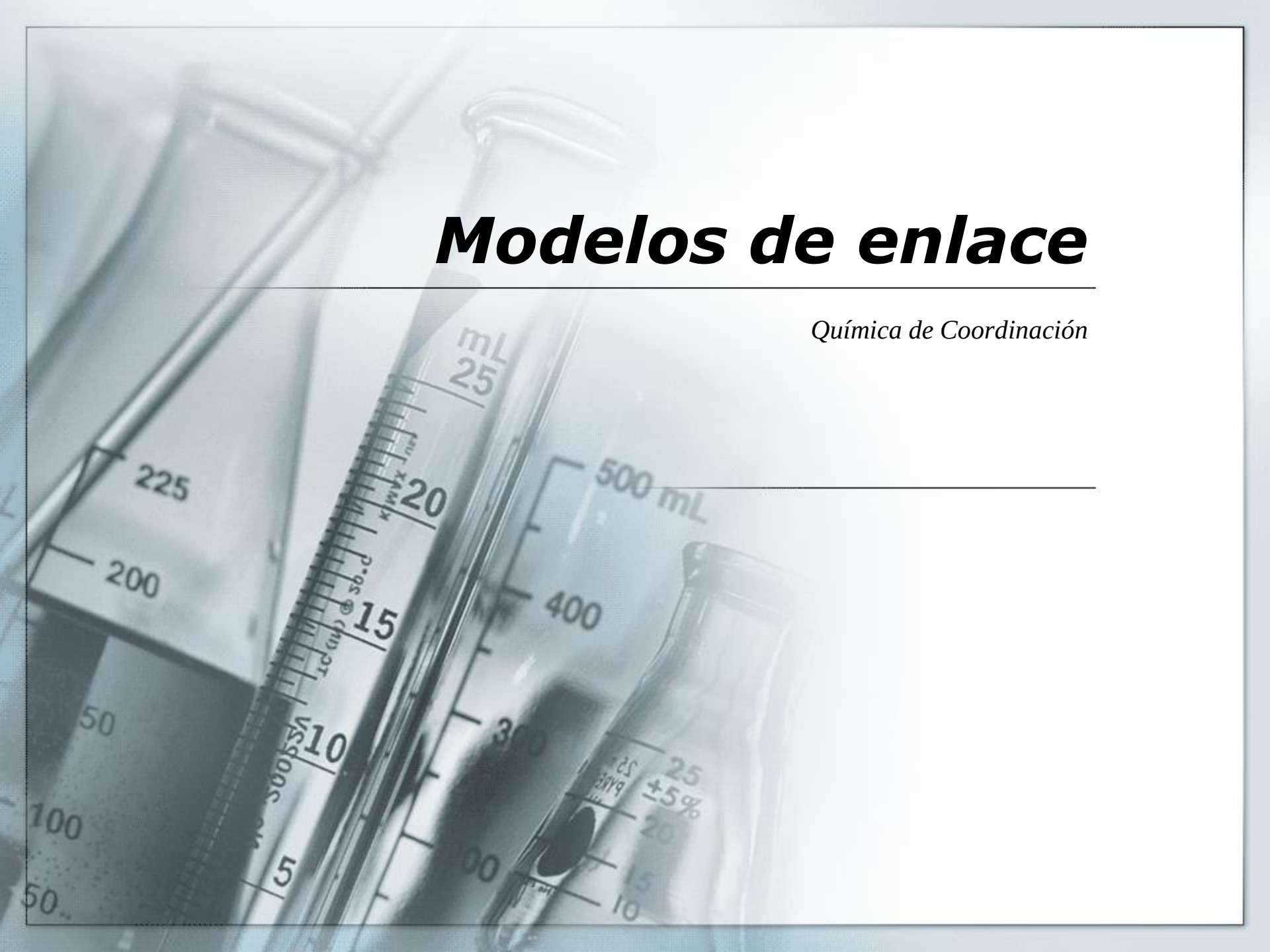
Modelos de enlace

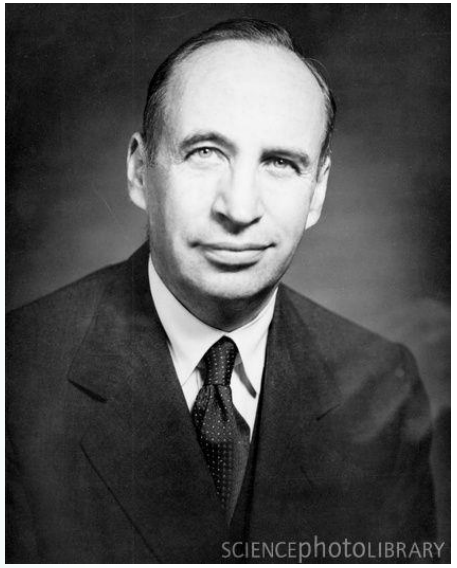
Química de Coordinación



Teoría de campo cristalino TCC

La idea principal es simple:

“Que le pasan a los orbitales atómicos de un elemento central cuando otras especies interaccionan con este átomo en una dirección preferente”



