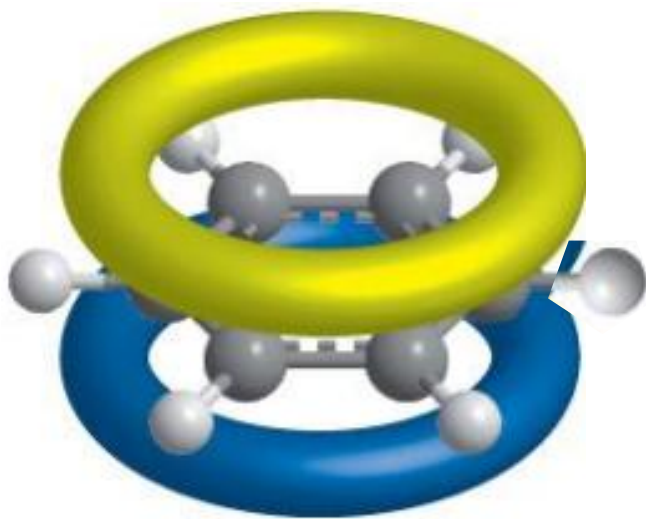
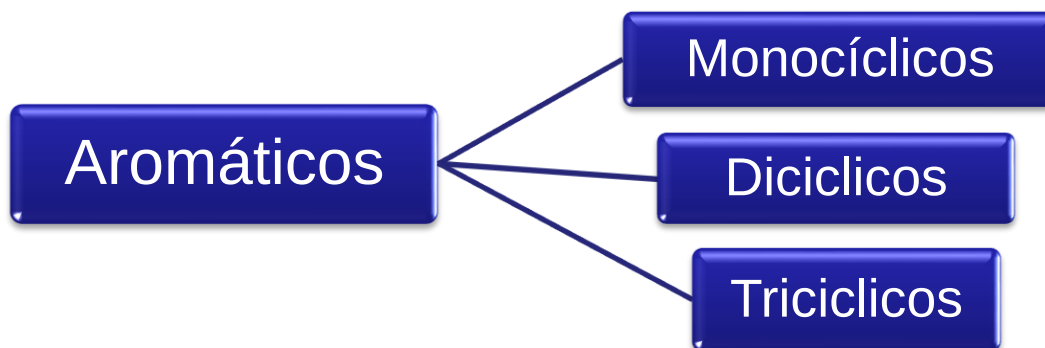


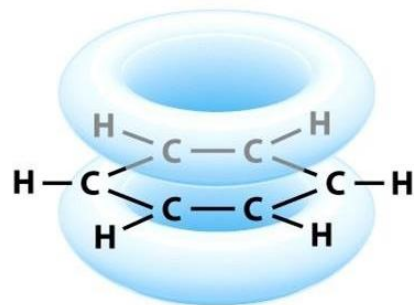
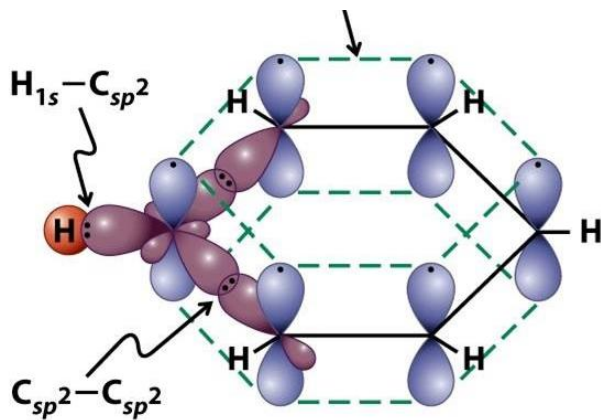
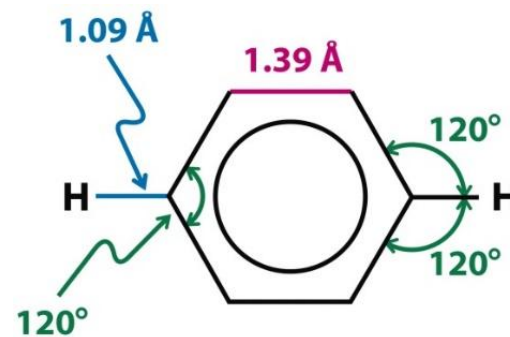
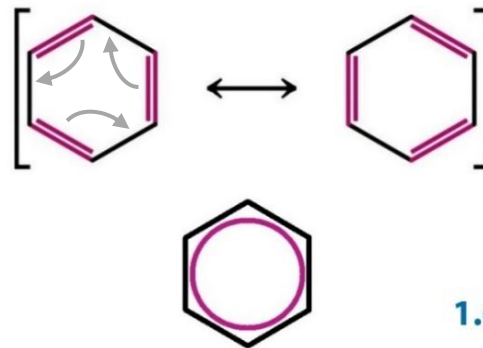
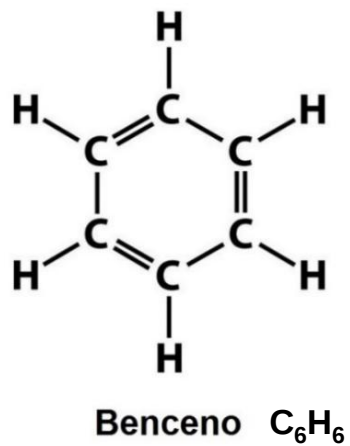
HIDROCARBUROS AROMÁTICOS



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Depto. Oncol Básica y Clínica
Facultad de Medicina,
Universidad de Chile



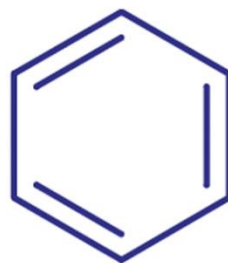
Benceno



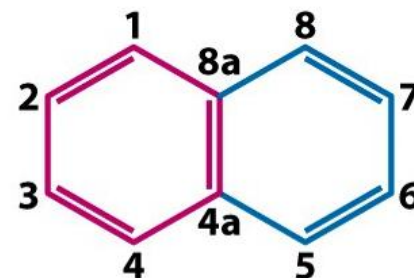
Regla de Hückel (simplificada)

Una molécula es **aromática** cuando:

