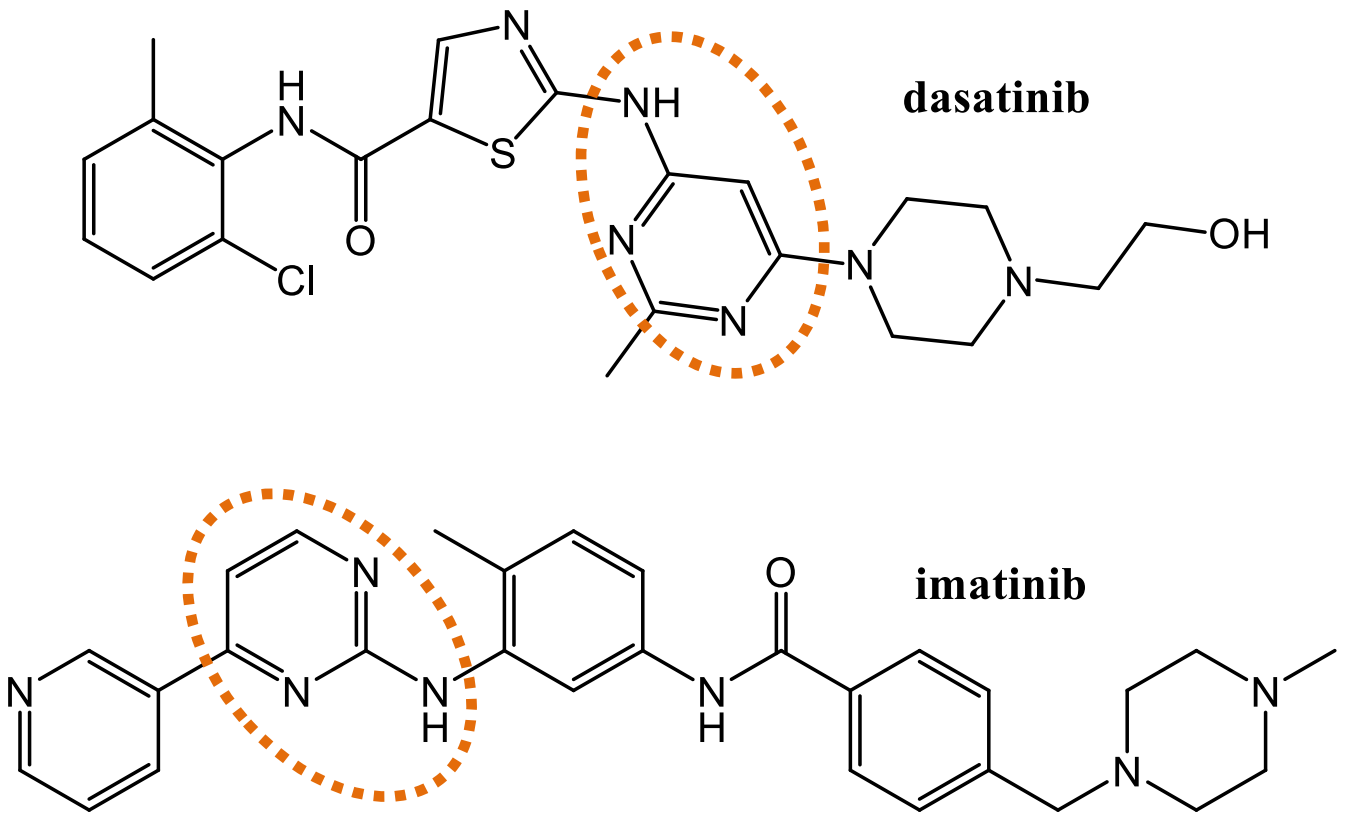


$pK_a = 3.44$

Exemplos de heteroaromáticos

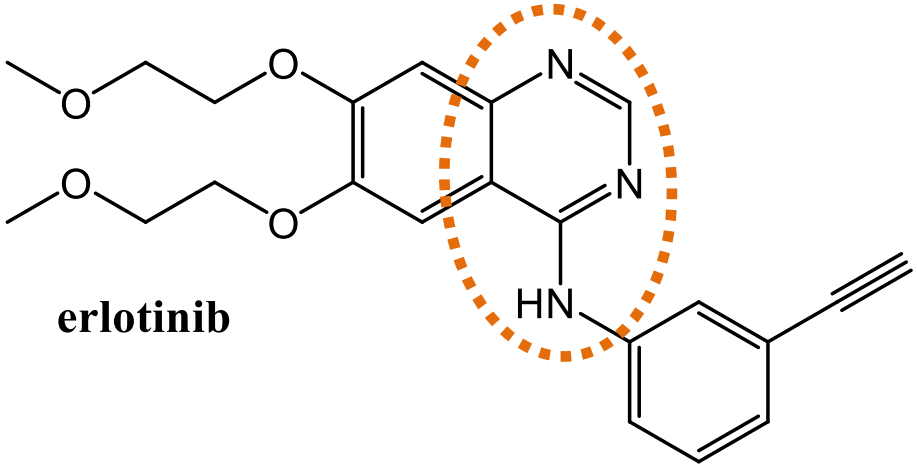


Exemplos de grupos funcionais

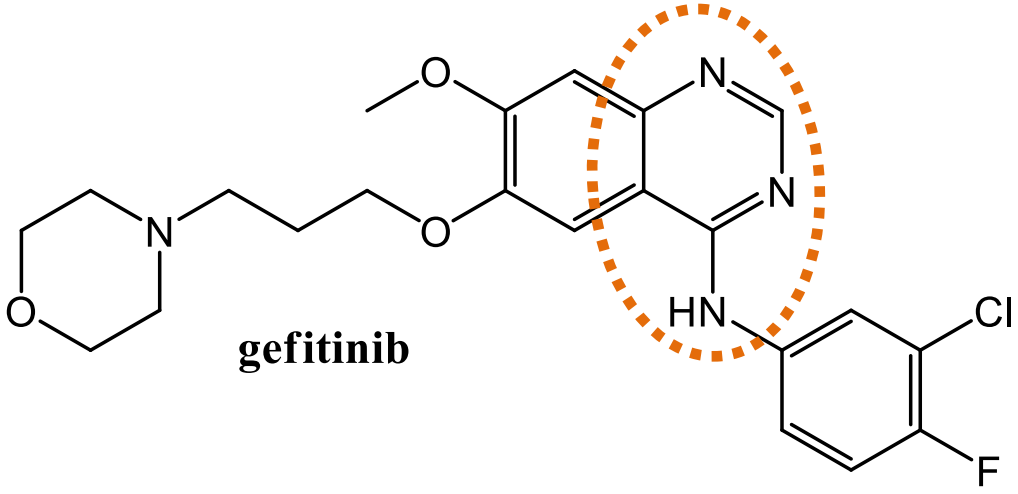


Hadjuk, P.J.; Greer, J. *Nature Rev. Drug Discov.* **2007**, *6*, 211

Exemplos de grupos funcionais (2)



erlotinib



gefitinib

Hadjuk, P.J.; Greer, J. *Nature Rev. Drug Discov.* **2007**, *6*, 211