John Hasbrouck van Vleck en 1930

TCC

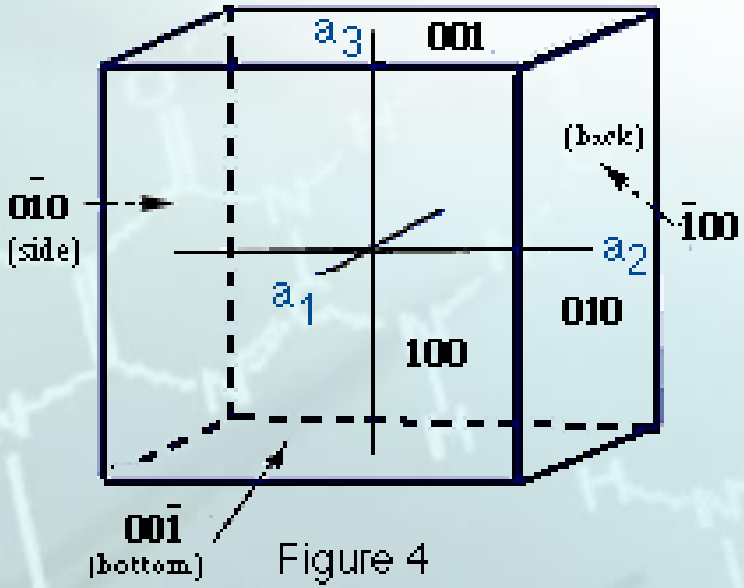
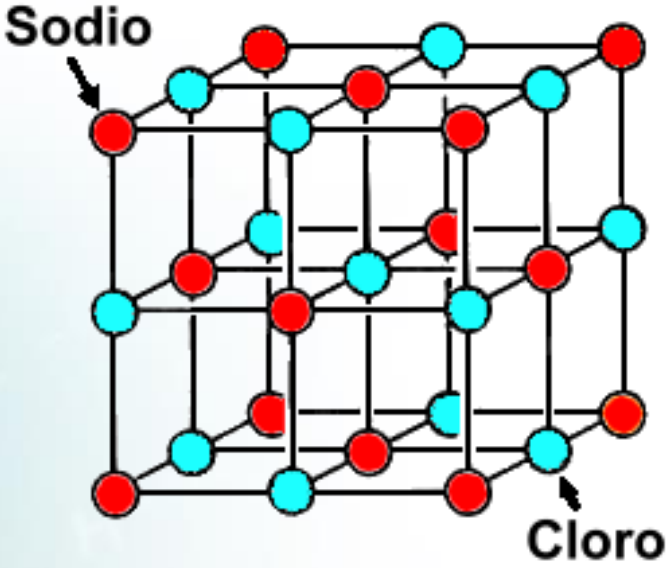
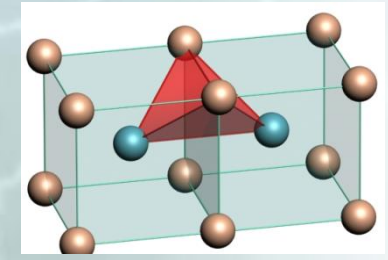
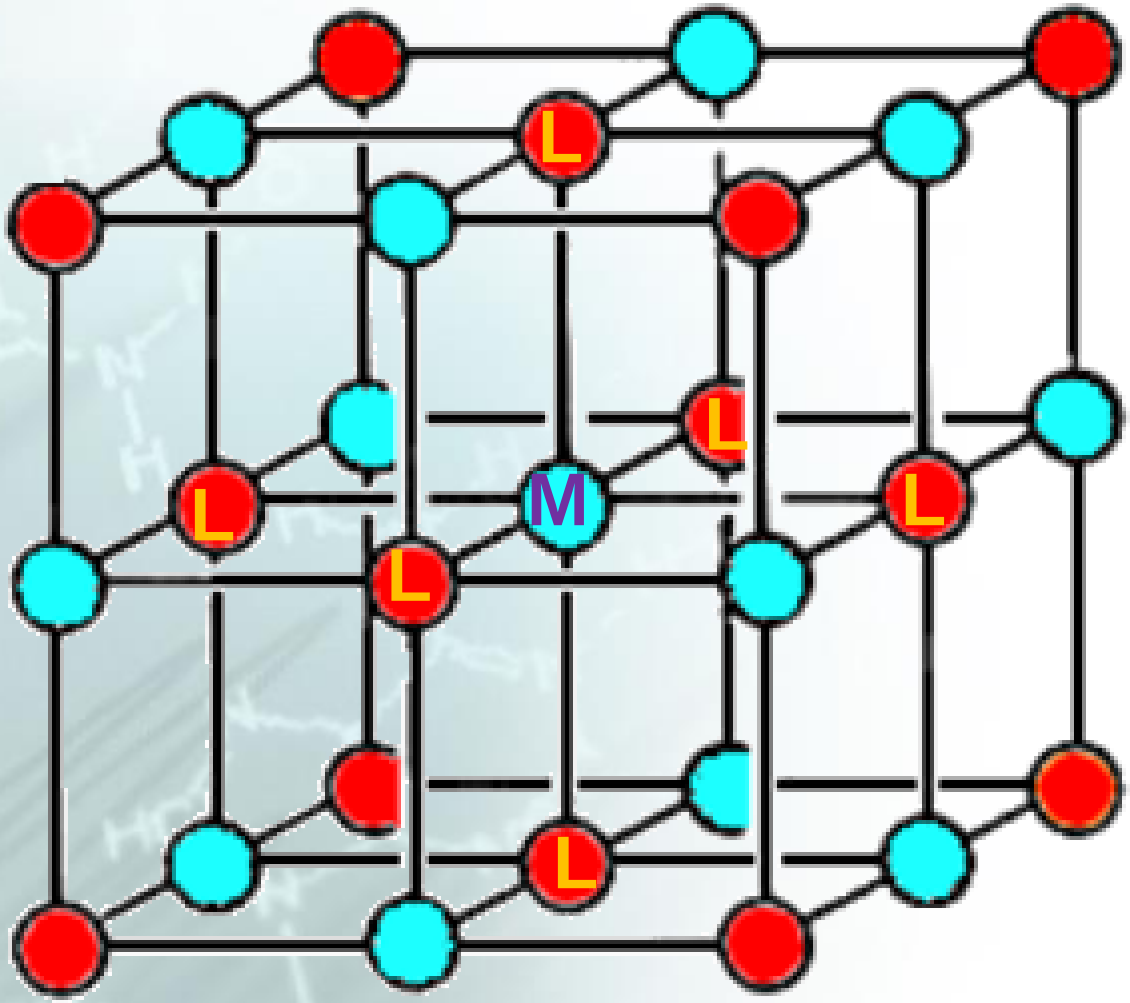