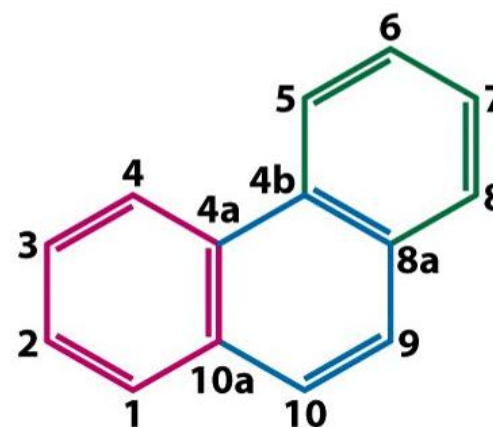
- Es **cíclica**
- Posee **enlaces π** conjugados (orbitales p en todos los C).
- Es **plana**
- Contiene un total de **$4n+2$** electrones en los orbitales *p* (donde $n \geq 1$)



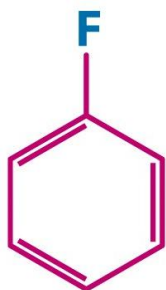
Benceno



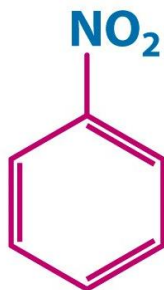
Naftaleno



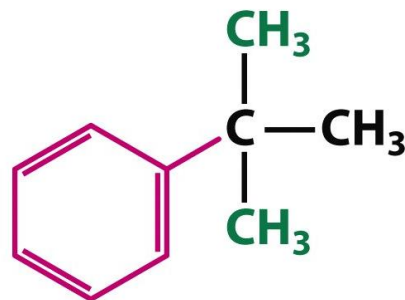
Fenantreno



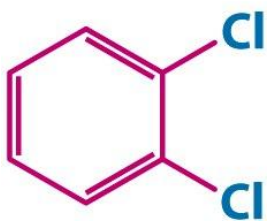
Fluor**ben**ceno



Nitro**ben**ceno



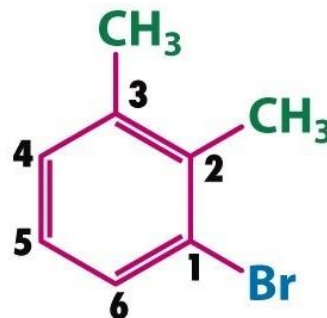
(1,1-Dimethiletil)**ben**ceno
(*tert*-butilbenceno)



1,2-Dicloro**ben**ceno
(*o*-Diclorobenceno)



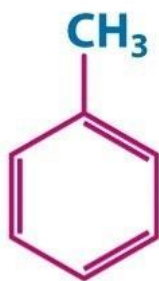
1-Bromo-3-nitro**ben**ceno
(*m*-Bromonitrobenceno)



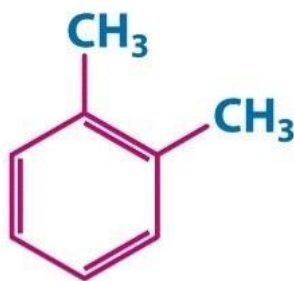
1-Bromo-2,3-dimetil
benceno



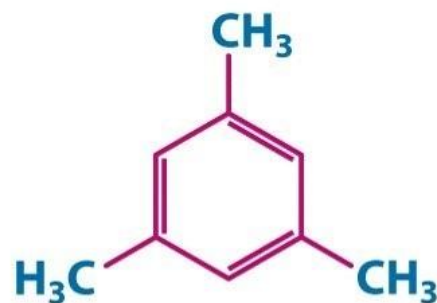
1,2,4-Trinitro**ben**ceno



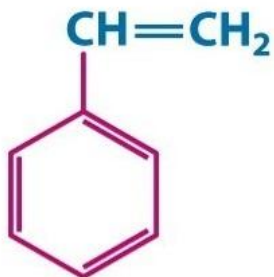
Metilbenceno
(Tolueno)



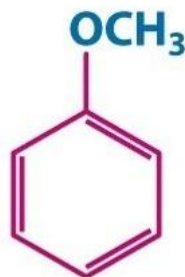
1,2-Dimetilbenceno
(o-Xileno)



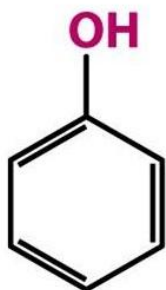
1,3,5-Trimetilbenceno
(Mesityleno)



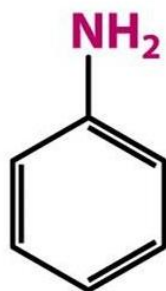
Etenilbenceno
(Estireno)



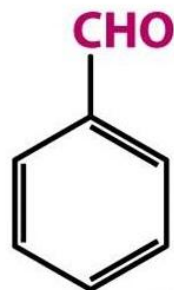
Metoxibenceno
(Anisol)



