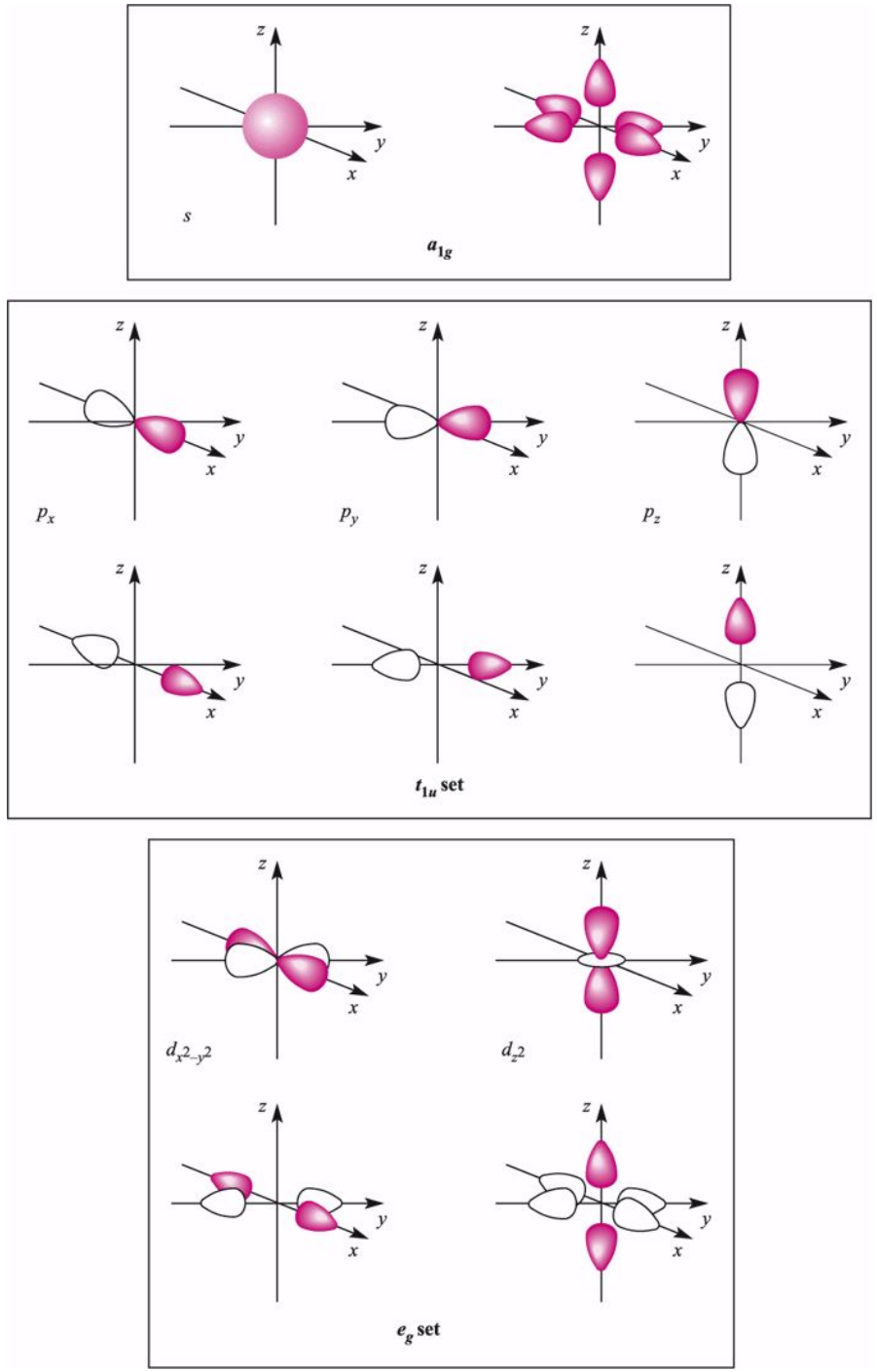
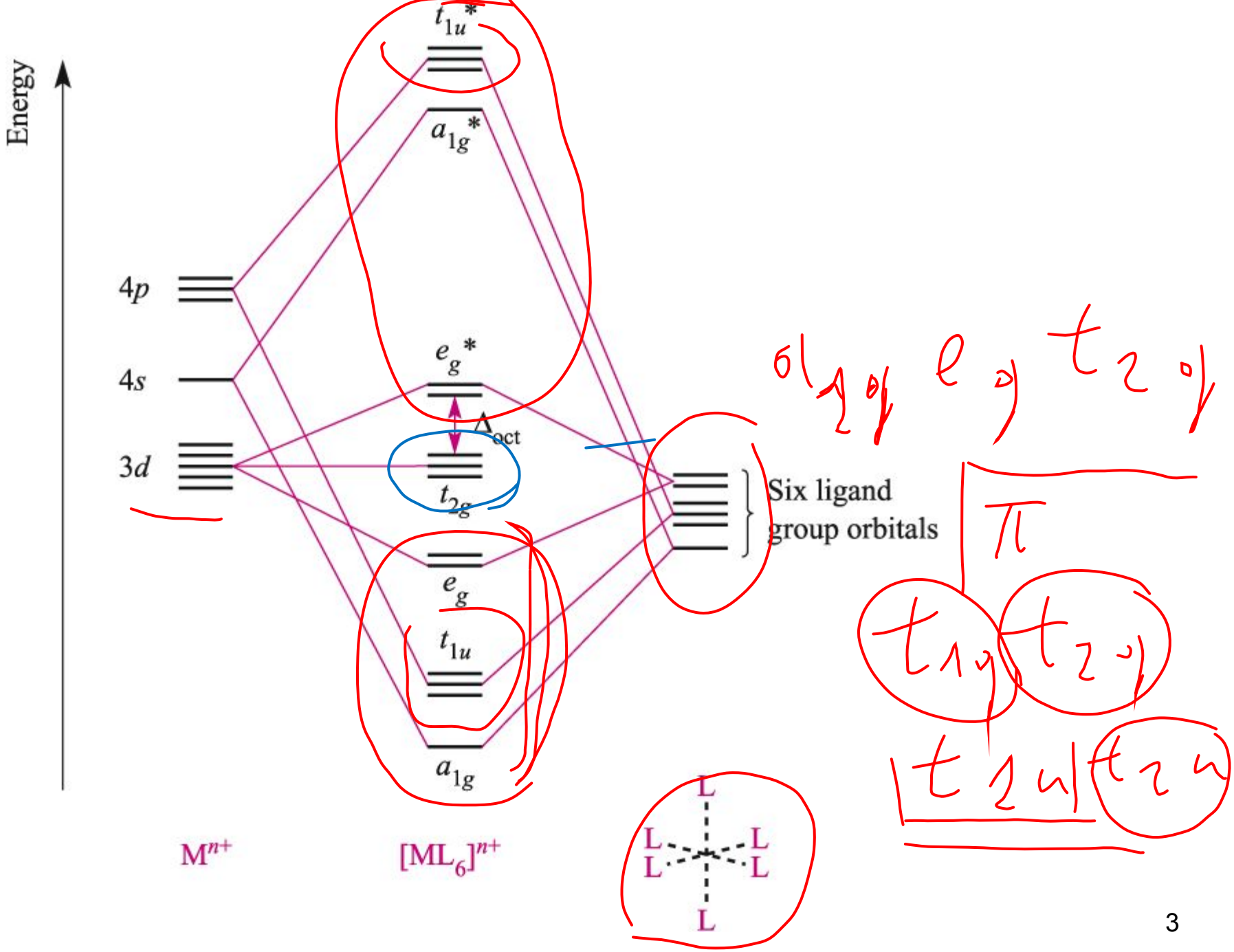
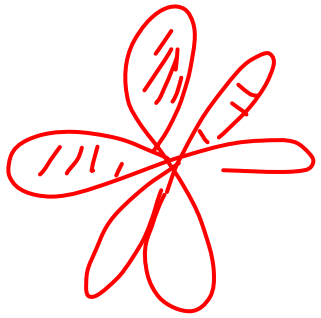
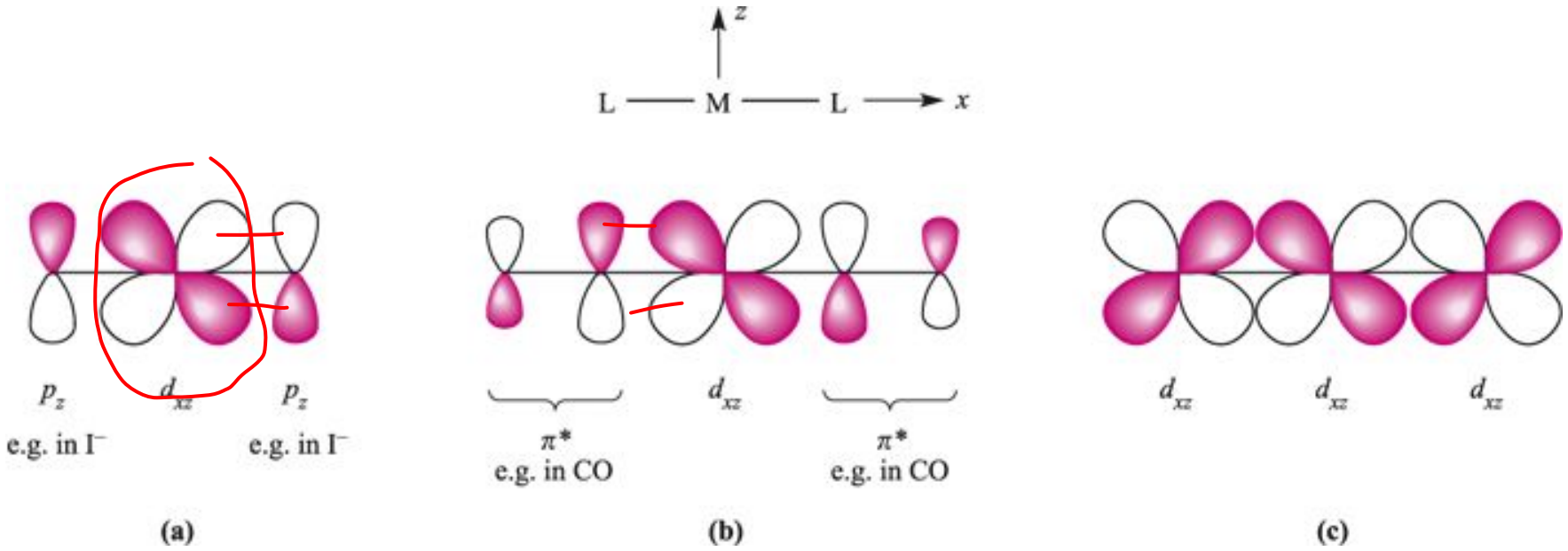
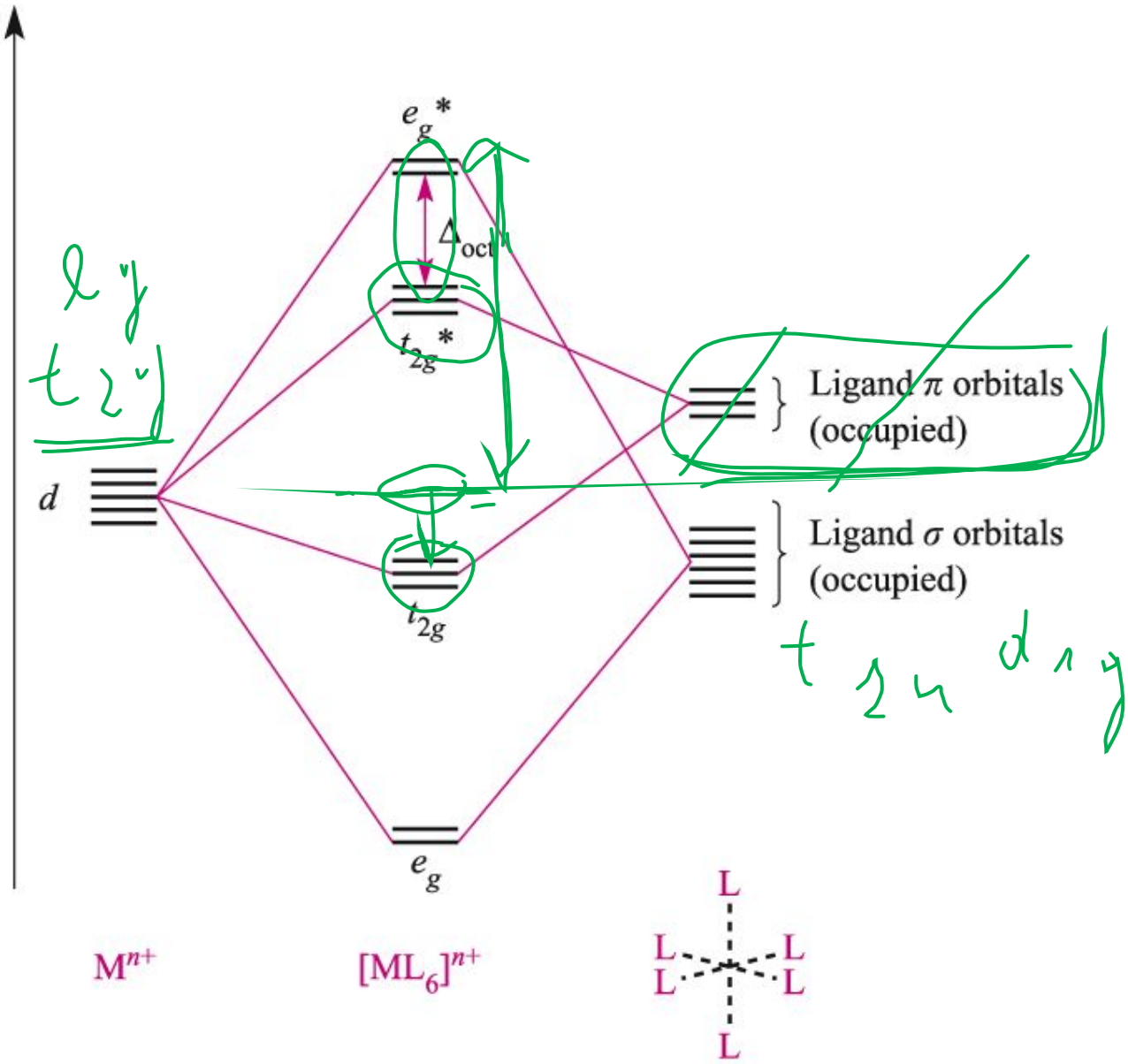