Figure 4

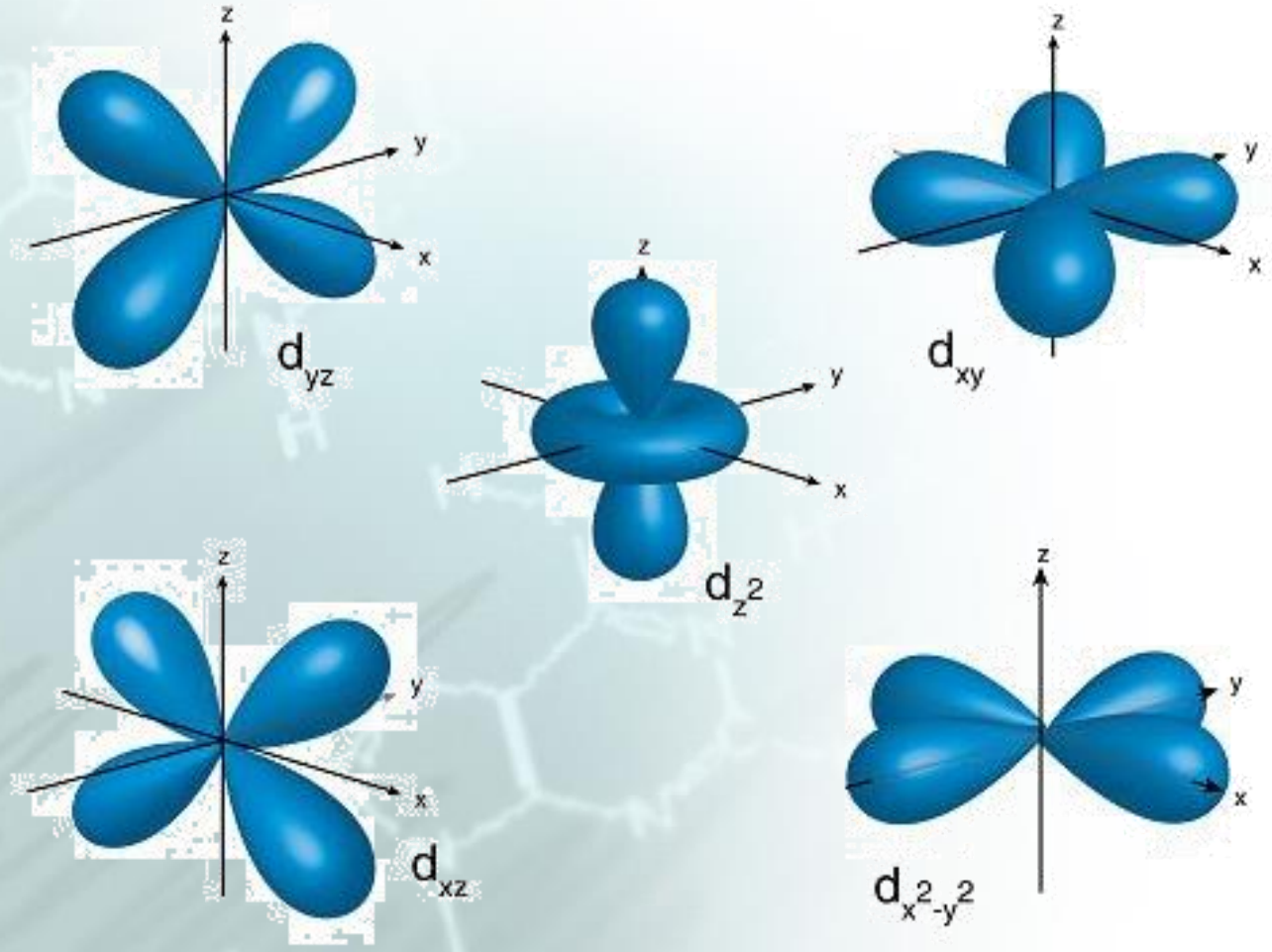




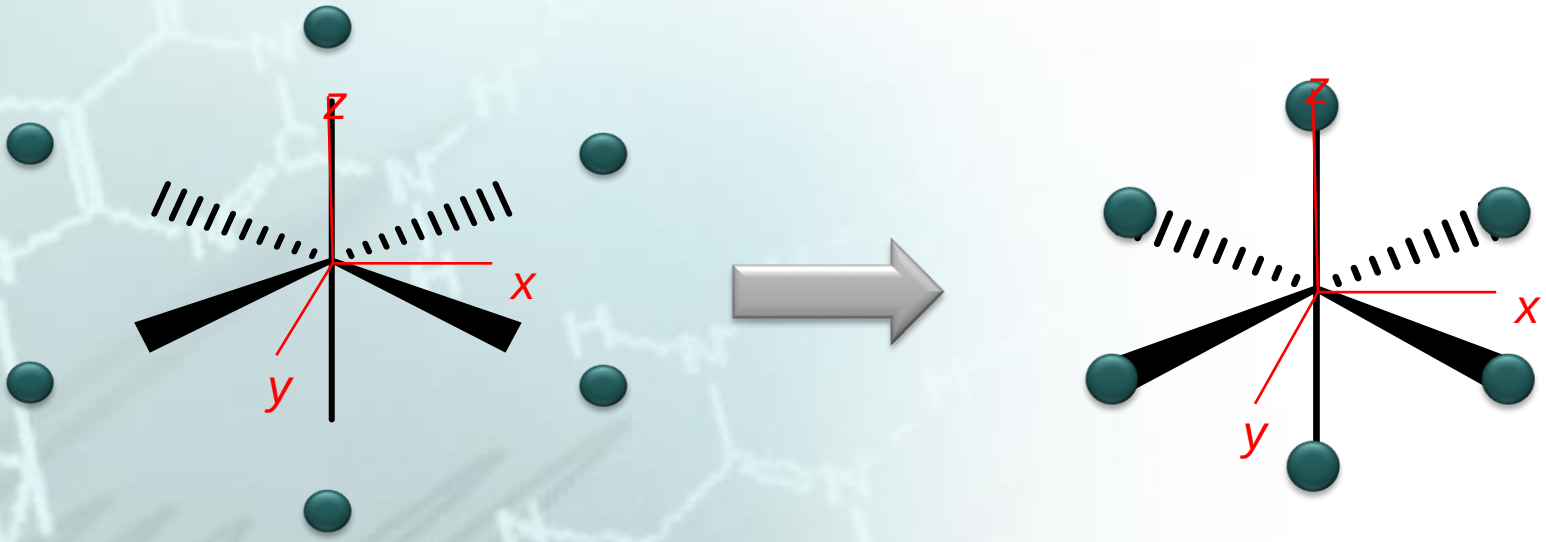
Ahora pasamos de sólidos a CC



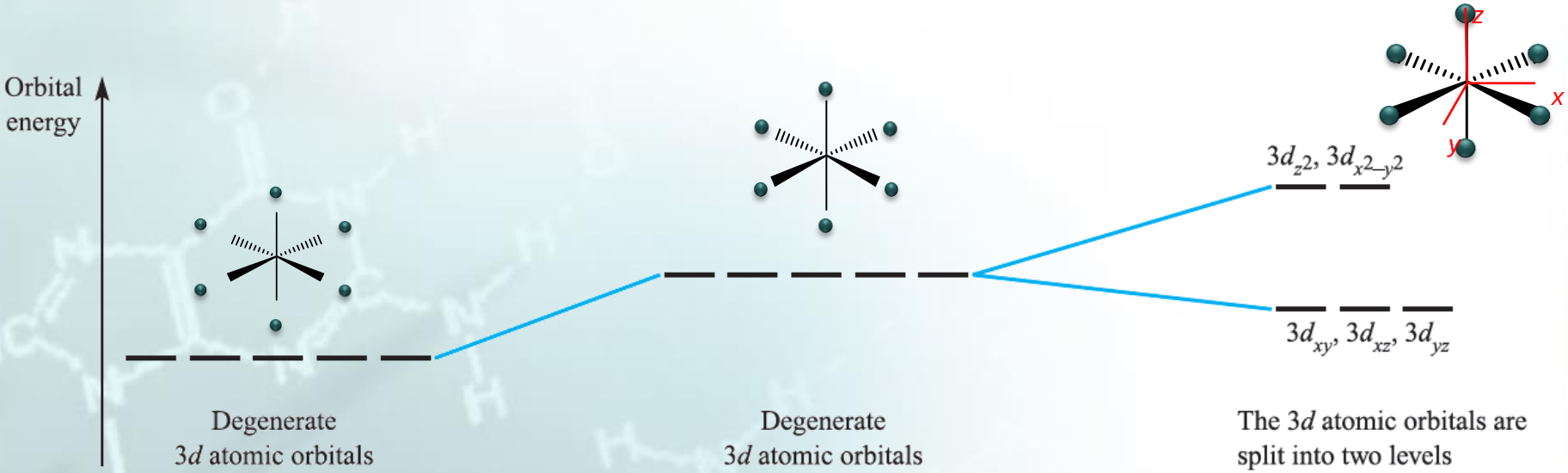
Como se orientan los orbitales «d»