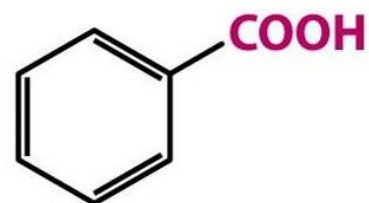
Fenol



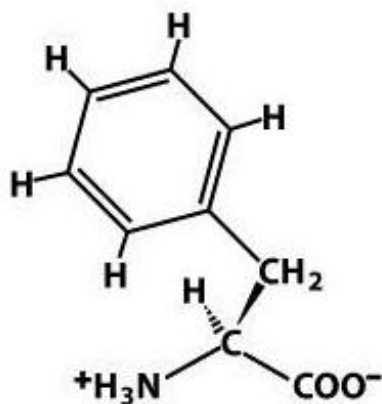
Anilina



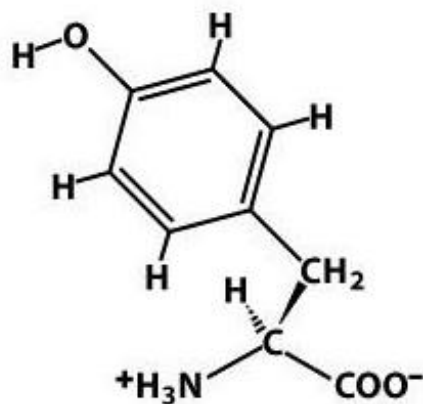
Benzaldehido



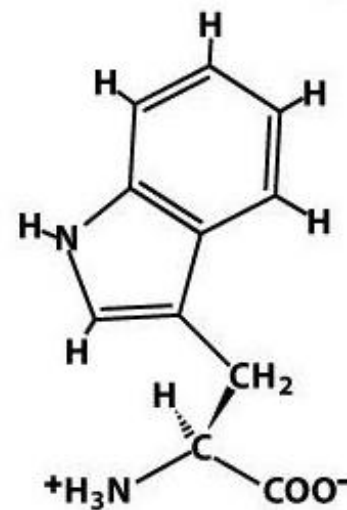
Acido Benzoico



Fenilalanina



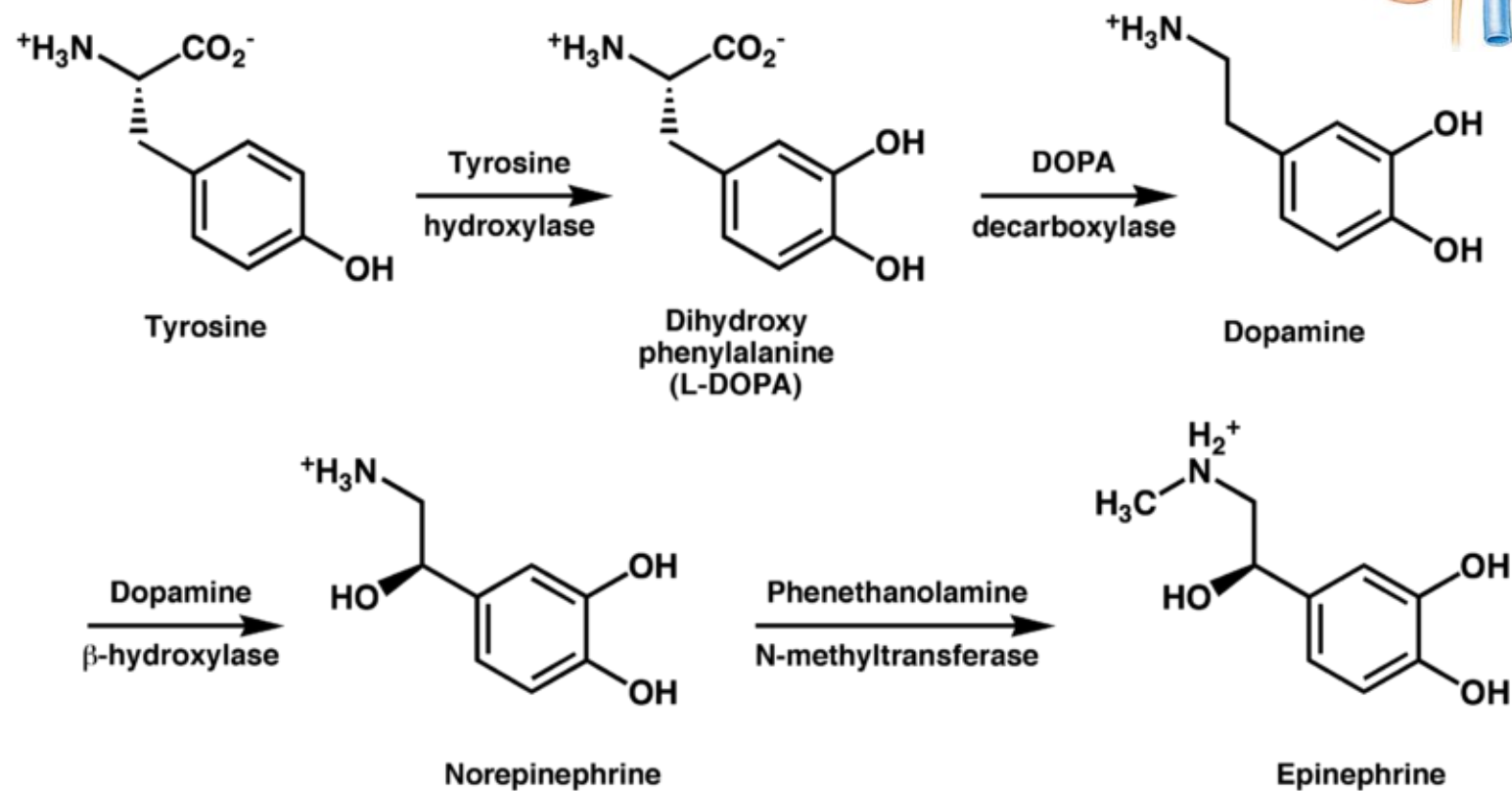
Tirosina



Triptofano

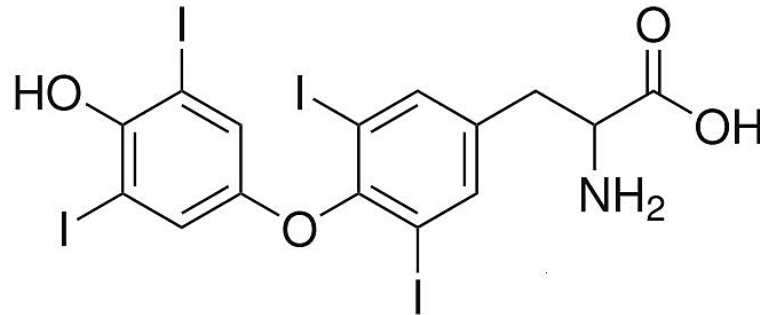
Fenoles - usos y abundancia natural

- La tirosina es precursor de catecolaminas

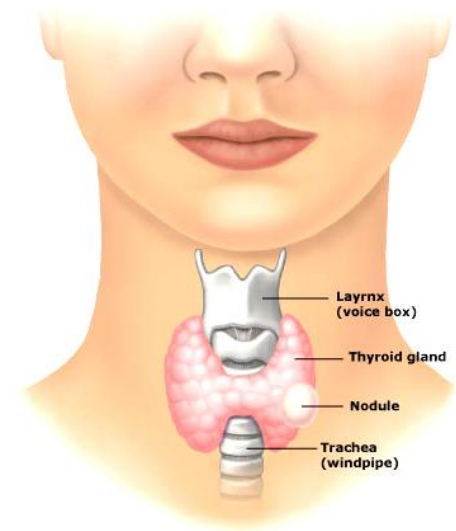
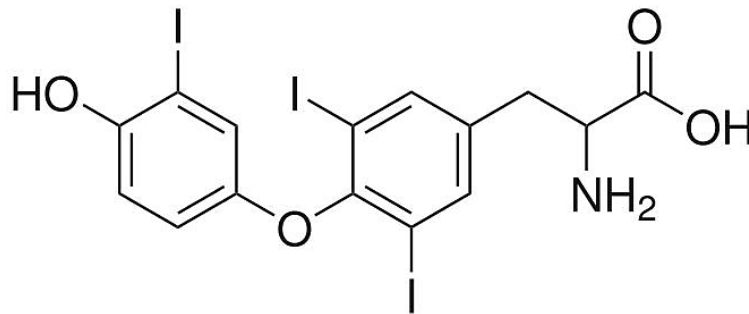