Метод молекулярных орбиталей для координационных соединений

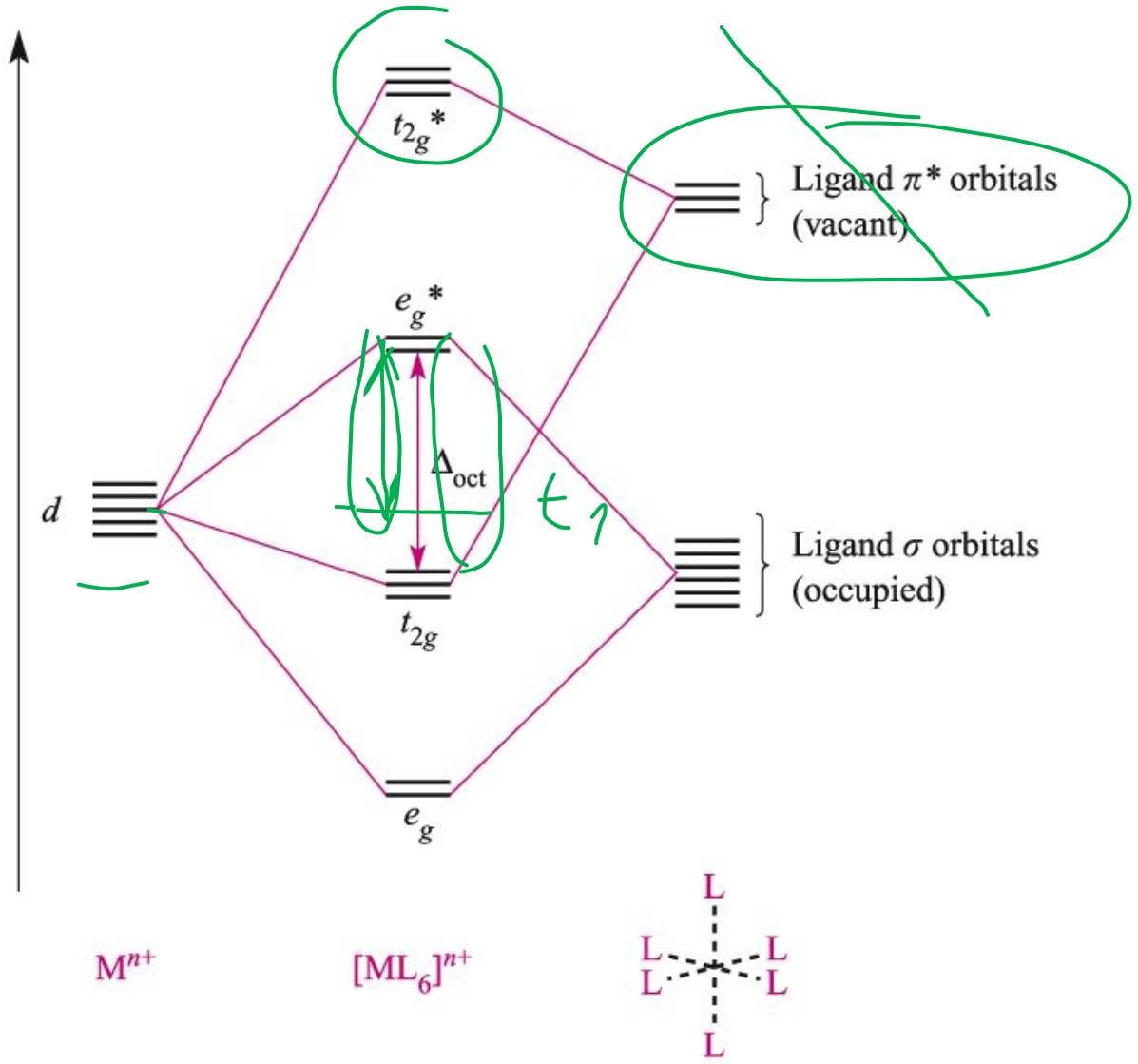

z
y
x
s
a_{1g}
p_x
p_y
p_z
t_{1u} set
$d_{x^2-y^2}$
d_{z^2}
e_g set

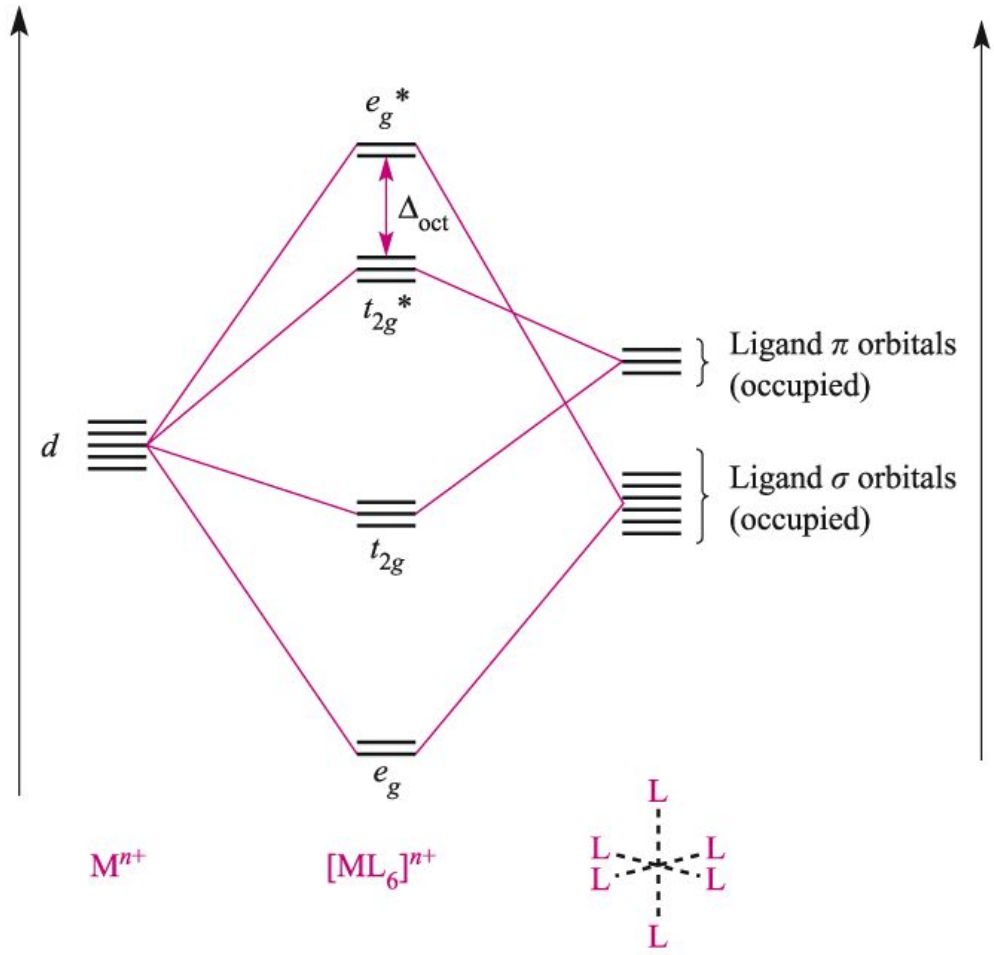

Energy