Como entran



TCC

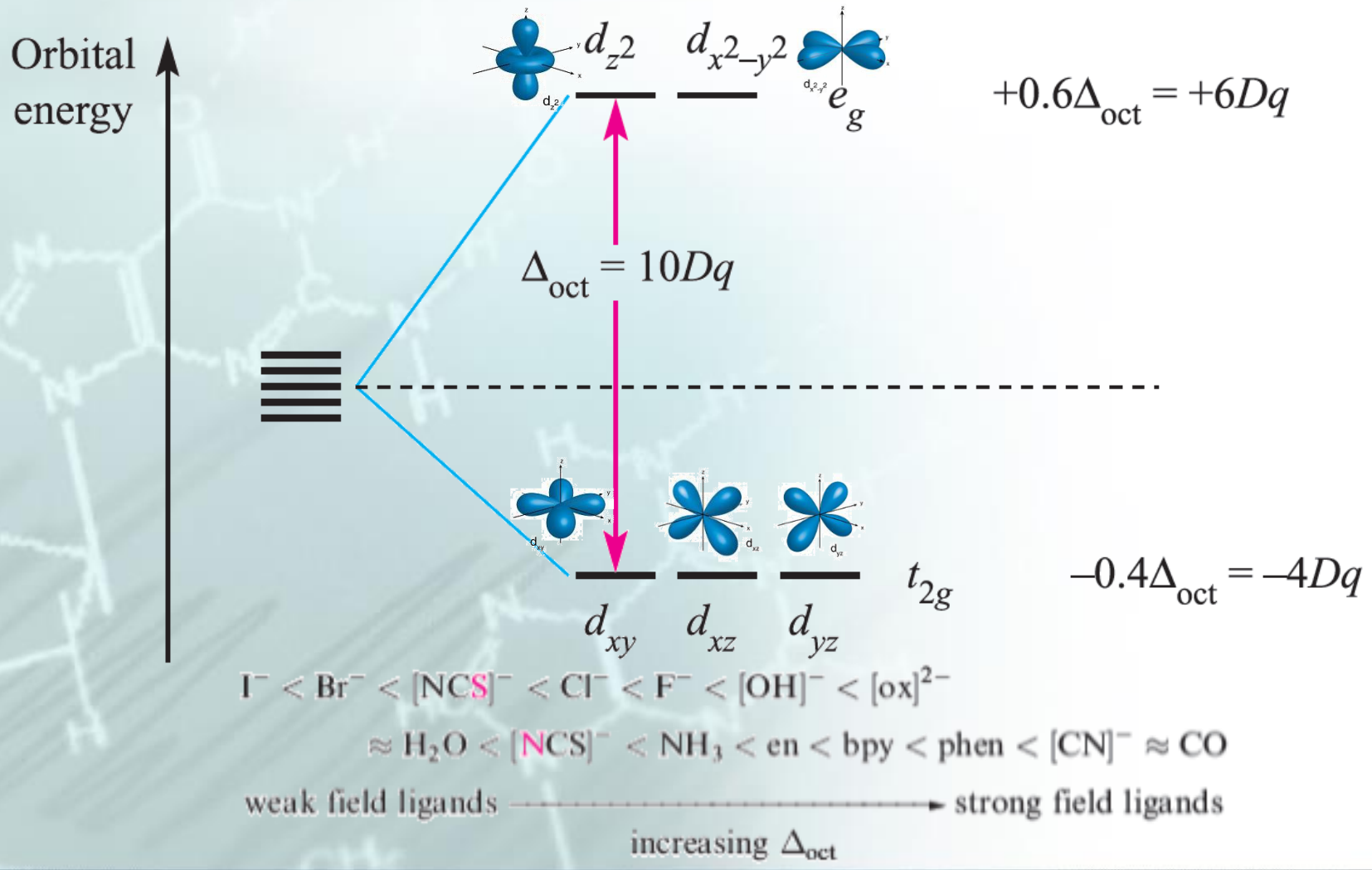


Metal aislado

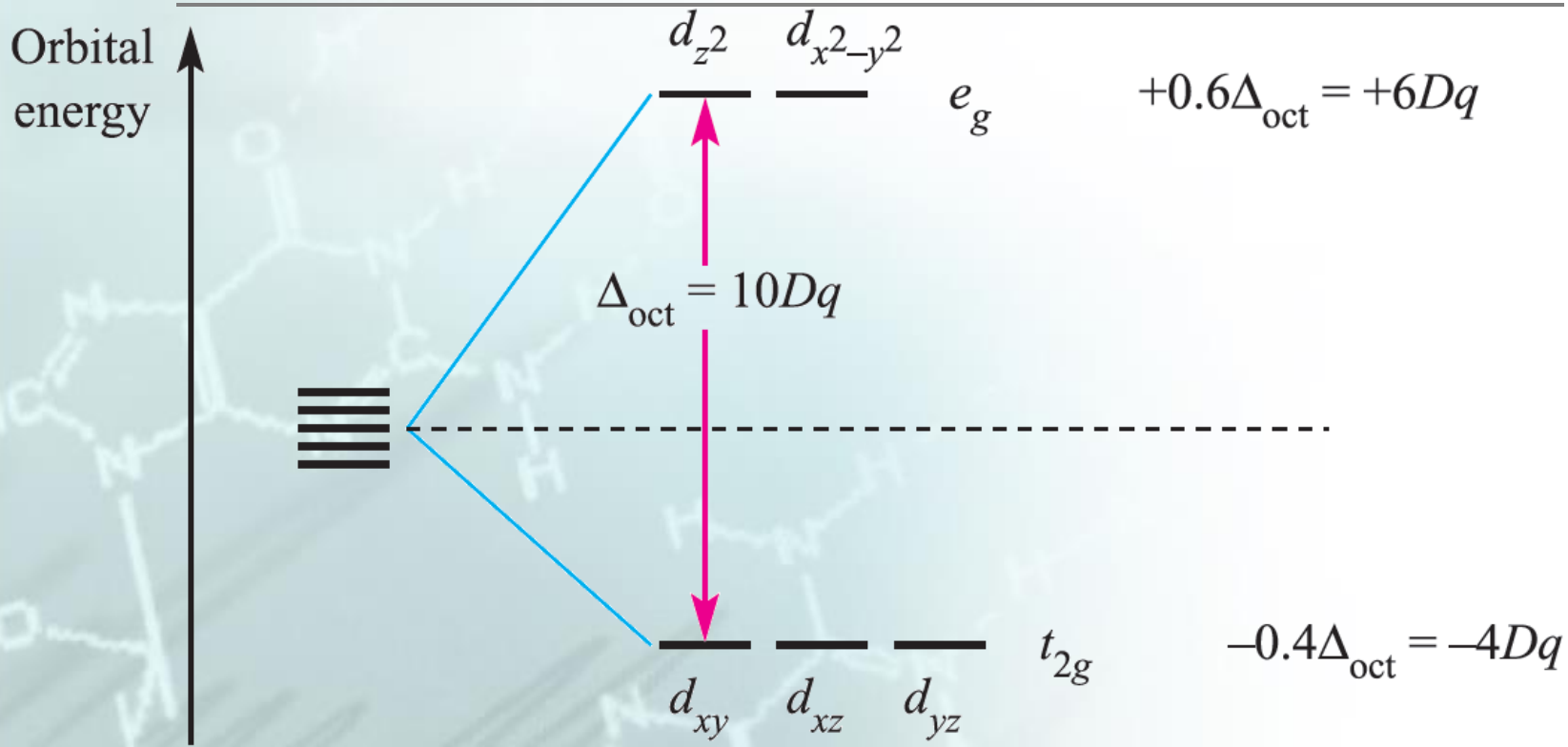
Se acercan los ligantes

Ya se nota cuantos son y de donde vienen

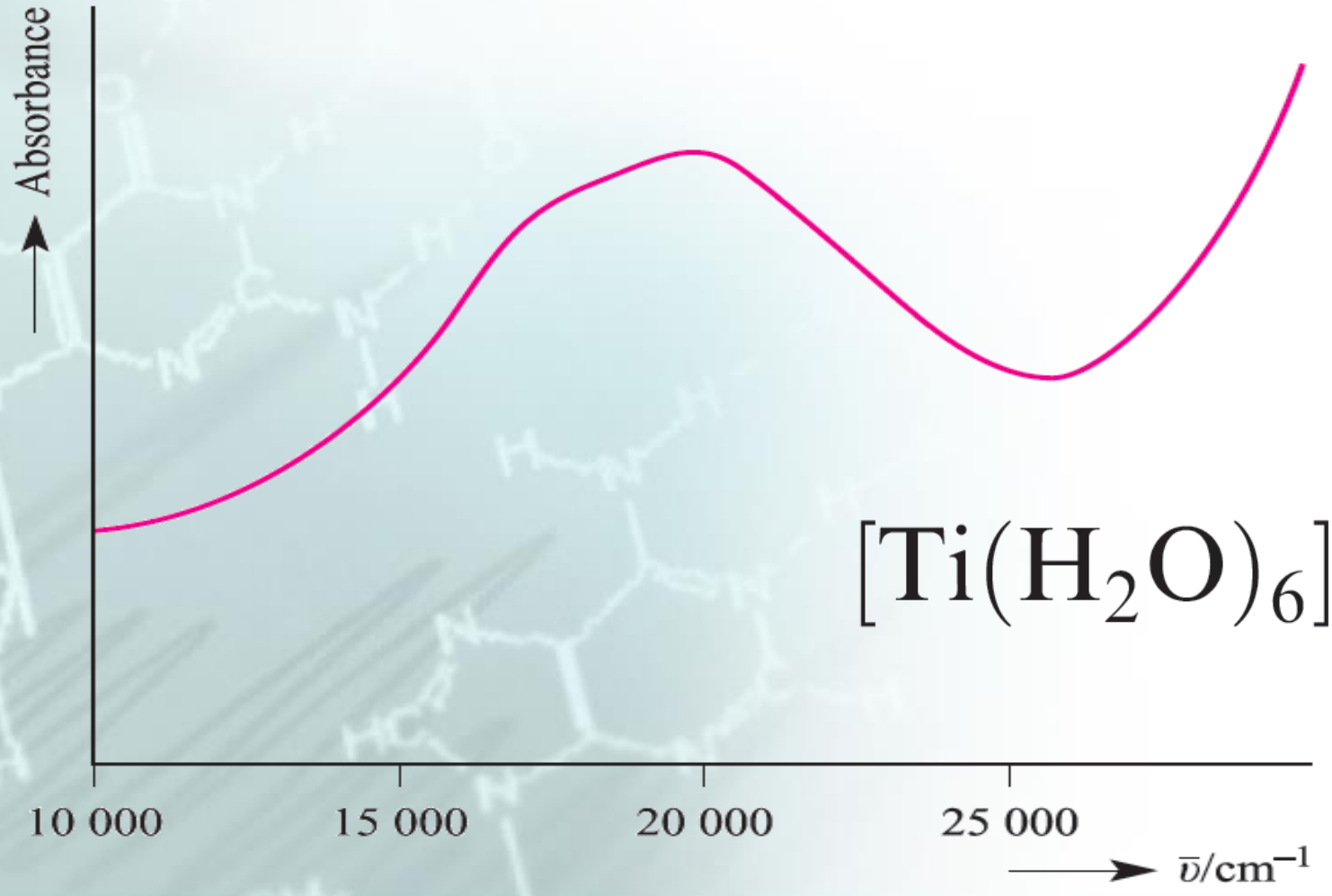
TCC


Orbital energy
d_{z^2}
$d_{x^2-y^2}$
e_g
$+0.6\Delta_{oct} = +6Dq$
$\Delta_{oct} = 10Dq$
t_{2g}
$-0.4\Delta_{oct} = -4Dq$
d_{xy}
d_{xz}
d_{yz}
$I^- < Br^- < [NCS]^- < Cl^- < F^- < [OH]^- < [ox]^{2-}$
$\approx H_2O < [NCS]^- < NH_3 < en < bpy < phen < [CN]^- \approx CO$
weak field ligands
strong field ligands
increasing Δ_{oct}