Fenoles - usos y abundancia natural

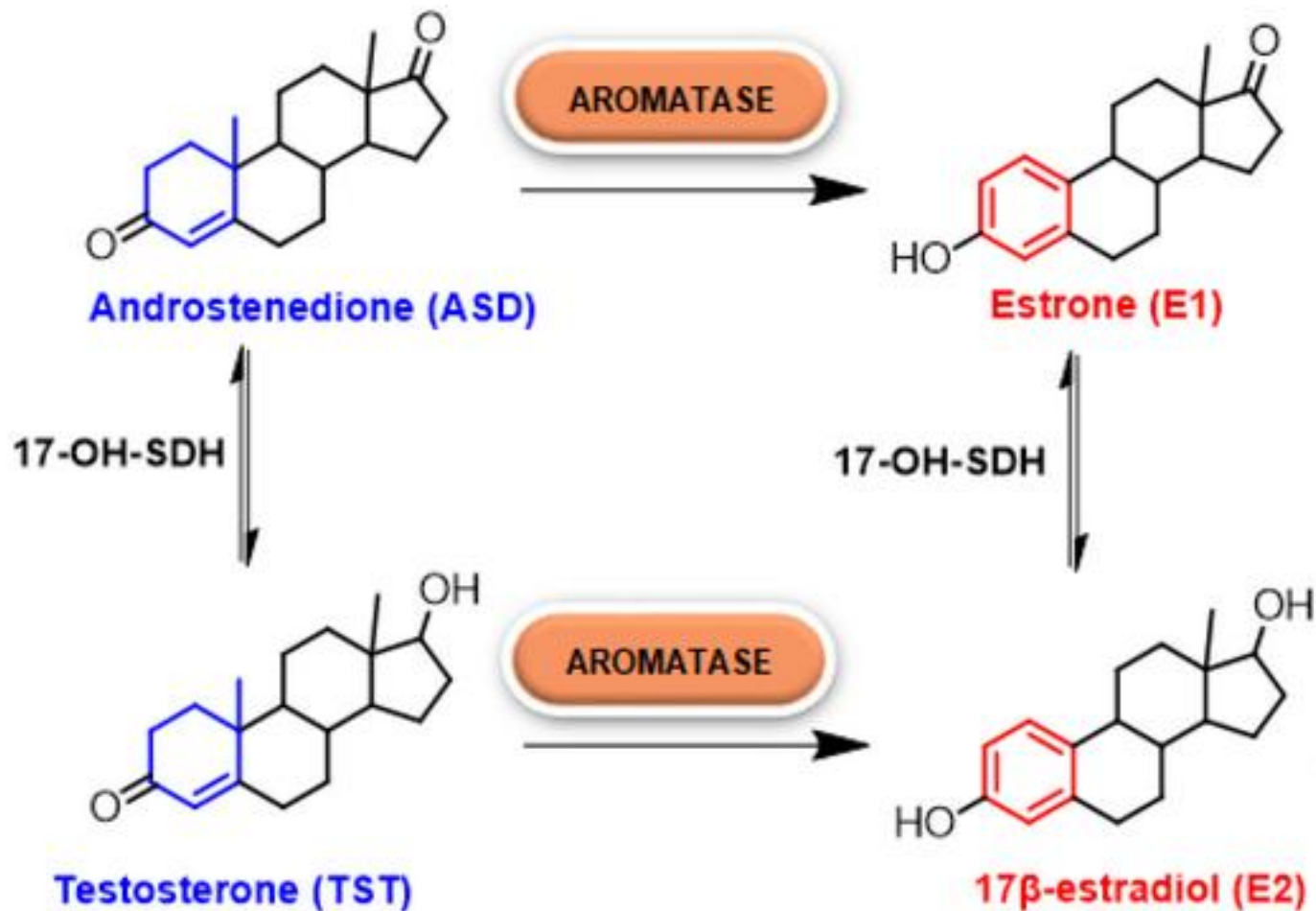
- **Tiroxina (T4)**



- **Triyodotironina (T3)**

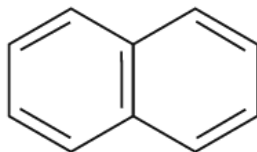


Fenoles - usos y abundancia natural

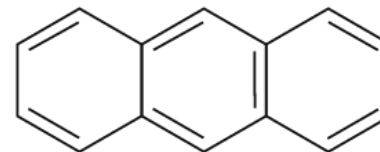


PAHs

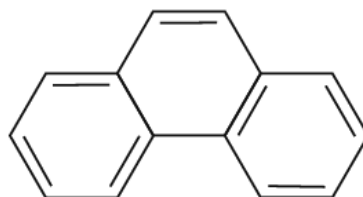
Naphthalene



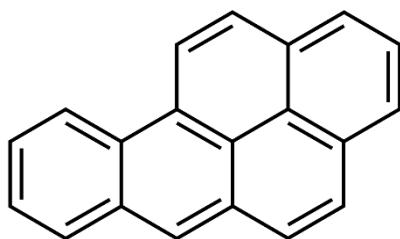
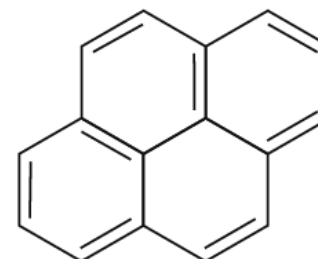
Anthracene