t_{1u}*
a_{1g}*
4p
e_g*
4s
Δ_{oct}
3d
t_{2g}
Six ligand group orbitals
e_g
t_{1u}
a_{1g}
M^{n+}
$[ML_6]^{n+}$
L
L
L
L
L
L
a_{1g} e_g t_{2g}
π
t_{1u} t_{2u}
t_{2u} t_{2u}

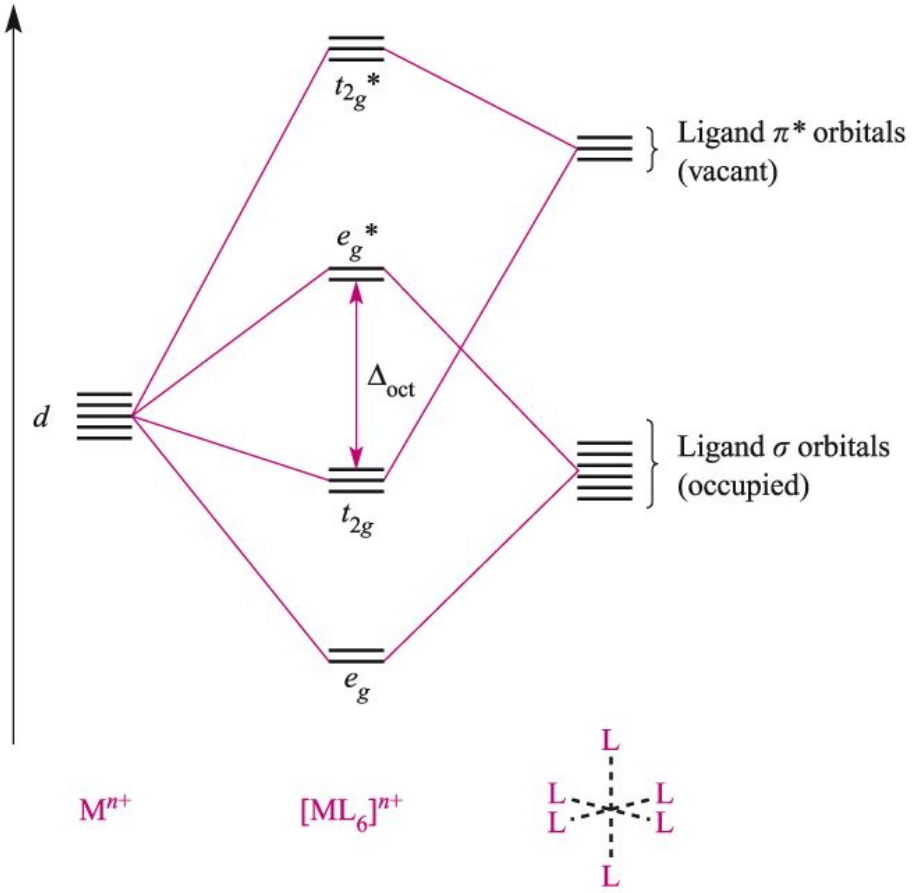



z
L — M — L → x
p_z
d_{xz}
p_z
e.g. in I^-
e.g. in I^-
d_{xz}
π^*
e.g. in CO
π^*
e.g. in CO
d_{xz}
d_{xz}
d_{xz}
(a)
(b)
(c)


e_g *
Δ_{oct}
t_{2g} *
Ligand π orbitals (occupied)
d
Ligand σ orbitals (occupied)
t_{2g}
e_g
M^{n+}
$[ML_6]^{n+}$
L
L
L
L
L
L


t_{2g}*
Ligand π* orbitals
(vacant)
e_g*
Δ_{oct}
d
Ligand σ orbitals
(occupied)
t_{2g}
e_g
M^{n+}
$[ML_6]^{n+}$
L
L
L
L
L
L


e_g*
Δ_{oct}
t_{2g}*
Ligand π orbitals
(occupied)
d
Ligand σ orbitals
(occupied)
t_{2g}
e_g
M^{n+}
$[ML_6]^{n+}$
L
L
L
L
L
L


t_{2g}*
Ligand π* orbitals
(vacant)
e_g*
Δ_{oct}
d
Ligand σ orbitals
(occupied)
t_{2g}
e_g
M^{n+}
$[ML_6]^{n+}$
L
L
L
L
L
L