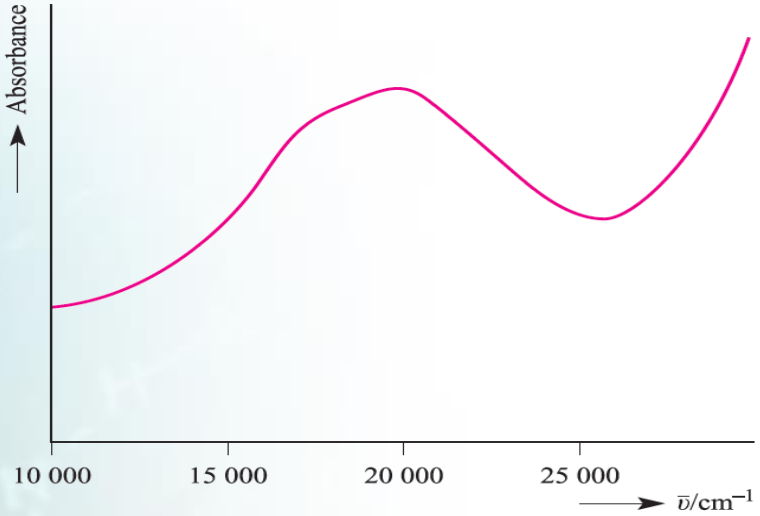
Energía de estabilización del campo cristalino



¿Como sacamos la energía?