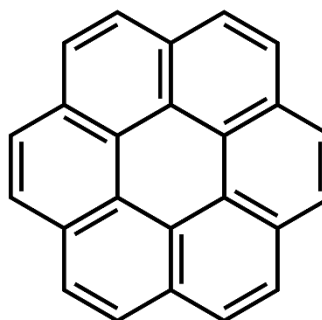
Phenanthrene



Pyrene

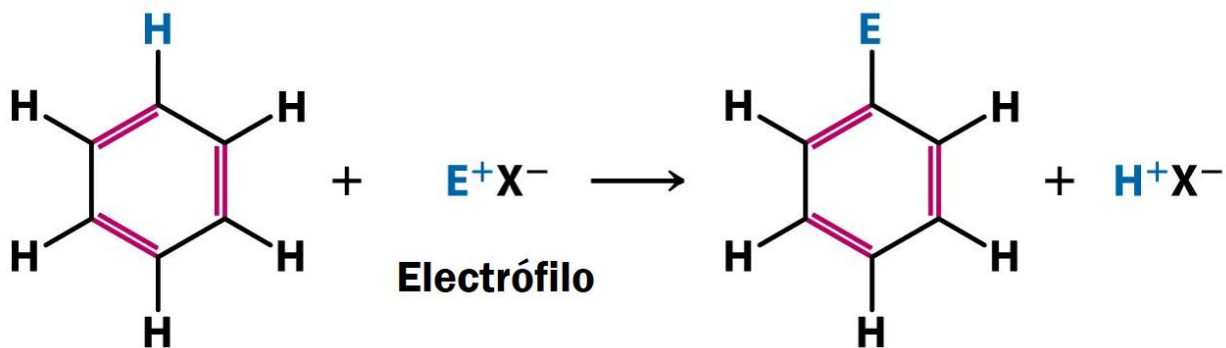
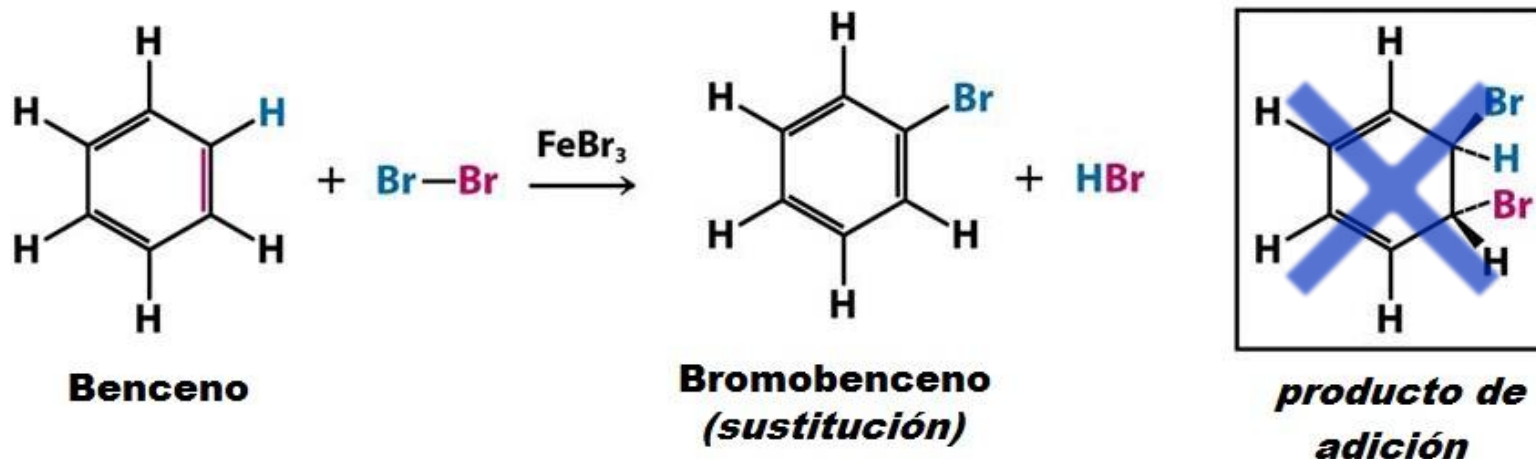


Benzopireno

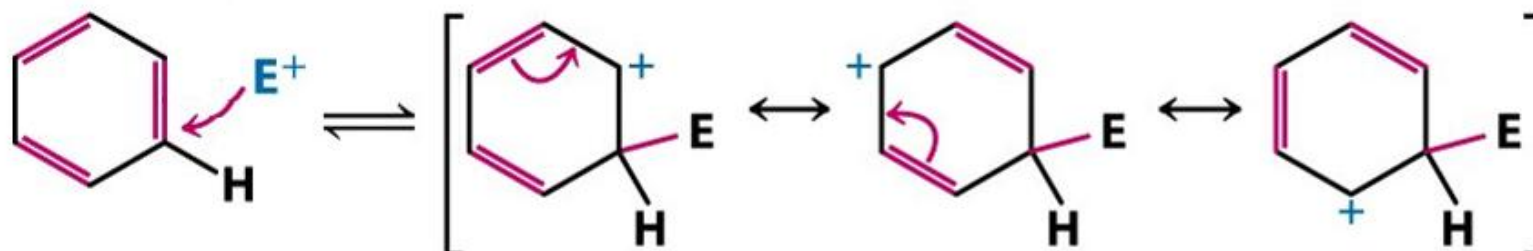


Coroneno

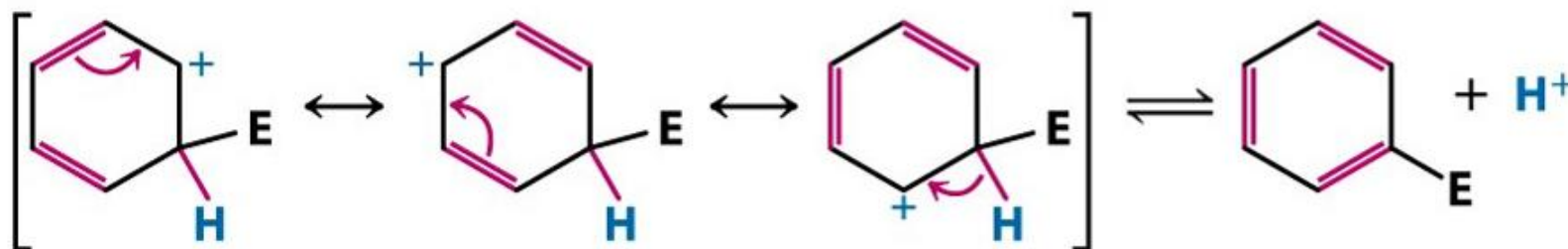
Benceno – Sustitución electrofílica aromática (SEA)



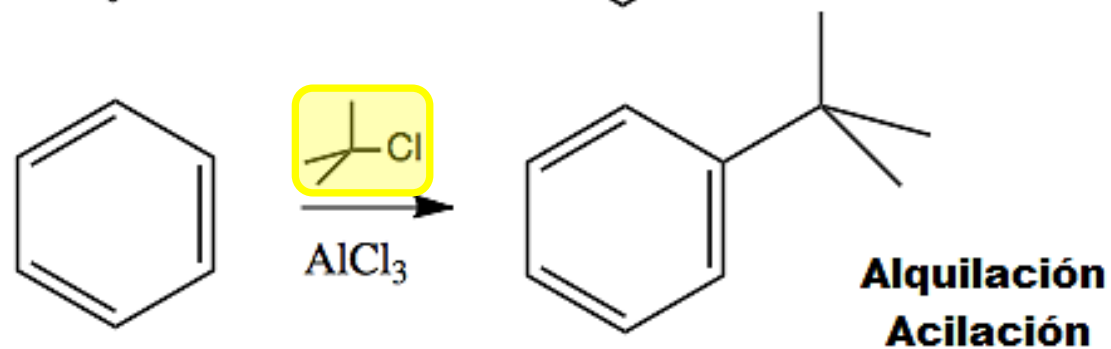
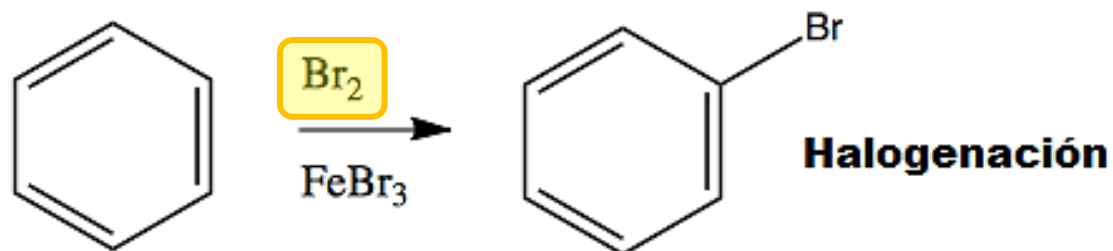
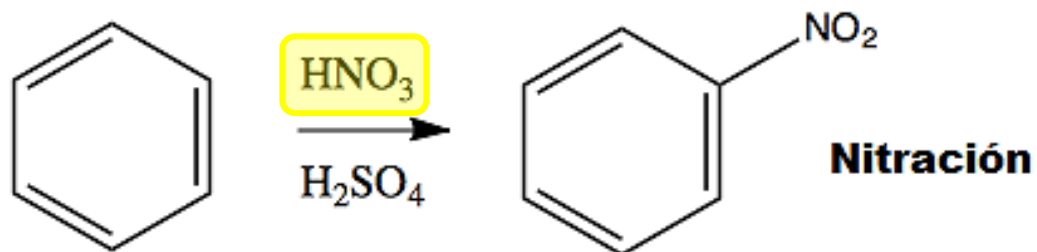
Paso 1: Ataque del electrófilo (limitante de v)



Paso 2: Eliminación de un protón



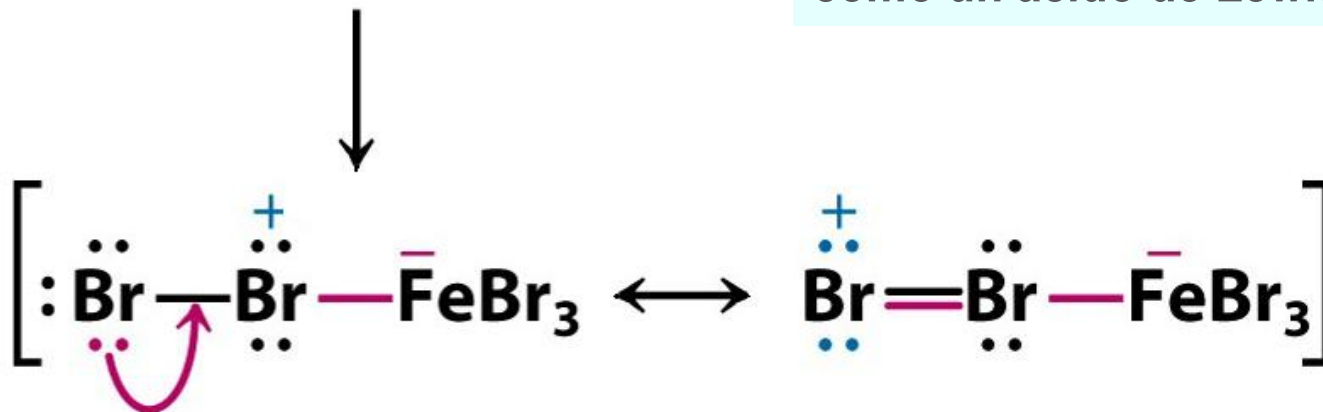
SEA - ejemplos



Paso 1 – Activación del Br₂ con FeBr₃

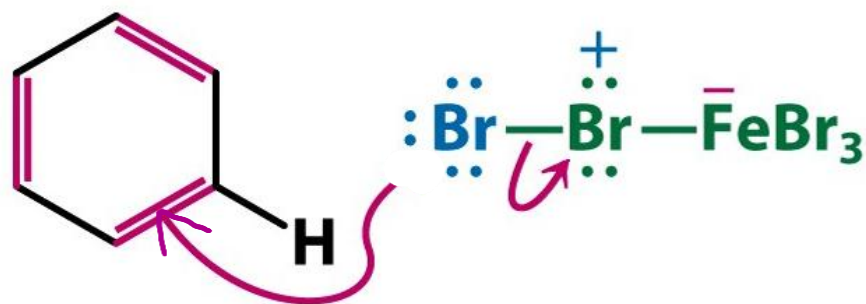


El FeBr₃ acepta un par de electrones de uno de los átomos de Br del Br₂ (actúa como un ácido de Lewis)



Se forma un intermediario que contiene un átomo de Br con carga positiva.

Paso 2 – Ataque electrofílico del Br_2 activado sobre el benceno

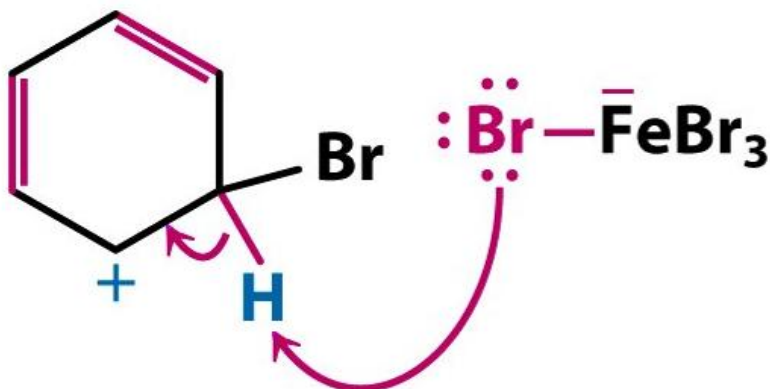


El Br terminal realiza el ataque electrofílico sobre el benceno.

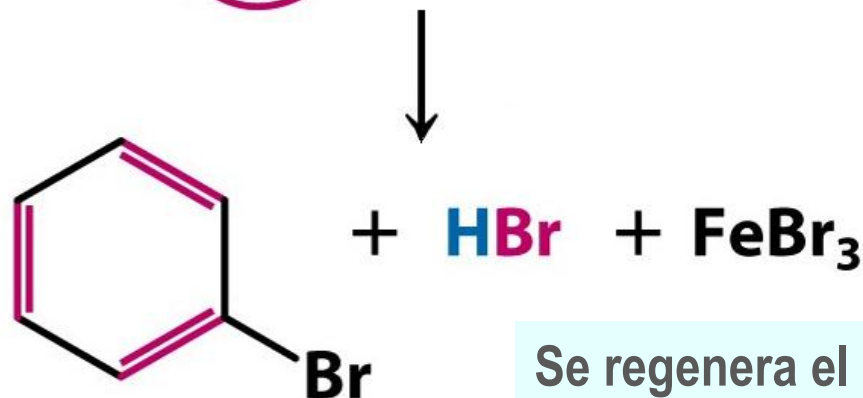


El Br central queda enlazado al FeBr_3 formando el grupo saliente FeBr_4^- .