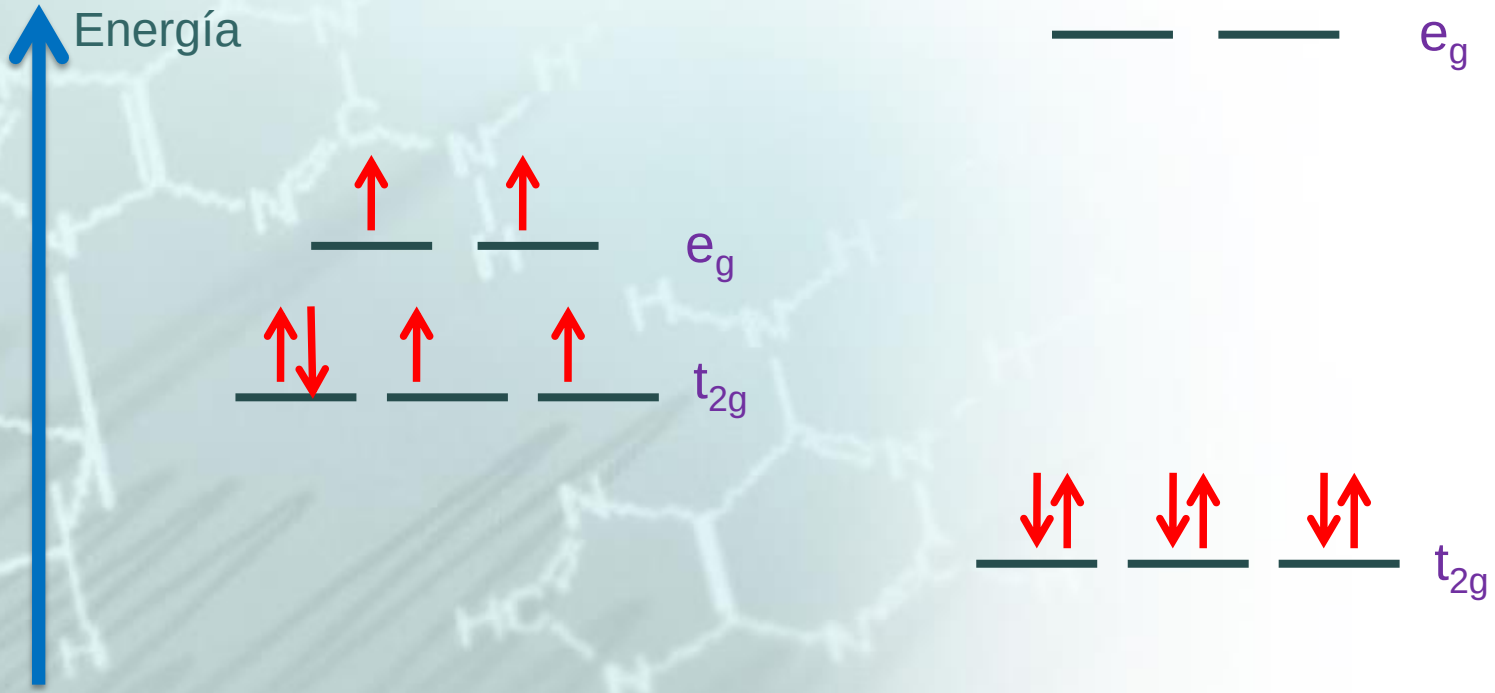
El espectro



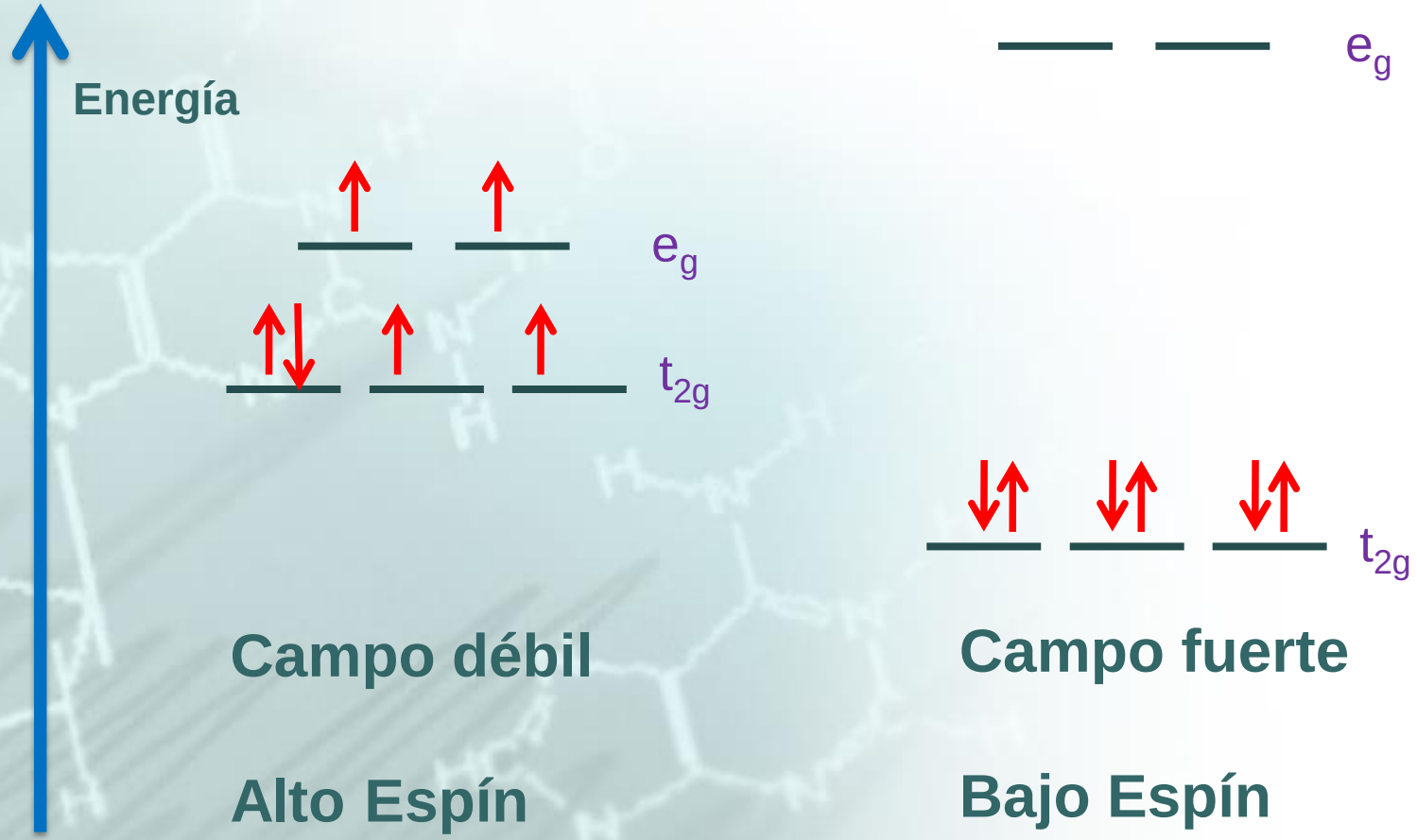
$t_{2g}^{1}e_{g}^{0}$ ⟹ $t_{2g}^{0}e_{g}^{1}$