Paso 3 – Formación del bromobenceno

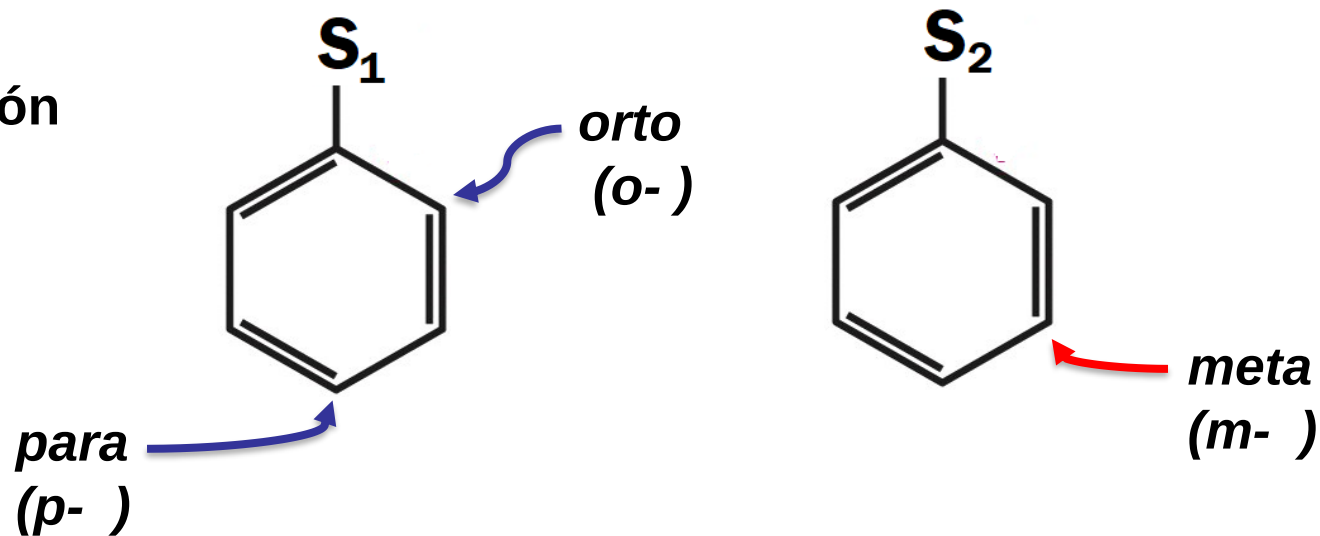


El FeBr_4^- actúa como base extrayendo un protón del intermediario (catión ciclohexadienil).

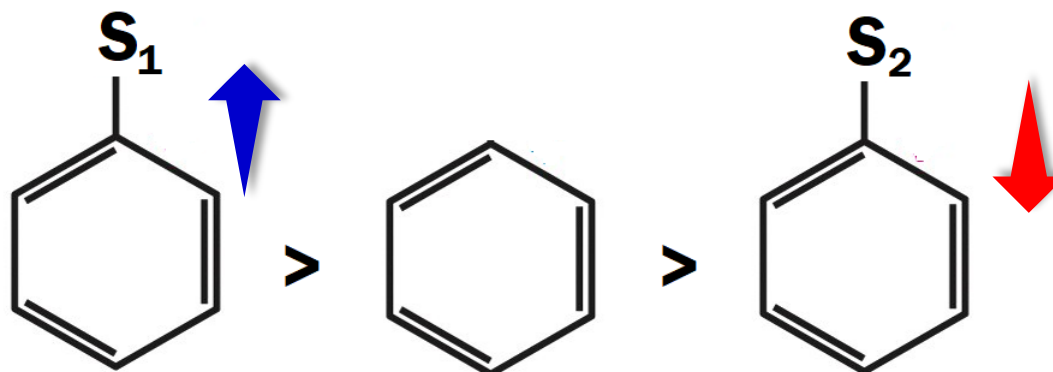


Se regenera el catalizador FeBr_3 y se forma HBr como producto inorgánico secundario.

Orientación



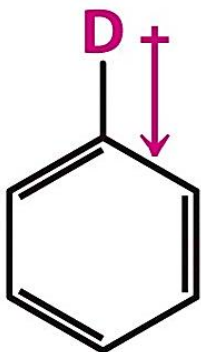
Reactividad



Sustituyentes – inducción

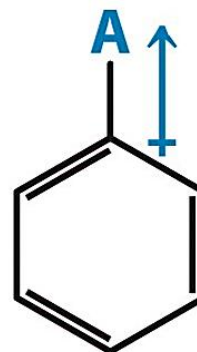
- El sustituyente ya presente (D o A) puede generar un efecto inductivo mediante la polarización de un **enlace sigma** por diferencia de *electronegatividad* entre C–D o C–A

Dadores



D = $-\text{CH}_3$;
otros alquilos

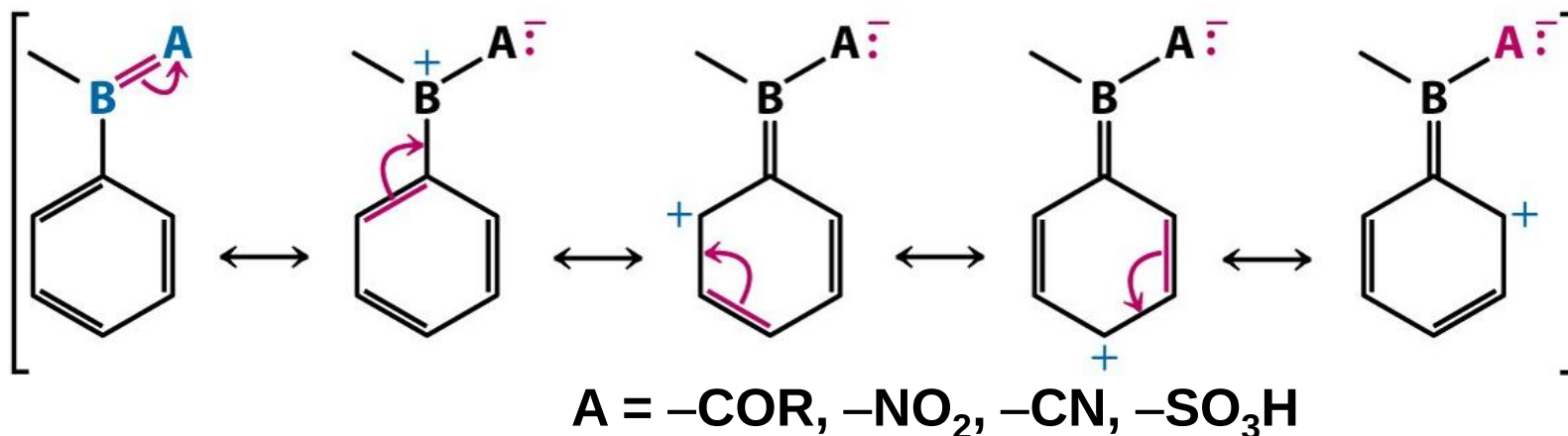
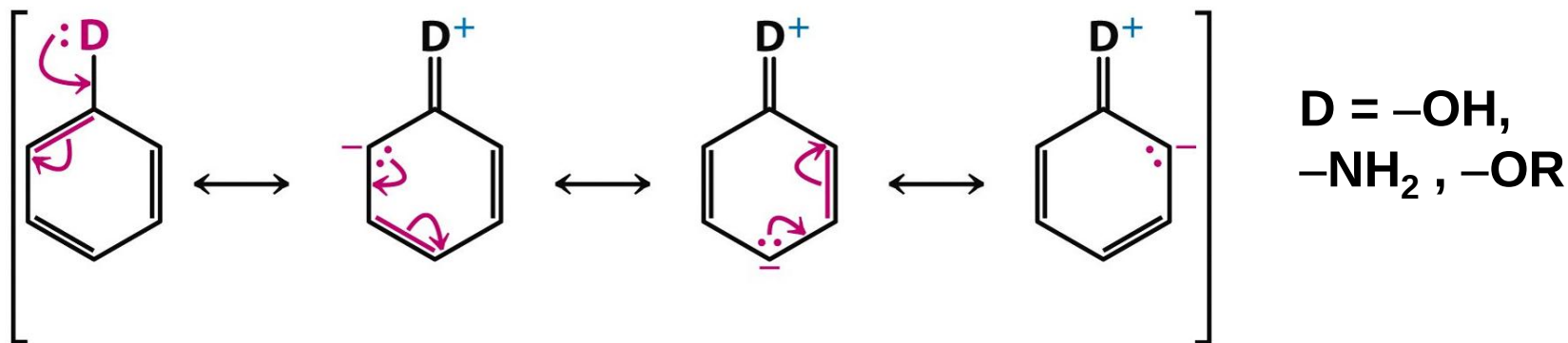
Atractores



A = $-\text{X}$, $-\text{OR}$, $-\text{COR}$,
 $-\text{NO}_2$, $-\text{CN}$, $-\text{SO}_3\text{H}$

Sustituyentes – resonancia

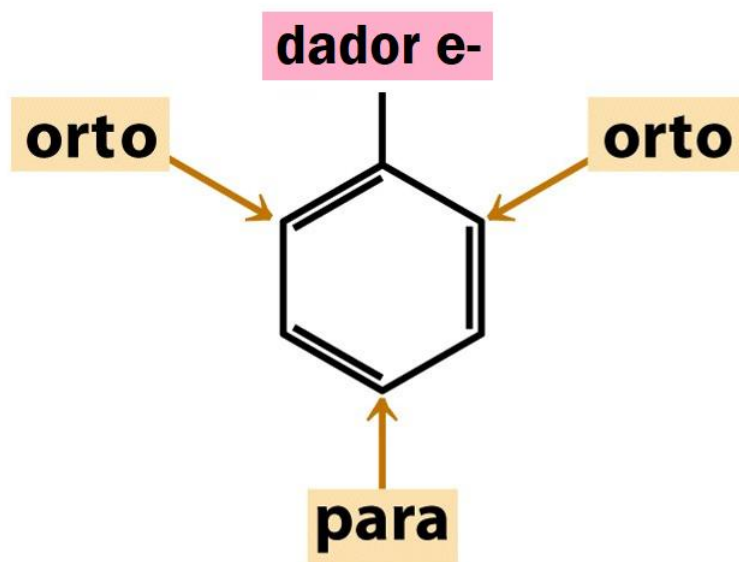
- Los electrones de los orbitales π del anillo aromático pueden deslocalizarse por efecto del sustituyente



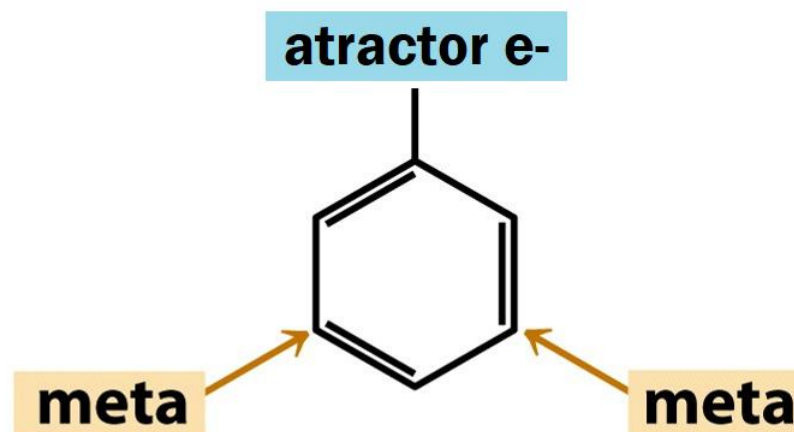
Reactividad y orientación - Resumen

<i>Sustituyente</i>	<i>Nombre</i>	<i>Orientación</i>	<i>Reactividad</i>
-NH ₂	Amino	orto, para	Activa (++)
-NHR, -NR ₂	Alquilamino	orto, para	Activa (++)
-OH	Hidroxilo	orto, para	Activa (+)
-OR	Alcoxi	orto, para	Activa (+)
-R	Alquil	orto, para	Activa
-Ar	Aril	orto, para	Activa
-H	Hidrógeno	----	<i>Estándar</i>
-X	Halógenos	orto, para	Desactiva
-COR	Acil	meta	Desactiva (+)
-COOH	Carboxi	meta	Desactiva (+)
-SO ₃ H	Sulfónico	meta	Desactiva (+)
-CN	Ciano	meta	Desactiva (+)
-NO ₂	Nitro	meta	Desactiva (++)

En resumen.....



El anillo se activa



El anillo se desactiva

GRACIAS !

Bibliografía

Bailey & Bailey, 5a Ed 1998

Vollhardt-Schore, 5a Ed 2007

Schmid, 1ª Ed, 1996

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Block E zócalo