Ahora ya podemos empezar a llenar

El caso Fe^{2+} octaédrico



TCC



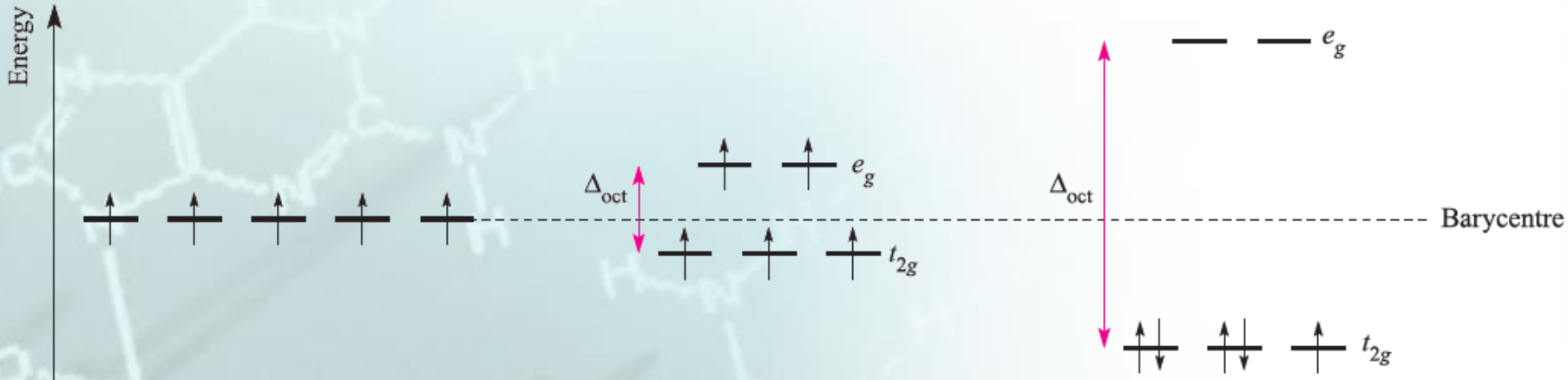
Campo débil

Alto Espín

Campo fuerte

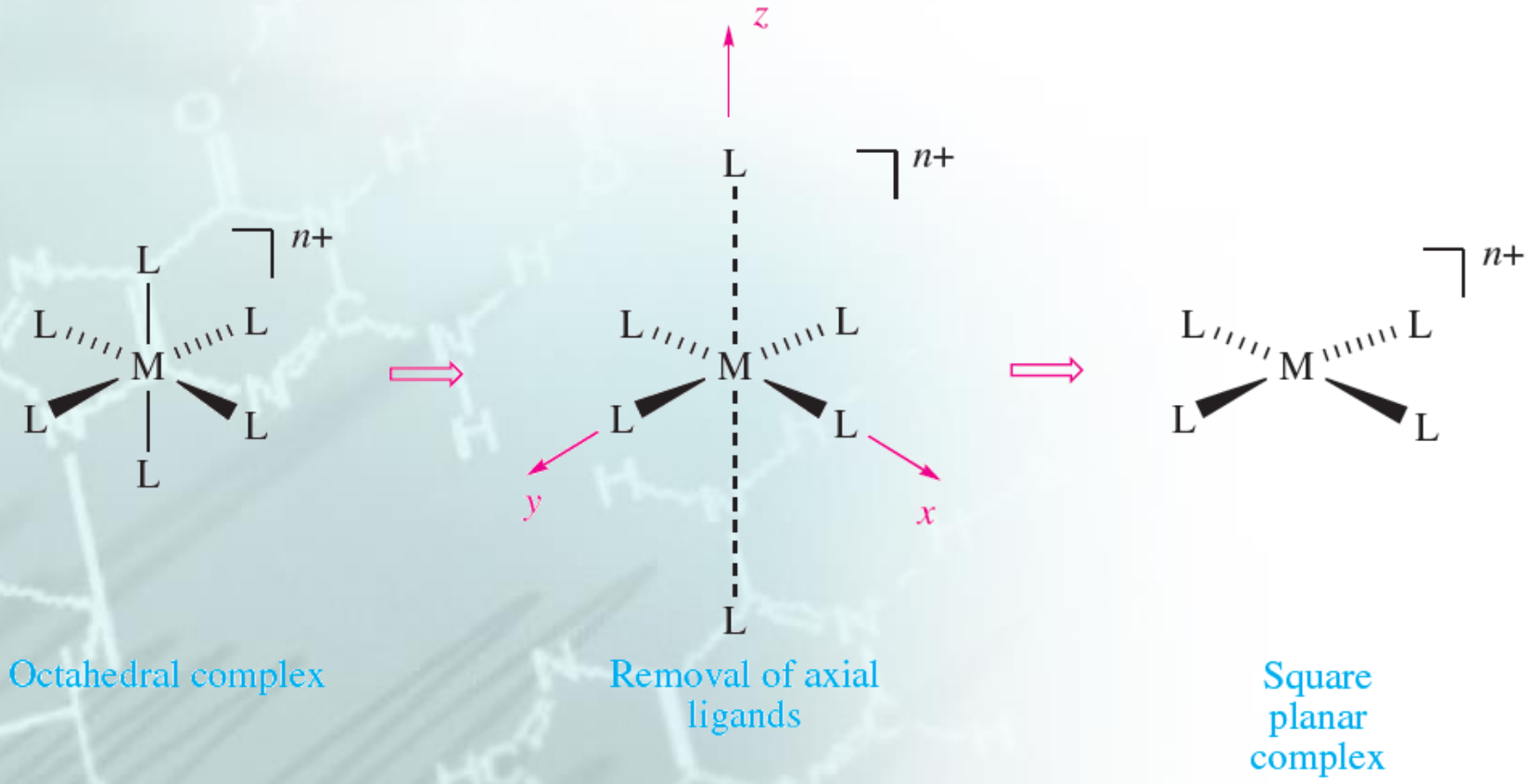
Bajo Espín

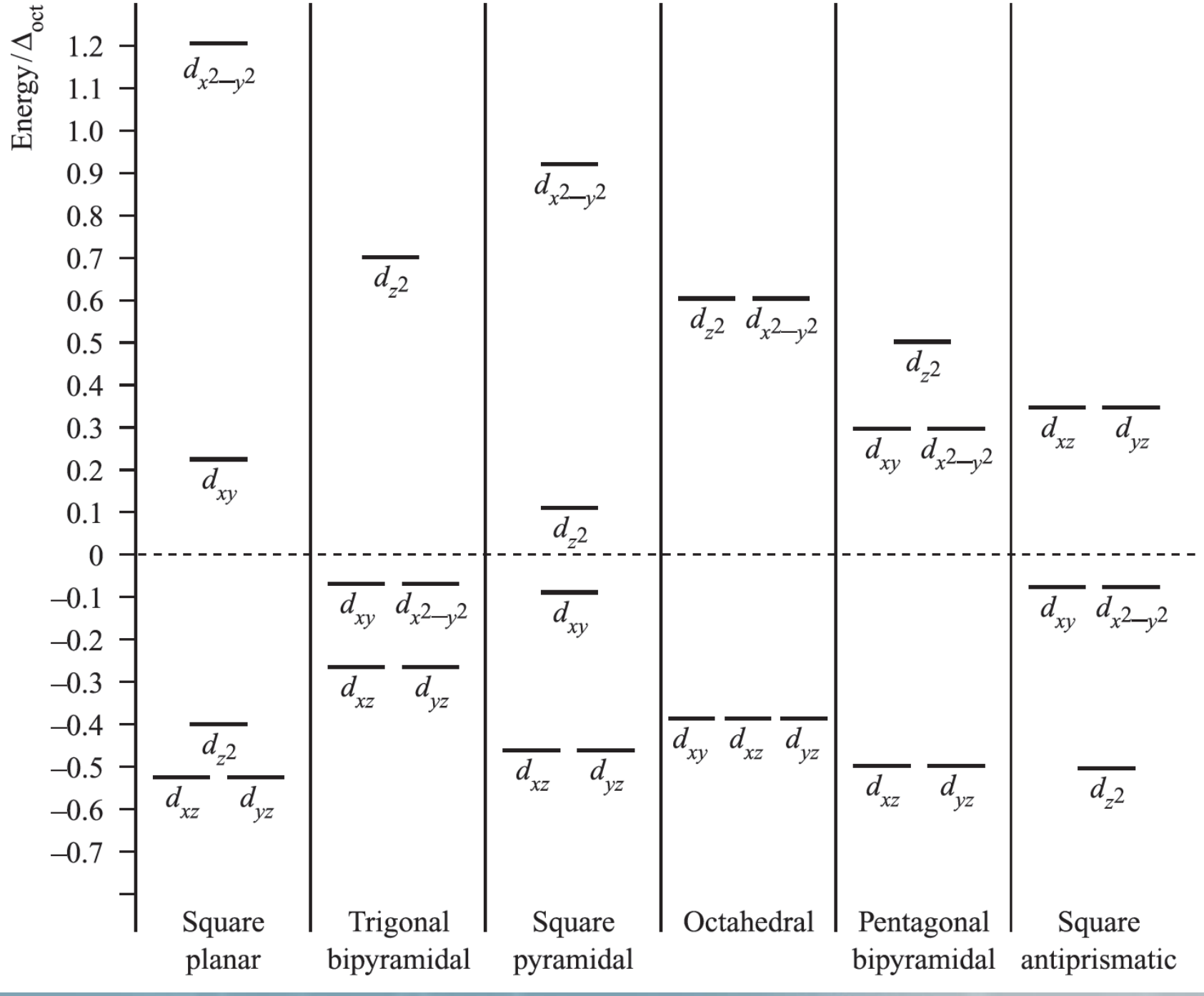
TCC



Si ahora son cuatro ligantes y es tetraédrico el complejo

Y los cuadrados




Energy/Δ_{oct}
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
–0.1
–0.2
–0.3
–0.4
–0.5
–0.6
–0.7
$d_{x^2-y^2}$
d_{xy}
d_{z^2}
d_{xz} d_{yz}
Square planar
d_{z^2}
d_{xy} $d_{x^2-y^2}$
d_{xz} d_{yz}
Trigonal bipyramidal
$d_{x^2-y^2}$
d_{z^2}
d_{xy}
d_{xz} d_{yz}
Square pyramidal
d_{z^2} $d_{x^2-y^2}$
d_{xy} d_{xz} d_{yz}
Octahedral
d_{z^2}
d_{xy} $d_{x^2-y^2}$
d_{xz} d_{yz}
Pentagonal bipyramidal
d_{xz} d_{yz}
d_{xy} $d_{x^2-y^2}$
d_{z^2}
Square antiprismatic